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IMLAUER HOTEL PITTER SALZBURG

Book of Abstracts

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PERED® TECHNOLOGY, SIMULATION AND COMPARE CAPITAL COST AND ENERGY SAVING WITH MIDREX® PLANT

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Abstract PERED® Direct Reduction technology is the new technology in the world. Iran country developed direct reduction PERED® technology for decreasing capital cost and energy saving. Iron oxide pellets reduced in the shaft furnace. Top gas return from furnace after cleaning in scrubber is divided to fuel and process gas. Process and natural gas mixed together (feed gas) after preheat in heat recovery system. Reducing gas is generated in the reformer by reacting methane (CH4) with water vapor (H2O) and recycled carbon dioxide (CO2) in reformer tube. Flue gas produced due to combustion of gases in the reformer box. Flue gas temperature is high therefore, preheats feed gas, main air and natural gas in heat recovery system. Some changes and improvement in equipment's has been done. Reformer tubes changed from 8 to 10 inch and reformer box volume is decreased. Process and seal gas compressors are changed from screw and Aerzen rotary lube type to centrifugal Siemens type. Shaft furnace has a new design and internal furnace diameter is variable vs. furnace diameter. China hat equipment replaced Upper Cluster breaker. Elimination of upper cluster breaker (huge maintenance and capital cost is reduced) is done without any problem for movement of material in the furnace. It is affirm that it didn't create any cluster in PERED® technology. Pellet and gas velocity distribution in the furnace is checked by fluent software. Tube bundles arrangement has been developed and one steam tube bundle installed. Reformer and Heat Recovery System is simulated with ASPEN HYSYS software. Energy, mass and momentum equations are solved together. Temperature, pressure and components composition of gases has been checked with plant experimental data. Mass and energy balance have been obtained for all streams. The overall condition of MIDREX® and PERED® technology is compared together.

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STOPPER RISE INDEX: PREVENTING CLOGGING IN THIN SLAB CASTER

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Nozzle clogging at thin slab caster leads to quality issues and, in certain cases, losses in production. Clogging in and around nozzle and stopper rod is one of the major concerns for thin slab caster at Tata steel Jamshedpur plant which produces aluminium killed steel through BOF-LF route. Stopper Rise Index Model has been developed which forecasts the tendency for stopper rise, which is an indicator for detecting clogging, for the incoming steel ladle. This model helps caster operator to take preventive actions for clogging. The model utilizes binary logistic regression and uses process parameters from different stages of steelmaking which affect alumina morphology in steel. 87.5% of nozzle clogging cases were successfully detected by this model.

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STUDY AND REDUCTION OF CAMBER IN SLABS BY IMPLEMENTING AIR MIST COOLING AT THIN SLAB CASTER

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Camber in slabs is one of the major concerns in the Thin Slab Casting & Rolling process route. The camber in slab caused stuck up of slab in mill entry guide while taking slabs for rolling, resulting without order generation and sometimes chopping as well in the newly commissioned plant. A systematic data and metallurgical analysis has been done to find out the camber formation mechanism and related design & process parameters. Cooling by water plays an important role in extracting heat from both the mold and solidifying liquid steel during the continuous casting of steel. It is characterized by complex boiling phenomena. Heat extraction rates during water cooling, which have strong dependence on the metal surface temperature and it can rapidly change with time as the strand cools down. Hence uncontrolled cooling may cause fluctuations in the temperature gradients inside the solidifying shell of steel and generate tensile thermal stresses at the solidification front that can ultimately lead to the appearance of cracks, camber and centerline segregation in the final product. Air mist cooling (AMC) in secondary cooling zone of continuous casting machine is a step in this direction. Air mist nozzles utilize compressed air in combination with water pressure to atomize secondary cooling water. This provides a much wider turn down / control ratio which is necessary in case a product mix covers a wide range of steel grades. Air Mist Cooling (AMC) leads to less camber results, less core segregation and more uniformity of temperature is attained. It helps in more equiaxed zone growth which helps in less core segregation. Key words: Thin slab casting & Rolling, Camber, on-line measurement

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STUDY OF ELASTO-PLASTIC DEFORMATION IN CAST AlCu7 ALLOY

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The need for efficient and clean technology puts high demands on modern combustion engines, to compete in a market with alternative drive concepts. Downsizing and weight reduction require light alloys with superior thermo-mechanical properties for high temperature exposure. Cast Al-Si and Al-Cu alloys are competing last generation light materials to increase high temperature strength, creep-resistance and long term stability of engine components. In such alloys with heterogeneous microstructures a composite-like deformation behavior is responsible for superior high temperature properties. Stiff Si or Al2Cu particles, respectively, reinforce a ductile alpha-Al matrix to a composite with improved thermo-mechanical strength. However, different Young's moduli and coefficients of thermal expansion are responsible for high microstress gradients and unpredictable microcrack formation under operation. These micro-mechanical deformation mechanisms in Al-Si and Al-Cu systems, responsible for crack initiation and growth, are unknown by far.
Therefore, the current work describes an experimental approach of combining non-destructive diffraction and imaging techniques to investigate the elasto-plastic deformation behavior of two competing light alloy classes. Al-Si hyper- and hypo-eutectic are compared to Al-Cu in as cast and T6 heat treated conditions. Microstrains, stresses and crack formation were investigated, using Photons, Electrons and Neutrons as probe particles. High resolution imaging of the phases, selected microstrain analysis and 3D visualization of crack formation reveal information of deformation mechanisms, internal architectures and damage propagation under operation conditions.

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CAPILLARY-MEDIATED SOLID-LIQUID ENERGY FIELDS: THEIR DETECTION WITH PHASE-FIELD METHOD

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Grain boundary grooves (GBGs) are common features on polycrystalline solid-liquid interfaces. Stationary GBGs, of course, support distributions of their Gibbs-Thomson thermo-potentials along their curved interfaces, but, surprisingly, the vector gradients of these potential distributions excite *persistent* capillary-mediated energy fluxes. Moreover, these steady interfacial fluxes exhibit vector divergence, and therefore can add, or remove, small rates of thermal energy along their interfaces. These previously undetected flux divergences affect the energy budget and modulate the local speed of moving solid-liquid interfaces, thereby acting as auto-perturbations stimulating pattern formation and influencing the evolution of solid-liquid microstructures. The existence of active energy fields on GBGs was exposed using precision multiphase-field simulations, as capillary energy fields induce small, proportional changes to the thermo-potential along a solid-liquid interface. These non-linear components of the interface potential were determined along simulated solid-liquid interfaces on a variety of GBGs as measured residuals of their thermo-potential. Quantitative phase-field measurements of persistent interface energy fields on stationary GBGs independently confirm prior analytical predictions based on sharp-interface thermodynamics and field theory. Self interactions of stationary GBGs with their own capillary fields will be shown to cause only minor modifications to the profiles of variational GBGs, the analytical profiles for which have been used extensively to estimate solid-liquid interfacial energies for many materials.

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MICROSTRUCTURE EVOLUTION OF AN Al-Cu ALLOY IN THIN-SAMPLE POLYCRYSTALLINE SOLIDIFICATION: IN SITU SYNCHROTON X-RAY RADIOGRAPHY IMAGING AND FULL-SCALE PHASE-FIELD SIMULATIONS

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The growth dynamics of multiple equiaxed dendrites in a thin metallic sample is studied using *in situ* synchrotron X-ray imaging of Al-4 wt.%Cu alloy solidification experiments and corresponding full-scale three-dimensional (3-D) phase-field (PF) simulations. The tip growth velocity V, tip radius ρ, the secondary dendritic arm spacing (SDAS) λ_2 and the total solid fraction f_s, are analyzed systematically in a relatively large range of cooling rate R_c. Through an in-depth comparison of the growth dynamics with experiments, including the tip velocity and the primary arm length, the nucleation undercooling for each grain is estimated. Quantitative agreements in V of several selected grains and f_s between experiments and simulations have been achieved. The tip velocity, followed by free growth from the melt that is cooled continuously at constant R_c, decreases first at the very beginning of solidification in both experiments and simulations. Subsequently, V increases up to a peak value until the grains interact with each other by solutal effect. Moreover, an oscillation growth of the dendritic tip is observed during the soft-impinged growth stage in both experiments and simulations, featured by an acceleration of V after it goes down to a minimum from the peak value. With increasing R_c, V will be enlarged while ρ will be reduced, due to the narrowed solute boundary layer ahead of the tip. Furthermore, ρ and λ_2 show good agreements between simulations and dendrite growth theories, with $\rho \sim V^{-1/2}$ and $\lambda_2 \sim R_c^{-1/3}$. However, experimental measurements of λ_2 are generally larger than λ_2 in PF simulations, and this discrepancy could be attributed to liquid convection in experiments, despite the thin sample configuration. We incorporate liquid flow dynamics into the computationally

less-demanding 2-D PF simulations. It has been found that with the gravity-driven convection the sidebranches are more developed and coarsened, thereby enlarging the spacing between the secondary arms.

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INFLUENCE FACTORS ANALYSIS OF THE BLOCKING LAYER IN THE ELECTROMAGNETIC INDUCTION CONTROLLED AUTOMATED STEEL TEEMING SYSTEM

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Abstract: In the electromagnetic induction controlled automated steel teeming (EICAST) technology of ladle, the position and thickness of the blocking layer are critical factors to determine the coil installation position and the coil length. Therefore, it is also an important factor affecting the successful implementation of this new technology. In this paper, the influence of the molten steel refining temperature and the ladle containing time of molten steel on the position and thickness of the blocking layer were studied by numerical simulation method. The molten steel refining temperature and the ladle containing time are determined by the steel grades and the production processes, the position and thickness of the blocking layer can only be adjusted by changing the elements of alloy filled in the nozzle. Therefore, the influence of alloy compositions on the position and thickness of the blocking layer was also analyzed. To verify the accuracy of numerical simulation results, a large experimental platform was used to imitate the actual working condition of the ladle with the electromagnetic steel teeming system. The results show that the position of the blocking layer moves down with the increase of the molten steel refining temperature and the ladle containing time of molten steel. The thickness of the blocking layer decreases with the increase of the molten steel refining temperature, however, it increases with increasing of the ladle containing time of molten steel. In addition, the position and thickness of the blocking layer can be largely adjusted by changing the elements of the alloy filled in the nozzle, which is very important for the industrial implementation of the EICAST technology.
Keywords: EICAST, refining temperature, containing time of molten steel, blocking layer, numerical simulation

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EFFICIENT MODEL FOR THE PREDICTION OF DENDRITIC GRAIN GROWTH USING THE LATTICE BOLTZMANN METHOD COUPLED WITH A CELLULAR AUTOMATON ALGORITHM

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An efficient model for the prediction of dendritic grain growth is developed coupling the lattice Boltzmann method for solving the transport of solute and a cellular automaton algorithm for determining the evolution of grains' envelope and the release of solute during phase change. In contrast to solving equations from the field of continuum mechanics the new model is more related to particular occasions what is more similar to the behaviour of cellular automaton algorithms.

The resulting dendritic grain growth shows qualitative correctness, although the consideration of solute conservation is still missing. It is shown that neglecting proposed conditions regarding the choice of time step size can destabilize the solid-liquid interface resulting in secondary and ternary dendrite arms.

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SIMULATION OF MACROSEGREGATION AND COLUMNAR TO EQUIAXED TRANSITION IN A NUMERICAL SOLIDIFICATION BENCHMARK PROBLEM

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The simultaneous prediction of macrosegregation and columnar to equiaxed transition (CET) in metal casting is still an important challenge. One of the open questions is the role of melt convection on the CET and the effect of the CET on macrosegregation. A three-phase Eulerian volume-averaged model for macrosegregation and CET is developed. The model uses our recently-developed accurate constitutive relations for equiaxed solidification. It accounts for columnar dendrite tip undercooling and nucleation of equiaxed grains ahead of the columnar tips. The model is used to perform macrosegregation and CET simulations for a numerical benchmark problem involving solidification of a lead-18 wt. pct. tin alloy in a side-cooled cavity. Simulations are performed for different values of the dendrite tip selection and nucleation parameters. As the value of the dendrite tip selection parameter is increased, the predicted number and depth of channel segregates decreases significantly and the grain structure transitions from mixed columnar/equiaxed to fully columnar.

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ADVANCES IN MODELING OF STEEL SOLIDIFICATION WITH IDS

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IDS (InterDendritic Solidification) is a thermodynamic-kinetic software package, which simulates phase changes, compound formation/dissolution and solute distribution during solidification of steels and during their cooling/heating process after solidification. The software package also simulates solid state phase transformations related to the austenite decomposition process (ADC module), at temperatures below 900/600 °C, and calculates important thermophysical material properties (enthalpy, thermal conductivity, density, etc.) from the liquid state down to room temperature. These data are needed in other models, such as heat transfer and thermal stress models, whose reliability heavily depends on the input data itself.
The present IDS software package consists of six calculation modules: 1) SOL: simulation of solidification, 2) ADC: simulation of austenite decomposition, 3) MAT: calculation of temperature functions for material properties, 4) GAS: calculation of hydrogen and nitrogen solubility, pressure and diffusivity, 5) PRF: simulation of precipitate formation at the ferrite/austenite phase interface, and 6) SCA: simulation of oxide scale formation in the strand surface. The software package also features a data bank for material properties, including parameters for Gibbs energy, enthalpy, diffusion, microstructure, thermal conductivity, density and liquid viscosity.
SOL module – the main module of the IDS software package – is applicable for the temperature range from 1600 to 900 °C (low-alloyed steels) and from 1600 to 600 °C (high-alloyed steels). The module applies thermodynamic chemical potential equality equations (all components), interfacial

material balance equations including Fick's 1st diffusion law (solutes) and a finite difference application of Fick's 2nd diffusion law (solutes).
The development work of the software package started in 1984 and has since validated with extensive data of solidification experiments with good results. Owing to the short calculation times, the IDS tool is suitable for on-line applications. So far, it has been installed to four slab casters for on-line use. In this presentation, the IDS and its modules are presented with the latest developments and validations along with examples of modelling results. Special attention will be given to SOL module.

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CONTROL OF SOLIDIFICATION PATTERN OF CAST IRONS BY SIMULTANEOUS THERMALS AND CONTRACTION/EXPANSION ANALYSIS

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An experimental device was developed with a technique to simultaneously evaluate cooling curves and expansion or contraction of cast metals during solidification. It conducts thermal analysis and volume change measurements in a single ceramic cup so that mould media as well as solidification conditions are constants, with cast iron quality as the variable. The recorded data are processed using specialized software, which conveniently displays both cooling and contraction/expansion curves and their specific parameter values. Experiments compared solidification patterns for white [WI], grey [GI] and ductile [DI] cast irons, focusing on the early stages of solidification, to correlate the most important events between the cooling curves [the start of eutectic freezing (nucleation), the beginning and the end of eutectic reaction and the end of solidification] and contraction curves, to evaluate the sensitivity to chill [carbides] and shrinkage formation. The maximum expansion, reached between the end of the eutectic reaction and the end of solidification, depends on the carbides/graphite ratio and graphite morphology: WI-0.465%, GI-0.552%, DI-1.032%, as averages. Graphitic expansion, absent for WI, increased to 0.109% [GI] and up to 0.596% [DI]. For both GI and DI the expansion at the end of solidification is only 6% lower compared to the maximum level, while for WI it decreased more than 50%. Specifically the increasing speed of the graphitic expansion up to the maximum level [Kgr1] is different compared to it decreasing up to the end of solidification [Kgr2], and also are different for irons being tested, GI versus DI. Nodular graphite led to the [Kgr1] factor being 2.5 times higher, compared to GI, whereas only a slight difference was observed between GI and DI for the Kgr2 factor. Higher graphitic expansion in DI led to higher shrinkage sensitivity, compared to GI, as measured in furan resin mould test castings.

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OPTIMIZATION OF ULTRASONIC CAVITATION PROCESSING IN THE LIQUID MELT FLOW

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Ultrasonic processing (USP) during direct-chill casting of light alloys is typically applied in the sump of a billet. This approach, though successful for structure refinement and modification, has two main drawbacks: (a) mixture of mechanisms that rely heavily on dendrite fragmentation and (b) limited volume that can be processed by a single ultrasonic source. We suggest moving the location of USP from the sump to the launder and applying it to the melt flow for continuous

treatment. The apparent benefits include: (a) degassing of the melt, (b) grain refinement through activation of non-metallic inclusions, fragmentation of primary crystals, and deagglomeration of grain refining substrates, and (c) a possibility to use a single ultrasonic source for processing large melt volumes. To optimise this process with regard to the acoustic intensity and melt residence time in the active cavitation zone, a flow modification with baffles as well as informed location of the ultrasonic source are required. In this paper, we demonstrate the results of experimental trials where the degassing degree and grain refinement have been the indicators of the USP efficiency for two alloys, i.e. A356 and AA7050. The results are supported by acoustic measurements and computer simulations.

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NUMERICAL SIMULATION OF WAVE-LIKE NUCLEATION EVENTS

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The Interdependence model [1] predicted that nucleation would occur in waves of events with regions of no nucleation in between each wave. The waves continue to form until nucleation covers the sample. The cause of this phenomenon was attributed to the formation of a nucleation-free zone which incorporates solute suppressed nucleation and inhibited nucleation zones. Recent real-time synchrotron x-ray studies by Prasad et al [2], Liotti et al [3] and Xu et al [4] have confirmed that nucleation of equiaxed grains does not occur continuously but in a step wise fashion with a number of events occurring followed by no nucleation for a short period before another set of events occurs. This process is more clearly observed under conditions of a relatively low temperature gradient. A microscale solidification model that predicts diffusion controlled dendritic growth has successfully shown the effect of the developing constitutional supercooling on the selection of nucleation events. In this study, we use this model taking into account particles with nucleation potencies similar to those provided by a grain refining master alloy, to predict the solidification behaviour under the conditions experienced during the above published real-time synchrotron studies.

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FORMATION OF METASTABLE MICROSTRUCTURES IN Al-45wt%Cu ALLOY QUENCHED IN HIGH MAGNETIC FIELD

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The rapid solidification processing is frequently used to fabricate novel microstructures. In this work, the formation of novel microstructures in two Al-Cu alloys, i.e. hypoeutectic Al-26wt%Cu and hypereutectic Al-45wt%Cu alloy, in a steady magnetic field (SMF) was investigated using the conventional quenching technique. It was found that the application of the SMF led to appearance of a bulky ϑ-Al2Cu phase in Al-26wt%Cu and bulky supersaturated α solid solution Al-45wt%Cu alloy, respectively, which are impossible to appear under normal solidification conditions. The cooling curves of the quenched samples show that the cooling rate with a SMF is significantly higher than that without a SMF, and a larger undercooling before the onset of eutectic solidification was achieved in the SMF. The microstructure formation in the SMF can be explained using the phase diagram with metastable extensions.

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NUMERICAL SIMULATION OF FORCED FLUID FLOW IN THE MUSHY ZONE WITH THE EXISTING OF INTERMETALLIC PHASE IN AlSi7Fe1 ALLOY

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The presence of small amount of the Fe in the Al-Si alloy causes the formation of the platelet-shaped Al5FeSi intermetallic phase, which is detrimental to the alloy mechanical properties. A series of directional solidification experiments on Al-Si-M alloy were performed under diffusion or controlled convection to study the interaction of fluid flow and the formation of the intermetallic phase and their effect on microstructure and segregation[1]. The blocking effort of the intermetallic phase on fluid flow in the mushy zone leads to the decrease of the permeability of the mushy zone both in flow normal and parallel to the primary dendrites and a decreased species transport. A two-phase model is used to study the effect of the intermetallic phase on the fluid flow and segregation. In the two-phase solidification model, the columnar dendrites are approximated by step-wise growing cylinders with constant primary and secondary arm spacing. The growth kinetics of the columnar phase is governed by the diffusion of the rejected solute ahead of the solid-liquid interface. The conservations for mass, enthalpy, momentum and species are solved respectively. The influence of the intermetallic phase on the fluid flow in the mushy zone is approximated with the anisotropic permeability law with an additional coefficient (where represents the impact factor of the intermetallic phase). Due to the insignificant amount of the Fe in the alloy, the simplified binary alloy Al-7%Si alloy is used to perform current simulation. The unidirectional solidification process can be qualitatively reproduced with the two-phase solidification model. Two inward circulation flow pattern ahead of the mushy zone, which induces the strong positive segregation in the center of the sample, is observed. The fluid velocity in the mushy zone is suppressed due to the decrease of the permeability caused by the formation of the intermetallic phase. At the same time, the segregation severity is reduced for the decreasing of the mass transfer in the mushy zone. The decreasing of the velocity will decrease the feeding ability, which makes it more likely to form some pores and porosities.
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EFFECT OF PORES ON TENSILE FRACTURE OF DIE-CAST AlSiMgMn ALLOYS WITH 3D X-RAY μ-CT AND

FE SIMULATION

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Die casting process is widely used in making Al and Mg alloy components, especially in automotive industry. In the process, due to high speed filling of liquid metals gases in die cavity are prone to be entrapped resulting in final pores in the castings. The pores are detrimental to the casting properties and performance.
In this study, the pores in die-cast AlSiMgMn alloys were inspected and reconstructed with high resolution 3D X-ray micro computed tomograpgy (μ-CT) technique. Finite element (FE) meshes were built with consideration of the pore actural morphorloges from the μ-CT inspection. Based on dutile damage model, the FE simulation of tensile fracture at the velocity of 1 μm/s of the alloys was carried out. The simulation results were compared and verified with the tensile of in-situ scanning electron microscopy (SEM). The two results are agreement in the main crack path and pores on the fracture. With the pore-scale FE simulation, the effects of pore characteristics including size, sphericity and locations et al. on the stress distributions, crack initiation and growth during the tensile were analyzed and discussed. It was found that the pores of lower sphericity and larger volume easily formed secondary cracks and promoted main crack deflection; the pores near surface or minimum cross section resulted in serious stress concentration hence accelerating crack initiation. The results showed that aggregation of brittle alpha-Fe intermetallics of the alloys also had important influence on the main crack propagation.

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3D DENDRITE NEEDLE NETWORK MODELING AND X-RAY RADIOGRAPHY OF EQUIAXED ALLOY SOLIDIFICATION IN GRAIN-REFINED Al-3.5wt.-%Ni

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Multiple dendritic equiaxed grain formation is common to solidification in many technical alloys in industrial solidification processes. We investigate this type of grain formation and competition during directional solidification of grain-refined Al-3.5wt.-%Ni at various solidification conditions by comparison of experimental data and 3D dendrite needle network (DNN) modeling. For the experiments in-situ x-ray radiographic characterizations in thin samples reported in literature [1] are used. DNN modeling makes use of heterogeneous nucleation, branched dendritic growth and solutal interaction between branches and multiple equiaxed grains. Here, a first comparison using a 2D modeling approach valid at low Péclet numbers [2] is extended to account for thin samples in 3D, higher Péclet-number, as well as different grain orientations.
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MESOSCALE ENVELOPE MODELLING OF COLUMNAR GROWTH AND CONDITIONS FOR CET IN NPG-DC ALLOY

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Mesoscopic envelope models rely on the description of the complex morphology of a dendritic grain by an envelope, which is a smooth surface connecting all of the dendrite tips. This simplification in the description of the grain shape enables to reduce requirements on spatial resolution and allows for modelling of larger number of grains or domains, when compared to more detailed microscopic approaches. Mesoscopic envelope modelling has already shown its capability of simulate columnar growth in transparent alloy systems during directional solidification, including misorientation between columnar grains [1], as well as equiaxed grains [2]. Here, we apply 3D mesoscopic envelope modelling to simulate columnar dendritic growth in the transparent alloy Neopentylglycol-(D)Camphor (NPG-DC) during directional solidification under microgravity conditions. Experimental results for comparison are taken from the « TRACE-3 » experiment [3], conducted on a TEXUS sounding rocket. Special emphasis is put on a comparison of characteristics of columnar growth and the conditions for columnar-to-equiaxed transition CET. [1] Viardin A., Založnik M., Souhar Y., Apel M., Combeau H., 2017, Acta Materialia 122, 386-399. [2] Souhar Y., De Felice V.F., Beckermann C., Combeau H. and Založnik M., 2015, Computational Materials Science 112A, 304–317. [3] Zimmermann G., Hamacher M., Sturz L., 2017, Proc. Of the 23 rd ESA Symposium on European Rocketr and Ballon Programmes and related research, A-035.

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INVESTIGATION ON BAND SEGREGATE FORMATION DURING THE ELECTROSLAG REMELTING OF H13 DIE STEEL

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Band segregation has been found in the H13 die steel produced by the electroslag remelting (ESR) technology. Chemical and metallographic studies have been carried out on a one ton ESR ingot of H13 die steel, so as to understand the formation mechanism of the band segregation. The results indicate that the oxygen and nitrogen contents in the ingot increase by 47.2% and 15.7%, while the sulfur content decreases by more than 50% after the treatment of the ESR process. Most of the sulfide inclusions are effectively removed during the ESR process. The original Al2O3 or MgO•Al2O3 inclusions would be modified to the CaO•Al2O3 inclusions. The overall removal ratio of the inclusion is around 65.8%. The Vickers hardness number of the samples is around 170 HV. The segregation of the vanadium carbide is found in the ESR ingot, and lots of the sulfide segregations are detected around the segregation of the vanadium carbide. Besides, black and white segregation bands can be observed on the samples after etching, and the microstructure of the samples is identified as the granular pearlite. More granular cementite occurs in the black band than that in the white band.

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SOLIDIFICATION ASSESSMENT OF COMMERCIAL STEEL GRADES WITH THERMODYNAMIC DATABASES

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One of the most powerful tools for studying the development of microstructures is the CALPHAD (Calculated PHAse Diagrams) method because it comprises information derived from thermodynamic principles, presented in a form that makes the data readily accessible. It is much easier and less time consuming to perform these thermodynamic calculations with any of the available software rather than trying to experimentally identify the phase transformations during solidification, but one has to be sure that the temperatures calculated are close to the real system. Even when the thermodynamics tells us what should happen in equilibrium, it does not guarantee that it is what will happen, as the real system may be influenced by kinetics. However, when dealing with complex systems like commercial grades of steel, where many phases may be formed during solidification through various reactions, it is necessary to perform more complex calculations.
In this publication two examples will be shown on how the CALPHAD method is used to evaluate the castability of commercial steel grades where complex phases appear during solidification and cooling.
The first example will focus on the different phases that can appear in HSLA steels (High Strength Low Alloyed) where the microalloying elements (Nb, V, Ti, Al, etc.) that precipitate as carbo-nitrides at different stages during and just-after solidification are related to the so-called second ductility trough and may cause cracking at the last stages of the casting process.
Further, the second case show the possible castability issues for AHSS (Advanced High Strength Steels) that are related to the phase transformation and how the CALPHAD method can help on designing new steels.

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INFLUENCE OF THERMOELECTRIC-MAGNETIC EFFECT ON SOLIDIFICATION OF ALLOYS

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During solidification of alloys with a temperature gradient in a stati magnetic field, the thermoelectric magnetic(TEM) force may be induced. The TEM force will produce convection in the molten metal and stress in the solid during the solidification. The convection and stress may play an important role in the formation of the micro-and macro-structures of the alloy. The influence of the thermoelectric magnetic force on the unidirectional solidification of Al-Cu alloys under a static magnetic field has been investigated experimentally. It is shown that the TEM force induced the instability of solid/liquid interface, which is the sound verification of the ATG instability model proposed by Asalor, Tiller and Granfield in 1990‘s. The experiments showed that the dendrite growth was modified seriously and the dendrite spacing increased along with increase of the magnetic field. The columnar- equiaxed transition during directional solidification of the alloy was promoted by the imposing of a astatic magnetic field, due to the TEM force and convection. The static magnetic field was imposed in the additive manufacturing of superalloy with laser melting. It is shown that the magnetic field accelerated the CET transition and the crystal grains were refined. The result was attributed to the strong TEM force in the process.

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DENDRITE GROWTH DIRECTION MEASUREMENTS: UNDERSTANDING THE SOLUTE ADVANCEMENT IN CONTINUOUS CASTING OF STEEL

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Open Source Phase-Field based Bulk Flow with Solidification Model for Steel
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Abstract:
Micro-scale solute transport due to fluid convection during an alloy solidification is of paramount importance in an industrial casting process due to the fact that how the excess solute governs the non-uniformity of chemical composition in the cast product. Experimental observation [1] being challenging, previous authors utilised commercial modelling [2, 3] though the information on the bulk fluid flow behaviour for Fe base alloys is limited. Hence the authors have developed an open source phase-field based solidification model which has been validated for pure Nickel melt as well as for binary Fe-0.1wt% C alloy. Moreover, the model has been coupled with incompressible bulk fluid flow. The effect of interface growth velocity on the dendrite bending angle due to fluid convection has been studied for different Fe-C binary alloy compositions, providing the potential for being used for materials research applications.
Keywords: binary alloy, solidification, phase-field, dendrite bending, open source
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INVESTIGATION OF THE COLUMNAR/EQUIAXED TRANSITION (CET) DURING THE UNIDIRECTIONAL SOLIDIFICATION OF Al4Cu ALLOY AT DIFFERENT CONSTANT COOLING RATES

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Unidirectional solidification experiments were performed according to the vertical, upward Bridgman method by using Al-4 wt.% Cu alloy. The diameter of the cylindrical samples was 8 mm and their length was 120 mm. Three different constant sample-movement velocities were used during the experiments. The temperature of samples was measured by 13 pieces of NiCr-Ni thermocouples located at different positions along the length of samples during the total solidification process. The positions of the solid/liquid interface at starting the solidification (ahead of the dendrite tip in the melt) and at finishing the solidification (at the root of the dendrites), the interface velocity and the temperature gradient were calculated from the recorded temperature-time data pairs by using an in-house software. The interface velocity changed between 0.2 mm/s and 1.6 mm/s, and the temperature gradient varied between 7 K/mm and 1 K/mm from the bottom towards the top of samples. So the values of cooling rate (1.5; 1.6 and 1.8 K/s) were near constant along the length of samples. The columnar/equiaxed transition was investigated on the solidified longitudinal sections. It was stated that the solidification started at the bottom of sample with the formation of a cellular structure. Afterwards a columnar dendritic structure developed which transformed into an equiaxial dendritic one above the interface velocity of 1.2 mm/s. The secondary dendrite arm spacing (SDAS) was measured on the longitudinal

sections in the sample axis where the movement velocities of the solid/liquid interface were the identical. By increasing the interface velocity, the values of SDAS decreased from 55 [U+F06D]m to 35 [U+F06D]m. After the Barker's colour etching, the change of the grain structure was analysed on the cross-section of samples as a function of the different cooling rates.

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TIME-RESOLVED X-RAY TOMOGRAPHY STUDIES OF DENDRITIC EVOLUTION IN Al-Cu ALLOYS

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Dendrites are ubiquitous structures that are central to setting material properties but the mechanism behind how dendrites grow is not fully understood. After x-ray synchrotron radiation experiments are performed, the dendritic growth of Al-12.6wt%Cu alloys is studied in 4-dimensions to track the evolution of the 3-dimensional structure as a function of time using novel x-ray tomography algorithms. Starting from a temperature above the liquidus, samples were cooled, at multiple cooling rates, to observe dendritic growth. These experiments provide information on the differences in dendrite tip growth rates, morphologies, branch spacing and interfacial curvatures due to different cooling rates. Two-point spatial correlations are used to investigate these quantities to provide a better insight into the process of dendritic growth.

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SOLIDIFICATION PATH OF CAST IRON ALLOYED WITH 9.0%Al

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The oxidation properties of cast iron were reported to sharply increase if the aluminum content exceeds 6–8%, but the applications of such alloys are still limited due to the formation of free complex carbides of iron and aluminum which renders the alloy very brittle and unmachinable. However, the factors affecting the structure of such alloys are still far from being well studied. This paper deals with the different parameters affecting the solidification path of the cast iron containing 9-10% Al. Preliminary results show that the structure of this alloys is rather sensitive to Si-content, cooling rate, inoculation practice as well as alloying with copper. Formation of primary Fe-Al carbides could be considerably eliminated by using the proper combination of the above mentioned parameters. Differential thermal analyses as well as repeated quenching from different temperatures were used to study the solidification behavior of this alloy. Alloys containing up to 3.5% Si solidified with the complex carbide formed as primary phase. Inoculation with Ca Si and alloying with 1% copper suppressed the primary carbide formation and solidification starts with primary austenite crystals. The solidification of – alloys containing up to 3.5% Si ends with the invariant 5-phase reaction: With increasing Si-content to 5.0%, the alloy solidifies through one eutectic reaction: (at 1220°C) $L + \varkappa \rightarrow \gamma + \alpha + G$ and ferrite together with graphite are the only existing phases down to the room temperature. $L \rightarrow \alpha + G$ In the second part of this report, the effect of solidification under elastic vibrations, both in the low frequency of mechanical vibrations (˜ 50 Hz) or in the ultrasonic frequency of 20 KHz on the solidification path of the same alloy was investigated. The microstructural characteristics of the dynamically solidified alloy were compared to those of statically solidified ones. Dynamic solidification leads to structural refinement as well as remarkable increase in the graphitization potential and significant decrease in the complex carbides formation in the structure.

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EFFECT OF MAGNETIC STIRRING BY RMF ON THE MICROSTRUCTURE OF UNIDIRECTIONAL SOLIDIFIED Al-6wt%Si-4wt%Cu-2wt%Fe ALLOY

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The unidirectional solidification of Al-6Si-4Cu-2Fe alloy was performed in a vertical Bridgman furnace with bottom cooling. The diameter of cylindrical samples was 8 mm and their length was 120 mm. In the course of the experiments, a sample movement velocity of 0.1 mm/s was used and the experiments were performed by applying of RMF magnetic stirrings having different intensities. During the solidification process, the temperature of sample was measured by means of 13 pieces of thermocouples located along the length of sample. The cooling rate, the position of the solid/melt interface, its movement velocity and the temperature gradient were calculated from the recorded temperature-time data by means of an in-house software. The aim of experiments was to investigate the effect of magnetic stirrings having different intensity (RMF 2 – 100 mT) on the microstructure of solidified sample and on the developed grain structure in case of a sample movement velocity of 0.1 mm/s. The intensity of magnetic stirring at which the columnar microstructure changed to equiaxial microstructure (CET) was also investigated. Both longitudinal- and cross-sections were made of the samples. The sections were prepared by a hydrogen-fluoride etching in order to investigate the developed structure. The grain structure developing during the solidification process was investigated after the Barker electrochemical etching of the sections.

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CELLULAR-AUTOMATON SIMULATION OF MICROSTRUCTURE EVOLUTION DURING ADDITIVE MANUFACTURING

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Recently, Additive manufacturing (AM) has emerged as a disruptive technology to manufacture complex parts with greater scales of economy and also with a reduced need for post-machining. However, the influence of processing conditions and the alloy compositions on the strength, defect formation are not yet fully understood. A quantitative simulation of the microstructure morphologies and segregation patterns for a given alloy composition will help towards a better prediction of the physical and mechanical properties of the developed part. More particularly, properties such as the susceptibility to solidification cracking are directly related to the segregation behavior as well as the structure of dendritic network in the mushy zone.
In this work, a Cellular Automata based three-dimensional (3D) model was developed to simulate dendritic growth for the case of AM. The Thermocalc database was used to obtain the equilibrium multi-component phase diagram. Finite Difference schemes were used to obtain the temporal and concentration fields in the computational domain. The interface velocity and concentrations were obtained by simultaneously solving the corresponding Stefan conditions for individual components along with the Gibbs-Duhem condition assuming local equilibrium at the interface. A height-function based curvature technique was used to accurately estimate the curvature of the sharp interface. In order to achieve a nearly grid-independent growth in any specified crystallographic direction, a decentered-cube algorithm was incorporated. The model validation was performed by comparing the velocity and tip radius selection with analytical relations based on the marginal stability criterion as well as simulations results obtained using the phase-field method. Further, the code was parallelised using MPI libraries, thus enabling it to be run on larger domains.

Multi-dendrite simulations were carried out under directional solidification corresponding to AM conditions. The dendrite morphology, orientation and primary arm spacing selection were studied for different cooling rates and thermal gradients. This model can be used to simulate microstructure evolution for generic two-phase alloys under AM conditions.

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ONLINE MODELLING OF HEAT TRANSFER, SOLIDIFICATION AND MICROSTRUCTURE IN CONTINUOUS CASTING OF STEEL

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Computational simulation and modelling of different phenomena in casting has greatly helped to solve practical problems in industrial casters and to improve process practices and control. Altogether, we still need deeper understanding of the complex solidification phenomena and transformations of microstructure to respond to the increasing requirements. For this purpose, advanced numerical simulation models for continuous casting of steel have been developed.
The models developed are the transient three-dimensional heat transfer model, CastManager, and the solidification and microstructure model, IDS. The computing times of these models are short and they are now integrated together to one online concept. The start and the end of casting as well as the ladle change, steel grade change and width change are also included in the integrated system. This concept is now installed to the automation systems of four slab casters in Finland. Testing and validation work is now in progress. The system simulates the important phenomena in continuous casting online. The future aim is that this information will be used for on-line quality control and for optimizing the process conditions to avoid defect formations. Many quality indices have already been developed. A steady state version of CastManager tool is also developed, called Tempsimu.
CastManager and Tempsimu tools consist of two separate modules: the three-dimensional mould model and the three-dimensional strand model. IDS is a thermodynamic-kinetic software package, which simulates many solidification and cooling related microstructural phenomena as phase transformations, inclusions and precipitates, grain size, austenite decomposition and material properties. IDS has also a quality prediction module, which calculates quality indices for decisionmaking. The heart of the IDS model is the large thermodynamic, diffusion and microstructure data bank made through our own assessment work.
On-line IDS calculates also the material data for the CastManager for the steel to be cast from the ladle composition. This is important because for accurate results from the heat transfer simulations, accurate data on the thermophysical material properties are needed. The boundary conditions describing the heat transfer phenomena taking place along the strand surface is also of crucial importance for obtaining reliable results. In CastManager, the boundary conditions can be determined very accurately. Each spray nozzle and roll can be described separately and accurately.
In this presentation, the developed models and the integrated on-line concept are presented with the latest developments, validations and industrial case examples.

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INFLUENCE OF MINOR ADDITIONS ON ICOSAHEDRAL SHORT-RANGE ORDER (ISRO) AND ITS CONSEQUENCES

ON NUCLEATION AND SOLIDIFICATION GROWTH KINETICS IN FCC ALLOYS

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The present contribution reviews the recent progress related to the influence of Icosahedral Short-Range Order (ISRO) and icosahedral Quasicrystals (i-QC) formation on the solidification of fcc alloys through minor solute element additions. From intensive crystallographic analysis of multi-twinned region in as-cast Al-based and Au-based fcc alloys, it has been shown recently that a so-called "iQC-mediated" nucleation mechanism occurs when a few hundreds ppm of Cr and Ir, respectively, are added to the melt [1] [2]. Similarly, it appears that the growth directions of dendrites in Al-Zn:Cr is also influenced by ISRO in the liquid, thus showing an attachment kinetics effect [3]. Similar observations have been made recently in pink gold alloys with Ir-additions, when the solidification speed is increased [4].

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INVESTIGATION OF THE MICROSTRUCTURE ADJUSTMENT BY VELOCITY VARIATIONS DURING THE DIRECTIONAL SOLIDIFICATION OF Al-Ag-Cu WITH THE PHASE-FIELD METHOD

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The microstructural pattern evolving during directional solidification is of high interest as it directly influences the material properties. During the ternary eutectic directional solidification of Al-Ag-Cu, besides the evolution of different patterns the solubility of silver in the α-aluminum phase changes by 50 % directly below the eutectic point. This leads to a change of the phase fraction and to a pattern adjustment. To understand the influence of the various physical and process parameters on the solidification, phase-field simulations are conducted using the massive-parallel Pace3D-framework. A temperature dependent phase-field model based on the grand potential approach is used to investigate the evolving patterns during the solidification processes and the afterwards adjustments due to the solubility change. The model incorporates temperature dependent Gibbs energies and diffusion coefficients. With this model, the effects of cooling rate, temperature dependent diffusion, interface anisotropy and concentration variations

in the solid phases are investigated by systematic simulation studies. Based on quenched and then heat-treated experimental microstructures, studies are presented which show a similar behavior as the experiments. To quantitatively compare the microstructure evolution over time from the experiments and simulations, principle component analysis (PCA) based on two-point correlations is utilized. With this, the evolution of experimental microstructures could be quantitatively reproduced with phase-field simulations.

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PHASE-FIELD SIMULATION OF THE MICROSTRUCTURE EVOLUTION DURING DIRECTIONAL SOLIDIFICATION OF THE TERNARY EUTECTIC SYSTEM Bi-In-Sn

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Due to the significant effects of the underlying microstructure on the material properties, accurate understanding of microstructure evolution in solidification processes has attracted lots of attentions in recent years. The low melting point of the ternary eutectic Bi-In-Sn alloy has lead to accurate in situ observations of its solidification process in experimental studies. Although these observations have deepened our understanding of microstructure evolution, due to complexity of the procedure there are lots of open questions of ongoing mechanisms. In the current study a thermodynamically consistent phase-field model based on the Grand potential approach is utilized to simulate the pattern formation in directional solidification of the system. As the first step of simulation studies, CALPHAD database is benefited to model the Gibbs energies and derive the chemical potentials of associated phases and the driving forces of the solidification process. Based on the reported system and process parameters like interfacial energies, solidification velocities and temperature gradient, two and three dimensional simulations are performed. The experimentally investigated 2D lamellar microstructure with ABCB repeat unit (A: γ-Sn , B: $BiIn_2$, C: β-In) is achieved and the effects of material and simulation parameters on the phase arrangement is studied. Case studies of different instabilities like oscillations of phases boundaries, bifurcation and tilting of solidified phases are performed to investigate their stability ranges. The anisotropy of interfacial energies is considered as an effective parameter in pattern formation which is difficult to be controlled or measured in experimental studies. By means of different anisotropy models and the possibility of exact control of parameters,the effects of orientation and strength of the exposed anisotropy is determined. These effects can be summarized as changes in repeat unit and strength of the observed instabilities. Finally for each solidification velocity, the most stable conditions are introduced.

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PHASE-FIELD SIMULATIONS OF COUPLED DENDRITIC-EUTECTIC GROWTH

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The solidification of alloys shows a large variety of different microstructures depending on the material system and processing conditions. Since materials properties such as tensile strength are dependent on the microstructure, its prediction is a topic of high interest in order to produce materials with tailored properties. Whereas theory is capable of investigating simple geometries, simulations are utilized to ascertain the influence of processing conditions on complex

evolving geometries. An example of this is the coupled growth of dendrites and eutectics, which typically evolve at different length scales. % irgendiwe ohne example schreiben In order to simulate this coupled growth, the phase-field method is chosen as it has been established as a versatile tool to investigate microstructural evolution. The phase-field model is based on a grand potential approach with parabolic free energies approximating thermodynamic CALPHAD data of the system Al-Cu. With this the coupled growth of coarse dendrites and fine eutectics during directional solidification is investigated in two as well as three dimensional simulations. Depending on the process parameters, observations include: Closely-spaced dendrites turning into cells, stable coupled dendritic-eutectic growth, nucleation of eutectics on dendritic sidebranches as well as transitions to a completely eutectic state. Based on these results a tentative microstructure map is established. Finally, the influence of the dendritic growth direction on the microstructure is investigated.

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FINITE DIFFUSION MICROSEGREGATION MODEL APPLIED TO MULTICOMPONENT ALLOYS

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Macrosegregation phenomena in casting processes of metallic alloys generate freckles that limit manufacturing of parts with high mechanical properties. Freckles are particularly detrimental in single crystals (SX) produced for aeronautical applications, such as turbine blades. They generates both structural and composition inhomogeneities. The last generation Ni-based superalloys are more subject to freckle formation. The control of microstructure and composition homogeneities thus remains a challenge when producing SX turbine blade with always better in-service properties. Convective transport caused by buoyancy forces disturbs dendritic growth and results in segregation phenomena. Modeling of macrosegregation using usual local hypotheses (e.g., lever rule or Gulliver Scheil solidification paths) is able to describe solutal-driven convection and complex interactions occurring around the dendritic network. However, the coupling between dendrite growth and microsegregation phenomena provided by these simple approaches are not sufficient to predict the final as-cast distribution of species and phases at the scale of the SX part, yet required for further calibration of solution and ageing heat treatments. Finite diffusion of chemical species must be considered due to the need for precise as-cast state as well as the particularly long solidification time that characterizes directional casting processes. This present communication reports a microsegregation model that accounts for finite diffusion in phases as well as dendrite tip undercooling. Equations are generalised to multicomponent alloys. Experimental data are used for validation with different solidification conditions. Implementation in a finite element model solving heat and mass transfers is demonstrated. The microsegregation model is coupled with CALPHAD databases, yet not directly computing thermodynamic equilibrium. Instead, a tabulation strategy is developed. It thus provides with an efficient approach that avoids time consuming local equilibrium computations. Demonstration is given by simulation of a SX geometry produced by directional solidification.

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FINITE ELEMENT MODELING OF SOLIDIFICATION STRUCTURES IN STEEL INGOTS

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The industrial sectors of energy and transport require the development of equipment with high levels of safety and performance. These requests compel steelmakers to develop cast products with a high microstructural, chemical and mechanical homogeneity. As part of the SOFT-DEFIS project, collaboration between academic and industrials partners has been developed to optimize steel ingots quality in response to these expectations. The numerical modeling activity presented here is part of this project and aims at predicting the formation of solidification grain structures - columnar or equiaxed - and associated segregations. In addition, comparisons between simulation results and experimental analyzes of industrial ingots are planned as validation step.
A finite element approach is proposed for the modeling of grain structures development [1]. A level set method is applied in order to track the columnar front interface and a dendritic growth kinetics model is used to estimate its velocity. Equiaxed grains then develop in the undercooled liquid domain. A solid, an intra-granular liquid and an extra-granular liquid phases are associated to each columnar or equiaxed microstructure with specific chemical compositions. This original approach make possible to model the evolution of solidification progress at the level of elementary volumes and the exchanges between the two types of grain structure.
The conservation equations are solved using a splitting method [2]. Thus, their complexity is reduced by a sequential and time-decoupled resolution of the macroscopic transport and microscopic growth stages. Finally, at the scale of the ingot, the macrosegregation process is simulated considering the convective transport induced by buoyancy forces and the transport of equiaxed grains [3]. 1D and 2D simulation cases demonstrate the interest and efficiency of this approach. In addition, the importance to distinguish columnar and equiaxed grain structures is shown, in particular to predict the segregation processes and to improve the resolution steps. The model is applied, finally, to the scale of industrial foundry parts to predict the evolution of the developed structures and segregated zones, in comparison with the experimental analyzes of the project partners.
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PHASE-FIELD STUDY OF EUTECTIC COLONY FORMATION

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The properties of a material are mainly defined by their chemical composition and by the underlying microstructure. Depending on the process conditions during the directional solidification and the applied material system different microstructures evolve, which are suitable for the demands of specific applications. Instable growth conditions during the directional solidification can lead to an increase of microstructure regions with irregular phase arrangements. These areas can compromise the resulting properties of the material and hence their applicability. A result of instabilities is the growth of eutectic colonies in the microstructure. Eutectic colonies are mainly observed in ternary systems for alloy compositions in the vicinity of a binary eutectic reaction. The formation of colonies is driven by instabilities in the planar solidification front, which are caused by the ternary impurities diffusing from the two solidifying phases into the liquid.
To investigate the formation process of eutectic colonies in their complex spatial arrangement, two- and three-dimensional large-scale phase-field simulations based on a Grand potential formalism

are conducted. The formation of eutectic colonies is observed for two independent systems in different manners.
In a first study, increasing amounts of silver are added to the isothermal undercooled binary eutectic system Al-Cu, to study the influence of the third component concentration on the colony formation. Due to the different compositions, colonies in different shapes and sizes form. In an additional study, the composition of the high-performance material system NiAl-34Cr is set fixed, but the solidification velocity is systematically varied beyond the stability range of the microstructure to initiate the growth of colonies. Based on this the stability of the evolved eutectic colonies is analyzed by a systematic variation of the applied temperature gradient.
The focus of both studies is the investigation of the underlying mechanism of colony formation and of the correlation between the colony arrangement and the eutectic structure inside each colony. Furthermore the interactions in the contact zones between the colonies are studied as these are indicated to be the weak points for the applicability.

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THE EFFECT OF STATIC MAGNETIC FIELDS ON CRYSTAL-MELT INTERFACIAL FREE ENERGY IN SOLIDIFICATION

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Magnetic fields have varieties of ubiquitous influence on nucleation and growth in solidification. As long as plenty of experimental phenomenon and results respectively have been revealed and retrieved, the mechanism of effect of magnetic fields on nucleation and growth in solidification keeps ambiguous. Not only thermodynamics mainly clarifies mechanism of growth qualitatively in solidification under magnetic field, but also it try to explain nucleation qualitatively in vain. Crystal-melt interfacial energy, a crucial parameter of dynamics, plays a key role in nucleation and growth in solidification. Crystal-melt interfacial free energy represents an important material constant in[U+FB02]uencing various aspects of microstructural evolution and thus materials properties decisively. Static magnetic field performs a notable effect on the undercooling of pure Al and Bi and the morphology of crystal-melt interface of Al-Cu alloys. Several studies have inferred that static magnetic field may affect the absolute value and anisotropy of crystal-melt interfacial free energy. Herein, experiment determination of crystal-melt interfacial free energy of opaque metals and alloys is always difficult and the examination precision is fundamental to the absolute value and anisotropy of solid/liquid interfacial free energy. Grain boundary groove method and dihedral angle method are very plausible to determination of the absolute value and the relative value of crystal-melt interfacial free energy respectively. Equilibrium shape method is very reliable to measurement of the anisotropy of crystal-melt interfacial free energy. The absolute value, relative value and anisotropy of crystal-melt interfacial free energy in the Al-Cu system have been retrieved with and without static magnetic field in this work.
Key words: Crystal-melt interfacial free energy, Static magnetic fields, Solidification

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PARTICLE SCALE MODELLING OF POROSITY FORMATION DURING SELECTIVE LASER MELTING PROCESS USING A COUPLED DEM-CFD APPROACH

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Selective Laser Melting (SLM), the most advanced metal additive manufacturing (AM) process, produces metal parts directly from a CAD file. Currently, the main bottlenecks preventing the SLM parts from competing with traditionally manufactured metal parts include the defects, such as porosity, low surface finish quality, high residual stresses and anisotropy. Though post-build microstructural and mechanical characterizations of the SLM fabricated specimen provide an ample amount of information regarding the build quality but getting real-time information from the experiments about temperature, porosity generation mechanism, melt pool formation and its flow behaviour is very challenging. Also, real-time monitoring by infrared cameras or pyrometric techniques is not very useful as the SLM process is highly localized (melt pool size of the order of 60 μm – 200 μm), rapid (cooling rate of the order of 1.0e5 K/s), and transient (involving traversal speed on the order of 1 m/s - 5 m/s). Therefore, alternative strategies, such as mathematical modelling is becoming an effective tool to gain deeper insights of the SLM process.
Getting precise information about the powder bed (particle size and distribution) in the SLM process is critical for the particle scale modelling but determining it by experimental methods is not trivial. The current work uses a Discrete Element Method (DEM) based particle modelling approach to generate a realistic powder bed. For this purpose, the open source C++ DEM code LIGGGHTS is modified and extended. Once the powder bed geometry is obtained, the particle distribution on the powder bed is exported to an open source CFD C++ code OpenFOAM. A three-dimensional multi- phase heat transfer and fluid flow solver is developed in OpenFOAM to study the transport phenomena (convection, melting/ solidification phase change, shrinkage, remelting, etc) in the SLM process. The Volume of Fluid (VOF) method is used to identify and track the interface of the powder particles undergoing phase transition. Fluid convection, temperature gradient (G), solidification rate (R) and melt pool characteristics dimensions are calculated using this solver, which solves mass, momentum and energy transport equations. The developed DEM – CFD platform helps to understand laser/matter interaction, melting of particles, the formation of the fusion zone, porosity generation, effects of particle size and track morphology. The computational results were validated with the available experimental results on melt pool dimensions.
Keywords: Selective laser melting; Additive manufacturing; Particle scale modelling; Discrete element method; Volume of fluid; OpenFOAM

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SIMULATION OF THE MICROSTRUCTURE FORMATION DURING LASER MELTING ADDITIVE MANUFACTURING VIA THE MODIFIED CELLULAR AUTOMATA METHOD AND ITS EXPERIMENTAL VERIFICATION

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Abstract: A virtual submesh cellular automata method is established to reduce the computational mesh induced artificial anisotropy with high efficiency and the method is applied to simulate the microstructure evolution during laser melting additive manufacturing. The additive manufacturing process is divided into three parts during simulation: random powder deposition, laser melting and rapid solidification. The laser induced temperature field will be calculated by finite difference method and a uniform solute concentration filed will be used for the non-equilibrium solidification. The Lipton-Glicksman-Kurz and Kurz-Giovanola-Trivedi model will be used respectively for the growth of the molten pool boundary and grains nucleated in the bulk. In order to compare with the experiment, the simulation will be implemented with the pulse laser source and the nickel

base superalloy. The single crystal substrate was used and the processing parameter to produce single crystal part was predicted by simulation. The final microstructure of parts fabricated by the laser melting additive manufacturing has compared with the simulation result, which shows reasonable agreement.
Keywords: modified cellular automata simulation, laser additive manufacturing, artificial anisotropy, single crystal prediction

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STATIC MAGNETIC FIELD HAS IMPACT ON SOLIDIFICATION STRUCTURE OF METALLIC SAMPLES FABRICATED VIA ADDITIVE MANUFACTURING

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Additive manufacturing has been regarded as a highly potential method to produce metallic parts with complex geometry. Its basic process in fact is laser melting and the fast solidification afterward. Controlling such process or tailoring the solidification structure of the metallic samples fabricated via additive manufacturing is therefore the control of that fast solidification process. This is also the researchers desire to be realized. Several methods have been proposed such as rolling after several layers' deposited, adding grain refiner and applying ultrasound. They need to contact the sample or at least add another elements. Applying magnetic fields may give a method to affect the fast solidification process during additive manufacturing without any contact or elements added. In this work, Al-10wt.%Si, Inconel 718 Nickel based and Ti6Al4V alloys have been fabricated by additive manufacturing under a static magnetic field. The results show that all of their solidification structure has been affected by the magnetic field. In details, the dendritic growth tendency of primary phase was enhanced and the depth of each melting pool was decrease. These observations can be attributed to the results of compaction between the damping and accelerating (the thermoelectric magnetic flows) effect of static magnetic field on the melts.

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INITIAL RESULTS ON BENCHMARKING OF SOLIDIFICATION TRANSPORT PHENOMENA THROUGH COMPUTATIONAL AND REALTIME EXPERIMENTAL STUDIES ON TRANSPARENT AQUA AMMONIA SYSTEMS

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The current study is an effort to develop benchmark experimental and numerical settings for binary alloy solidification, and our initial results are presented in this paper. Controlled solidification experiments in a rectangular side-cooled cavity with analogue transparent aqua ammonia system (H2O+NH4Cl) are performed for different concentration (eutectic, hype eutectic, hyper eutectic solutions). Particle Image Velocimetry (PIV), High Speed (HS) imaging and thermocouples temperature measurement techniques are used for realtime measurement of flow field, solidified and mushy zone thickness and local temperature during the course of solidification. The measured solidification characteristics are described to obtain useful information for each of the solidification scenario (eutectic, hype eutectic, hyper eutectic solutions). Also, the quantified experimental data are detailed for each case. As known, in the hyper eutectic solution grain motion occurs, whereas in the hypo eutectic solution a fixed mushy zone is observed. An Opensource CFD software tool OpenFOAM is used for numerical simulations using models for each case. The model for the case of hyper eutectic solution considers multi-phase convection of both liquid and solid phases. The model predicts flow field, temperature, species and solid fraction distribution including the

solidification interface morphology for each case. The predictions from the model in each case are validated with the corresponding experimental data. Subsequently, the simulation results are used to obtain information on the evolution of solid fraction, temperature and velocity field, and the mushy zone. Keywords: Binary alloy solidification; Benchmarking; Particle Image Velocimetry; High Speed imaging; OpenFOAM; Fixed mushy zone; Grain motion.

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THE EFFECT OF FORCED MELT FLOW INDUCED BY ROTATING MAGNETIC FIELD ON THE STRUCTURE OF Al-Si EUTECTIC

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Al-Si alloys, which contains eutectic, are used in large quantities. Those are used not only like cast alloys but for base material of brazing technology as well. It is well known that too long Si lamellae can reduce the joining force of brazing, therefor it is necessary to produce finer eutectic structure. During manufacturing of brazing materials, the use of modifying agent (Na, Sr) is not always permitted. In these cases, we can perform to stir the melt. Eutectic and hypoeutectic Al-Si samples were solidified unidirectionally in a rotating magnetic field of different intensity and the developing structure was investigated. The regular investigation method for these irregular eutectics is the measure of the average distance of eutectic Si lamellae. But this technique is not saying anything about the size of lamellae and about the direction of growing them. Because that we worked out a measuring method by use of mosaic pictures. During our research work it was found that stirring of melt can change the microstructure of the sample radically: primary silicon and primary aluminum appear near each other and the structure of eutectic is very different around the primary phases. The size and the direction of eutectic lamellae were modified by stirring as well. Our study shows interesting effects of magnetic stirring and generate some question about the causes.

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THREE-PHASE NUMERICAL MODELING FOR EQUIAXED SOLIDIFICATION OF Sn-10 wt.%Pb ALLOY UNDER FORCED CONVECTION DRIVEN BY ELECTROMAGNETIC FORCE

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A three-phase equiaxed solidification model where macroscale heat transfer and fluid flow are coupled with microscale nucleation and dendrite growth, is applied to the simulation of the macrosegregation in binary alloy solidification subjected to the electromagnetic stirring. The investigated experimental solidification case is conducted in a cavity which has a precise control of the thermal boundary conditions. The proposed model is based on a three-phase approach and uses a double time step scheme to accelerate the solution. The calculation of the diffusion length at the interface between inter- and extra- dendrite liquid phases an approach proposed in [1] is

taken while the momentum exchange coefficient model is updated according to [2] to be adapted to wider conditions. It is demonstrated that both the two parameters have critical influence on simulation results. Electromagnetic force is interpolated from a solution of Maxwell's equations and introduced as a source term into momentum equation. A comparison between the results of simulation and experimental ones is made.

Acknowledgements

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ON THE USE OF HETEROGENEOUS THERMOMECHANICAL AND THERMOPHYSICAL MATERIAL PROPERTIES IN FINITE ELEMENT ANALYSES OF CAST COMPONENTS

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Cast components generally show a heterogeneous distribution of material properties, caused by variations in the microstructure that forms during solidification. Variations caused by the casting process are not commonly considered in structural analyses, which might result in manufacturing of sub-optimised components with unexpected in-use behaviour. In this paper, we present a methodology which can be used to consider both thermomechanical and thermophysical variations using finite element analyses in cast components. The methodology is based on process simulations including microstructure modelling and correlations between microstructural features and material properties. Local material data are generated from the process simulation results, which are integrated into subsequent structural analyses. In order to demonstrate the methodology, it is applied to a cast iron cylinder head. The heterogeneous distribution of material properties is investigated using experimental methods, demonstrating local variations in both mechanical and physical behaviour. In addition, the strength-differential effect on tensile and compressive behaviour of cast iron is considered in the modelling. The integrated simulation methodology presented in this work is relevant to both design engineers, production engineers as well as material scientists, in order to study and better understand how local variations in microstructure might influence the performance and behaviour of cast components under in-use conditions.

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IN SITU X-RAY IMAGING INVESTIGATION OF SOLIDIFICATION OF HIGH MELTING TEMPERATURE MATERIALS: SILICON AND SUPERALLOYS

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All growth and casting processes, used for example in the superalloy and photovoltaic industrial sectors, face challenges linked to the grain structure and crystalline defects left during the solidification step when aiming at improving the final desired properties. The post-mortem studies of the solidified ingots provide limited information on the mechanisms occurring during solidification, on their symbiosis or competition and on their kinetics which makes it difficult to control. As a consequence, it is essential to improve the understanding of the mechanisms of the formation of the final crystalline grain structure, of segregation and of the density of structural defects, namely dislocations.
Within this context, our contribution consists in characterizing the fundamental growth mechanisms of high melting temperature (up to 1800°C) materials using in situ X-ray imaging in a unique device named GaTSBI (Growth at high Temperature observed by X-ray Synchrotron Beam Imaging). Two imaging characterisation techniques are combined during solidification using X-ray synchrotron radiation at the ESRF (European Synchrotron Radiation Facility, Grenoble, France): X-ray radiography and X-ray Bragg diffraction. On the one hand, the X-ray radiography method brings information on the morphology and kinetics of the solid/liquid (S/L) interface as well as on solute segregation. On the other hand, the X-ray Bragg diffraction gives additional information about the evolution of the grain shape and structure, misorientation, defect formation and the local level of crystal lattice distortion during growth.
During the presentation, results concerning the solidification of Ni-Al alloys and silicon for PV applications will be presented. These experiments demonstrate the wide range of fundamental growth mechanisms that can be addressed and better understood with X-ray imaging applied during solidification. In metallic alloys, the formation of a dendritic network is studied as well as its interaction with convective flow. As concerns silicon for PV applications, essential features of twinning, grain competition and the origin and interaction of dislocations with grain boundaries in crystalline silicon are characterized.

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UTILIZING INCLUSION DATA IN CHARACTERIZATION OF OXIDE-SULFIDE STRINGERS IN HOT-ROLLED PLATES

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MATLAB is utilized to identify and locate detrimental oxide–sulfide stringers from the hot rolled plates. A method to estimate the inclusion phases of low carbon, aluminum-killed and calcium-treated steels is proposed. The inclusions are taken as a mixture of CaS, MnS, TiN and oxide (Al2O3-CaO-MgO) phases. The phase fractions and oxide phases composition are calculated from the elemental analysis for each inclusion. The phases present have a marked effect on the deformation of inclusions during hot rolling, and consequently, on mechanical properties of the steel.
Inclusion analysis data gathered with a scanning electron microscope and exported from IncaFeature software is analyzed. In the procedure, the sample area is first divided into narrow horizontal strips to determine the number of inclusions within them. If multiple inclusions on a strip are close enough each other, the inclusions are identified as a stringer.
The following properties are presented for each stringer: the number of inclusions and length of a stringer, phase fractions and compositions, and the composition of the unfragmented inclusion before hot rolling.

According to the results, the longest stringers have total lengths over 200 μm, with nearly 20 inclusions. The overall composition of the longest stringers is between C12A7 and C3A calcium aluminates with minor MgO contents. The diameters of the unfragmented inclusions in the slabs, forming stringers during hot rolling, were estimated to be around 20 μm for the longest stringers. From the dataset, plenty of CaO–CaS stringers were also characterized, obviously a result of excess calcium treatment.

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SOLIDIFICATION MICROSTRUCTURES IN LPBF PROCESSED IN718

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Additive manufacturing by Laser Powder-Bed Fusion (LPBF) is accompanied by solidification under large thermal gradients and cooling rates. As a consequence, solidification morphologies between dendritic with only limited sidebranches or rather cellular pattern are commonly observed. The growth regime is characterized by Péclet numbers of order or larger than 1 (with cell tip radii of order or larger than the length scale of the diffusive pile-up in the melt), and by significant kinetic effects at the solid/liquid interface. We will present results from 2D and 3D phase-field simulations of primary solidification of the Ni based alloy IN718 for a range of solidification rates (1 ... 10 cm/s) and temperature gradients (10^5 K/cm ... 10^6 K/cm) typically seen in LPBF. The operating state of the growth front will be discussed in terms of cell tip shapes, growth undercooling, primary spacing and the effect of crystallographic orientation. A general observation is that, for such high Péclet numbers, usual mechanisms of spacing selection and accommodation are less effective. Cellular morphologies and spacing variations show good agreement with experimental data for IN718.

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IN SITU STUDIES OF NATURAL CONVECTION DURING SOLIDIFICATION OF TERNARY MIXTURES

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Thermal diffusivity and individual solutal diffusivity of component play a significant role during natural convection dominated solidification of multicomponent alloys. In this study, in situ experimental observations of solidification of a ternary salt solution (water-potassium nitrate-ammonium chloride) are reported. The phase diagram of the ternary salt solution consists of three distinct regimes, distinguished based on the mode of heat transfer through the liquids. Each regime is divided into two subregimes on the basis of the primary solidifying component. In Regime II, the cotectic solidification leads to conduction dominated heat transfer through the liquid. The present study shows the real-time evolution of the convective flow in Regime II with different primary solidifying elements (ammonium chloride or potassium nitrate) using in situ optical techniques. A bottom-cooled experiment was performed using Mach-Zehnder interferometer (for thermal/solutal transportation) and particle image velocimetry (for flow field) in a rectangular cavity. The experiments show that the sub-regime II (with ammonium chloride as the primary phase) leads to the formation of double-diffusive convecting layers whereas the sub-regime-II leads to a more complicated convective flow with potassium nitrate as the primary solid. Furthermore, the mechanism of double diffusive convection in ternary mixtures is hypothesized.

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CHUNKY GRAPHITE IN SPHEROIDAL GRAPHITE IRON: REVIEW OF RECENT RESULTS AND DEFINITION OF A PREDICTING INDEX

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Graphite degeneracy in heavy-section spheroidal graphite cast irons is mostly associated with the formation of chunky graphite which consists of large eutectic cells with interconnected graphite strings. At low level, appearance of chunky graphite is limited to its anaesthetic effect on machined surfaces, while at higher level it is detrimental for mechanical properties of the components. Chunky graphite is often related to high silicon levels and too high cerium additions during the spheroidization treatment. The appearance of this defect may be limited by controlled additions of antimony that is thought to tight the excess of cerium, but other impurities and low level elements may have to be considered during melt preparation.
This contribution proposes a review of recent results and approaches on chunky graphite appearance, primarily but not exclusively in the case of heavy-section cast irons. Based on this literature review and series of experimental data, a predictive index for evaluating the risk of chunky graphite appearance is proposed. Lines for further research work aimed at a better understanding of graphite degeneracy are finally suggested.

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ROD-TO-LAMELLAR TRANSITION DURING DIRECTIONAL SOLIDIFICATION OF A MODEL TRANSPARENT EUTECTIC ALLOY

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Directionally solidified binary eutectics are of great practical interest as self-organized composite materials with tunable microstructural features. In a first approach, eutectic microstructures can be classified into rod-like and lamellar ones. Their formation dynamics, which results from a complex diffusion controlled dynamics of coupled-growth front patterns, has been extensively studied by in situ experimentation and time-resolved numerical simulations. Important results have thus been obtained on the morphological stability of eutectic growth shapes and some pattern selection processes. However, the problem of the possible coexistence of rod-like, lamellar, and other more complex shapes in a given sample, in brief, the lamellar-to-rod transition, still remains poorly explored. We have developed an in-situ experiment method that permits to visualize optically the evolution of coupled-growth front patterns in real time in transparent eutectic alloys. In the succinonitrile-(D)camphor system, we identified and located the stability limits (rod elimination, and rod splitting, respectively) of the stability interval of hexagonal eutectic-rod patterns. In this system, we also discovered a transition from rods to lamellae in the presence of a finite-size effect in semi-thin samples. These conclusions could be drawn from laboratory experiments during which thermosolutal convection in the liquid was negligible. On ground, this narrows the range of explorable parameters (composition, thermal field) and prevents one to undertake a systematic study of the lamellar-to-rod transition in large samples. We undertook a science-in-microgravity project (ESA/NASA) called TRANSPARENT ALLOYS (TA). An apparatus for in situ directional solidification experiments in large samples has been installed on board the ISS/MSG (Dec. 2017). We will present the results of the first TA campaign (January-March 2018 ; SEBA program) in collaboration with U. Hecht and V. Witusiewicz (Access e.V., Aachen, Germany).

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MODELLING OF MAGNETO-THERMO-ELECTRIC EFFECT ON SOLID GRAINS TRAJECTORIES DURING SOLIFICATION OF AlCu ALLOYS UNDER LOW FREQUENCY MAGNETIC FIELD

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Applying magnetic field during solidification of metallic alloys process under high thermal gradient may influence drastically microstructures of solidified metal. In fact, Magnetic Lorentz forces due to the coupling of electromagnetic field with thermo-electric currents are acting on the movement of solid grains and on the movements of fluid around grains, which finally produce re-organized and modified microstructures. We have developped 2D and 3D models to analyze and quantify numerically these effects. 2D and 3D Finite element models are based on non linear, time dependant algorithms, coupling electrokinetic to thermal and laminar fluid dynamic equations. Magnetic field is imposed and may be constant or varying at low frequency. Coupling terms coming from magnetism are Lorentz forces in fluid dynamic equations and induced currents in electrokinetics equation. Different approaches have been followed, working either with simplified geometrical grains (spherical, hexaedral ..), either with realistic grains coming from 2D X radiography or 3D tomography on Al7%Cu alloy sample. Solid grains are immersed numerically in the liquid using Chimera method. Results of simulation will present grain trajectories and movement during time and will be compared to analytical results on simplified geometries and to results coming from AlCu alloy solidification experimental processes.

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SOLIDIFICATION PATH AND PHASE TRANSFORMATION IN SUPER-AUSTENITIC STAINLESS STEEL UNS S31254

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Super austenitic stainless steels are widely used in hostile environments, as in seawater desalination and paper manufacturing plants, in which an excellent corrosion resistance is required. These steels require a fully austenitic microstructure at room temperature. During processing it may be possible to form Cr- and Mo-rich intermetallic undesirable precipitates that lower both mechanical properties and corrosion resistance. Particularly, as-cast ingots exhibit s phase (space group 136, tetragonal, [1]) in interdendritic regions, that has to be eliminated by further heat treatments. From the literature two main hypothesis are formulated for the s-phase formation in cast stainless steels: (i) it is formed during the last stage of solidification due to the enrichment of the liquid in s-forming element, (ii) the interdendritic regions are composed of ferrite that decomposes through a solid-state phase transformation. In this work, quenching during directional solidification (QDS) experiments was performed in order to determine the solidification and transformation paths of a (UNS31254) super-austenitic steel. Temperature recording during the QDS process allows to identify precisely the key transformation temperatures over the samples that were characterized in longitudinal and radial directions using SEM and EBSD. The results show that in the range of thermal gradients and solidification velocities investigated, s-phase forms from

interdendritic ferrite through the eutectoid reaction d → g + s at 1205±10°C. The solidification and transformation paths are discussed based on thermodynamic calculations. The observed orientation relationships between the different phases are discussed with regards to existing data of the literature.
[1] T. Koutsoukis, A. Redjaïmia, G. Foularis, Material Science and Engineering A 561 (2013) 477.

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A 3D DISCRETE-ELEMENT MODEL FOR SIMULATING LIQUID FEEDING DURING DENDRITIC SOLIDIFICATION OF STEEL

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A 3D meso-scale discrete-element model has been developed to simulate fluid flow during dendritic solidification of a binary Fe-C alloy. The model domain is a representative volume element consisting of hundreds of equiaxed dendrites along with corresponding liquid channels, where the final grain shape is given by a modified Voronoi diagram. Solidification of each dendrite is simulated via an average volume approach. The output of the solidification simulation at a given solid fraction is used as the input mesh for the fluid flow simulation. A single domain Darcy-Brinkman model is used to calculate the pressure field within the liquid channels, with Poiseuille flow assumed to occur in the extra-dendritic region, and Darcy flow assumed to occur within each dendrite. Mass conservation over each element is then used to derive a controlling equation that is solved via the finite element method. The results of this new model are first compared with a previously-developed granular model [Sistaninia, M., et al. Acta Materialia: 60.9 (2012): 3902-3911.] where fluid flow only occurs in the extra-dendritic region, and second analyzed for different boundary conditions. It is shown that the inter-dendritic liquid fluid flow plays a major role in the semi-solid pressure field, and thus needs to be included when investigating hot tearing susceptibility in engineering alloys undergoing dendritic solidification.

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DETERMINATION OF THE SOLIDIFICATION HEAT RELEASE IN THE LOCAL VOLUME BY FOURIER'S THERMAL ANALYSIS

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The Newtonian Thermal Analysis (**NTA**) is used quite often for analysis of the rate of heat released during the alloys' solidification. For the estimation of the solidification kinetics the cooling rate (approximated on the base of the temperature measurements) is compared with a base cooling rate diagram determined for the cooling of the same probe without exothermic transformation in the similar conditions.
Fourier's method of the thermal analysis (**FTA**) is based on the estimation of the heat released in the transformation time by comparison of the difference approximations of the first temperature derivative with time and second spatial derivative of the temperature (divergence of the temperature gradient vector). In the case of a unidirectional heat flux, a set consisting of only three thermocouples can be used for FTA measurements.

The results of NTA are averaged entire all the volume of the analyzed sample. The results of FTA are averaged for the local volume located between the isotherms passing through the positions of the two external thermocouples of the used set. That is why the FTA method brings the more precise data for the verification and validation of the modeling and simulation results.
The results of the FTA application for the estimation of the transformation rate is presented for casting alloys and composites. Methods are described for increasing the accuracy of measurements performed by the FTA.

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SOLIDIFICATION OF Ti-46Al-8Nb IN HYPER-GRAVITY AND MULTI-PHYSICS MODELLING

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Low pressure turbine blades (LPT) made by centrifugal casting from titanium aluminides require demanding process control, as to achieve desired solidification microstructures. The columnar-to-equiaxed transition (CET) and the related texture are of special interest. In the joint European Project "GRADECET" they were investigated in μg, 1g and hyper-g conditions. Solidification experiments of the alloy Ti-46Al-8Nb in EAS's Large Diameter Centrifuge (LDC) show that with increasing angular velocity the equiaxed grain formation is promoted, while also depending on alloy's composition and solidification pathway. Our numerical model handles thermal radiation and conduction in the entire furnace, the transient steps of melting and columnar solidification coupled with thermo-solutal flow. Furthermore, to understand the observed asymmetric CET event and distinct scenarios about the origin of equiaxed grains, motion of nuclei with flow under centrifugal condition was modelled by the Lagrangian approach. Taken together the simulation results reveal that the centrifugal and Coriolis forces affect the pattern and magnitude of the flow thus changing the growth conditions including undercooling, temperature gradient and nucleation ahead of the columnar front. When the angular velocity in the LDC increases, CET conditions based on Hunt' model are met more early, which is in good agreement with experimental observations.

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CELLULAR-TO-DENDRITIC AND DENDRITIC-TO-CELLULAR MORPHOLOGICAL TRANSITIONS IN A TERNARY Al-Mg-Si ALLOY

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Investigative efforts aimed at improving the understanding of the microstructural transitions in solidified metallic alloys are requested. Indeed, it is well known that the application properties of the metallic alloys will greatly depend on the final morphology of the microstructure. Determining the ranges of cooling rates associated with dendritic-cellular transition in multicomponent alloys is needed to control the final microstructure and thus the properties. The study presented focuses on the influence of the solidification thermal parameters upon the evolution of the microstructure of an Al-Mg-Si ternary alloy. As such, directional solidification experiments were conducted

using a Bridgman (steady state) device and another device that allows the solidification under transient conditions (unsteady state). As a consequence, a wide range of cooling rates (ψR), varying from 0.003K/s to 45K/s could be studied. This led to the identification of complete cellular/dendritic/cellular transitions. The range of experimental cooling rates associated with the steady state experiments was 0.003K/s $< \psi$R $<$ 0.17K/s. The regular cellular-to-dendritic zone remained for cooling rates lower than 0.03K/s and ended at about 0.005K/s, since no evidence of dendrites could be observed for this ψR value. For cooling rates between 0.03K/s to 0.17K/s only typical dendritic morphologies have been observed. For ψR lower than 0.005K/s a degenerate growth of α-Al cells was observed. From unsteady state conditions, the range of experimental cooling rates was about 0.2K/s $< \psi$R $<$ 45K/s. The observed growth of high cooling rate cells is related to ψR$>$ 2K/s whereas the dendritic region to ψR $<$ 0.8K/s. Values in between refer to a zone in which both cells and dendrites can be found. Therefore, a complete description of the low cooling rate cells transitioned to dendrites, which further converted to high cooling rate cells for the Al-3wt.%Mg-1wt.%Si alloy has can been carried out. Both cell spacing λC and primary dendritic spacing λ1 are related to ψR by power function growth laws characterized by a same exponent (-0.55). It can be seen that the experimental points fitted well the predictions of both experimental growth laws. This reinforces the proper application of this exponent in order to correlate the λC and λ1 evolutions with the cooling rate for both steady-state and unsteady-state solidification conditions.

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CHARACTERIZATION OF HEAT TRANSFER AND ITS EFFECT ON SOLIDIFICATION IN WATER COOLED LPDC OF WHEELS

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Computational process modeling has become an important engineering tool in the casting industry to predict the solidification sequence in complex castings. Used properly, this tool can help reduce manufacturing costs. One of the challenging issues in developing casting simulations for the low pressure die casting (LPDC) of automotive wheels is to quantify the heat transfer coefficients (HTC) within the cooling channels in a die. When water is used as the cooling media, the HTCs exhibit a complex, non-linear behaviour due to the boiling phenomena that occur making it possible to extract a significant amount of heat from the die in a short period of time and influence the solidification of a wheel. Primarily, constant heat transfer coefficients have been used to describe this heat transfer in casting models up until now, but an opportunity exists to improve the transient description of heat transfer in channels cooled with water. In this paper, HTC's in a lab-scale physical analogue model of die cooling will be characterized as a function of typical LPDC operational parameters such as flow rates, initial die temperatures and coolant temperature. The variation in solidification behaviour will then be assessed using an existing LPDC process model for wheels.

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DIRECT NUMERICAL SIMULATIONS OF FLOTATION OF LIGHT OXIDE INCLUSIONS IN STEEL MELT AND INTERACTION WITH GROWING DENDRITIC CRYSTALS

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The existence of oxide inclusions (e.g. Al2O3) in the steel melt is unavoidable. Most of these nonmetallic inclusions come from the steel-making process. During solidification, some of these

inclusions remain in the melt and interact with melt flow and the growing crystals. The movement of solid oxide inclusions in steel melt is directly numerically simulated through coupling the solid particle moving dynamics with the Navier-Stokes equations, which are solved using a vector-valued method based on the adaptive finite element method in three dimensions. Prior to this simulation, the settling of a single spherical Nylon solid particle in water is firstly calculated and then benchmarked by the experimental measurements, which shows a very good agreement of the terminal velocity between simulations and experiments. Then settling of many particles is performed to verify the treatments of collision between particles and collision between a particle and walls. With these benchmarks and numerical tests, the liquid-particle interaction dynamics are incorporated into the phase-field model for the alloy dendritic crystal growth. The natural convection due to the solutal buoyancy is also taken into account. Two-dimensional numerical simulations of flotation of many light oxide inclusions in the interdendritic region during solidification are performed. Simulations show that when considering the inclusion flotation, the interdendritic melt convection becomes orders of magnitude stronger than that only considers the solutal buoyancy. The inclusion flotation during directional solidification not only changes the flow strength but also alters the selection process of primary dendrites. In the multiple equiaxed solidification, the large-size inclusions lead to the flow of inclusion and melt, and thereby generating a flow passage between dendritic crystals. Most of the particles flow to the top along this passage when the dendritic branches are not well developed. While the dendritic arms become sufficiently large, more and more inclusions are blocked by the dendrites near this passage.

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IMPACT OF GRAVITY-RELATED PHENOMENA ON THE GRAIN STRUCTURE FORMATION: COMPARATIVE STUDY BETWEEN HORIZONTAL AND VERTICAL SOLIDIFICATION OF A REFINED Al-20wt.%Cu ALLOY

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The mechanical properties of materials are directly related to their solidification structures, so that a precise control of growth process is crucial in engineering. Two types of grain structures are commonly obtained during metal alloy solidification: a columnar grain structure with anisotropic properties, or an equiaxed grain structure with more isotropic properties. A fine and homogeneous grain structure is required in most aluminum-based alloys used in industrial applications. This feature is achieved by adding refining particles to the liquid metal before the solidification phase, which act as preferential nucleation sites for heterogeneous nucleation. The efficiency of refining particles and the final grain morphology depends on the solidification parameters, such as the temperature gradient, which is often present in many solidification processes and the cooling rate. On Earth, gravity-related phenomena such as thermo-solutal convection caused by density gradients in the melt, and buoyancy when the liquid phase is denser than the solid phase, are unavoidable and can affect drastically both the grain number and their morphology. It is for these reasons that fundamental studies comparing the influence of solidification parameters with and without gravity effects are important to obtain benchmark data useful to understand and then control the final structure of materials in industrial processes.
In the present work, the impact of the solidification parameters on the dendritic grain structure formation and on the final grain size and shape was investigated in-situ by using X-radiography for two different orientations with respect to gravity. Directional solidification experiments of refined Al-20wt.%Cu alloys were made using sheet-like samples (thickness $\approx$ 250 µm) in the laboratory device SFINX (Solidification Furnace with IN situ X-radiography). In a first step, experiments were carried out with various solidification parameters and with the furnace in horizontal position, with the main surface of the sample being perpendicular to gravity. This

configuration was chosen to limit gravity-related phenomena. In a second step, experiments were carried out with identical solidification parameters but with the furnace in a vertical position, and for two solidification directions (upward and downward). A comparative study between horizontal and vertical experiments have been carried out to analyze and highlight phenomena related to gravity. In addition, we will focus on the characterization of grain floatation during upward solidification and the interaction between dendrite growth and solute rich-plume evolution during downward solidification.

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MESHLESS PHASE FIELD MODELING OF DENDRITIC GROWTH BY USING AN H-ADAPTIVE COMPUTATIONAL NODE ARRANGEMENT

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A two dimensional model for the simulation of dendritic growth in binary alloys is developed. Phase field model is used to derive the system of partial differential equations describing the temporal evolution of the solid-liquid interface and concentration field. Quantitative modeling is assured by the use of thin interface limit of the isothermal phase field model. Meshless local radial basis function collocation method and explicit Euler scheme are used for the spatial and temporal discretization of the phase field equations, respectively. An h-adaptive computational node arrangement is developed in order to assure the high density of computational nodes near the solid-liquid interface. The model is verified and assessed by comparison with the analytical models. The influence of the node arrangement to the dendritic morphology at different preferential growth directions is analyzed. The speed-up of the simulation due to an h-adaptive computational node arrangement is assessed. The originality of the work is in the novel, adaptive approach to the efficient and accurate solution of the phase field model. Advantages and shortcomings of the novel adaptive meshless method as well as further developments are discussed.

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DIRECT OBSERVATION OF DENDRITE FRAGMENTATION IN THE SOLIDIFICATION OF UNDERCOOLED MELTS

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The fragmentation of dendrites immediately following the recalescence phase of growth during the solidification of undercooled melts has been invoked to explain various rapid solidification microstructures. Such fragmentation is thought to occur via the growth of a Rayleigh type instability along the dendrite arms. Despite this, little direct evidence of such a fragmentation process usually survives in the as-solidified material. Here we report on the rapid solidification of the single phase, congruently melting intermetallic Ni3Ge, processed via drop-tube. During equilibrium solidification this material solidifies to the chemically ordered L12 crystal structure. Conversely, during rapid solidification, disorder trapping results in solidification to a random fcc solid solution. We find that the L12 ordered variant is more resistant to chemical attack, meaning that etching will reveal the chemically disordered material only. Consequently, it is possible to image the material that grew during recalescence in the as-solidified sample. We present here results which show a range of microstructures in which the dendrite fragmentation process has been captured in progress. These include dendrite side-branches in various stages of fragmentation from intact, but with a clear Rayleigh instability modulation along their length,

to fully fragmented and spheroidised. Results from EBSD Euler mapping will be presented to elucidate the relationship between such fragmentation and grain refinement in samples solidified from their undercooled parent melt.

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DETERMINING GRAIN BOUNDARIES IN DIRECTIONALLY SOLIDIFIED DENDRITIC GRAIN STRUCTURES FROM OPTICAL MICROSCOPY IMAGES

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Analysis of grain structures as formed during directional solidification is of significant interest in the study of directionally solidification and the development of deeper understanding of grain selection. In the case of dendritic microstructures, different grains, as formed during solidification, can usually easily identified by just looking at micrographs from optical or electron microscopy and very reliable identification of different grains can be achieved by using EBSD. The latter identifies actual crystallographic orientations, but requires considerable technical effort and is commonly restricted to small parts of samples. Results from serial sectioning or tomography (micro CT) cannot be analysed this way. In this work a novel technique to identify grains and grain boundaries from dendritic structures is presented. Images form optical microscopy and micro CT are used as input for an automated method, implement into a computer. Application to directionally solidified Al-Cu and Ni-base superalloys are presented. It is seen that grains can be identified, and even small groups of dendrites separating from grain can be distinguished. When compared to EBSD results, it is found that the new method identifies the grain boundary as formed during dendrite impingement, while the EBSD result is affected by grain boundary movement after solidification was completed.

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PREDICTION OF CARBIDE PRECIPITATION USING A COMBINED PARTIAL EQUILIBRIUM-PARA-EQUILIBRIUM - LEVER RULE APPROXIMATION IN AUTOMOBILE GEAR MATERIALS

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In gear material in automobiles, both the wear-resistance around surface and the toughness in central part are required. By using gas carburization technique [1], it is possible to obtain a high carbon content that causes carbide precipitation at surface, while maintaining the original carbon content at base part. That is, the dual industrial demand is satisfied. In recent years, the requirements of both increase in gear hardness and reduction of the weight of automobiles have urged the researchers to test the substitutive elements to be added into the traditional materials. Here some VB group elements such as V etc and IVB group elements like Ti etc are selected as the newly added elements, because these elements can promote the formation of MC type carbides with relatively lighter densities and much higher hardness [2] than those of the usual M3C carbide. Partial Equilibrium (PE)- PAra-equilibrium (PA)- Lever Rule (LR) approximation [3,4] predicts the solidification path from liquid down to the room temperature with considering

the infinite diffusion of interstitials and the weak diffusion of substitutionals. It can also treat peritectic as well as eutectic transformations. Here the PE-PA-LR approximation was adopted to study the carbide amount and composition after the gas carburization. Some elements' effects were investigated on fulfilling the request of increasing the precipitation of carbides at surface and keeping none or little carbide precipitation in the base part. Results show that after gas carburization, the increase of carbon content mainly rises up the precipitation amount of M3C. And the addition of V or Ti element does help to precipitate the higher-hardness carbides such as (Mo,V)C and TiC.

KEY WORDS: Automobile gear material; Carbide precipitation; Effects of C, V, Ti elements; Partial Equilibrium- PAra-equilibrium - Lever Rule approximation.

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QUANTIFICATION OF β PHASE GROWTH IN Fe-CONTAINING 319 Al ALLOY WITH 4D X-RAY IMAGING AND MACHINE LEARNING

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To unearth the fundamentals in solidification requires the use of advanced experimental methodologies and computational modelling. On the experimental side, synchrotron based high speed X-ray tomography, which can capture a tomogram (3D volume) in seconds, is a powerful tool to study solidification in real-time, allowing the visualization of solidifying alloys as 3D movies or 4D (3D plus time) images. To take advantage of the technique in solidification, we have developed a unique directional solidification furnace coupled with strong magnetic fields, which we integrated with synchrotron beamlines with high speed X-ray tomography (I12-Diamond Light Source and ID19-European Synchrotron Radiation Facility). A large amount of data (tens of TBs) were collected in a series of beamtime experiment. However, it is a challenging task to analyse and correctly interpret the data effectively and efficiently. To provide a practical approach to the problem, we have applied machine learning and computer vision algorithms to automatically process the data. One example will be presented on measuring the kinetics of β intermetallic growth in Fe-containing 319 Al alloy, which demonstrates the advantages of using machine learning in 4D X-ray imaging. with the combined use of machine learning and advanced image quantification, the work reveals the nucleation and growth mechanisms of the intermetallic phase during Al alloy solidification.

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A NOVEL ROUTE TO THE COUPLING OF MOLECULAR DYNAMICS AND PHASE-FIELD SIMULATIONS OF CRYSTAL GROWTH

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In phase field modelling of solidification, one always assumes a smooth, symmetric, change between solid and liquid across the interface region in near equilibrium 1D solutions. Such a construction is usually motivated by computational convenience, and this is reflected by computational modelling where the gradient employed in the liquid-solid interface is much lower than realistic. To obtain quantitative results with a finite interface width, a phase field model can be constructed by asymptotic matching to a sharp interface model e.g. [Karma 2001 , Bollada et al 2018]. Yet ab initio and molecular dynamics reveal that the actual physical interface is not only finite, but also, non-symmetric - in fact, somewhat exponential in aspect . This paper addresses questions raised by assuming a phase field model to have a realistically shaped phase profile that matches ab initio or molecular dynamic phase profiles: How to model a non-symmetric profile? How to match a profile to given data? and, Does such a model have any consequences in speed of growth, dendrite shape, or, in the case of alloy models, in alloy concentration profile?

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DENDRITIC COLUMNAR GROWTH OF BBC BETA-(TiAl) IN MICRO- AND -HYPER GRAVITY: 1. EXPERIMENTAL RESULTS AND MACRO-SCALE MODELING

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The columnar growth of Ti-48Al-2Nb-2Cr alloy was investigated using power down directional solidification experiments under various gravity conditions, ranging from micro-gravity to 20 g. The g-vector always pointed in direction opposite to the growth direction. The columnar dendrite morphology and primary spacing was analyzed in longitudinal and transverse sections and for selected experiments in 1g and 15g also by X-Ray tomography. The results show that the primary dendrite arm spacing decreases with increasing gravity from an average value of 790 μm at μg down to 370 μm at 20g. Furthermore, the spacing evolution along the entire solidification length depends not only on the temperature gradient and velocity but also on the magnitude of the applied gravity. The experimental analysis was complemented by numerical simulations using among other an OpenFOAM code to couple solidification and fluid flow. We will present and discuss the observed spacing refinement and the associated refinement mechanisms based on current models of dendrite growth under the action of upward flow in the mushy zone. Key observations form phase-field modeling are presented in a second contribution.

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3D PATTERN EVOLUTION DURING DIRECTIONAL SOLIDIFICATION OF A TRANSPARENT ALLOY CONDUCTED ON DECLIC-DSI

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The microstructure formed during the solidification processing from the melt is a critical issue for industrial applications. Most of the mechanical properties of alloys are a result of these microstructures. Understanding and predicting both the microstructure formation and evolution are crucial for the development of performant materials. Since microstructures are strongly influenced by the history of the solid-liquid interface evolution during the solidification process, in situ observation of the interface patterns is an important tool to gain knowledge on microstructure formation.
To study the fundamental physical mechanisms in the dynamical formation of two-dimensional arrays under diffusive growth conditions, two experimental campaigns of directional solidification in a model transparent alloy - succinonitrile–camphor - have been conducted onboard the International Space Station using the Directional Solidification Insert (DSI) of DECLIC (Device for the Study of Critical Liquids and Crystallization) facility. This facility was developed by the French Space Agency (CNES) in collaboration with NASA. The solute concentration was changed between the two experimental campaigns so that both cellular and dendritic regimes could be explored up to highly-branched structures. The combination of in situ observation on transparent systems and microgravity environment which allows solidification experiments of unprecedented duration offered a very unique possibility to study solidification and the dynamics of patterns. This possibility puts us on the path to produce benchmark data needed to validate and develop theoretical and numerical models.
Experimental observations, supported by 3D phase-field simulations, demonstrate the influence of subgrain-boundary, misorientations and macroscopic heterogeneities of the thermal field on the primary spacing selection and pattern organization. Some of the most striking results from both campaigns regarding the pattern selection will be presented.

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DENDRITIC COLUMNAR GROWTH OF BBC BETA-(TiAl) IN MICRO- AND -HYPER GRAVITY: 2. PHASE-FIELD MODELING

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This second paper addresses the phase field modeling of columnar dendritic growth for different scenarios of fluid flow developing in response to gravitational forces. For this the experimental Ti-48Al-2Cr-2Nb alloy has been simplified to a binary alloy Ti-48 at.% Al. The 2D simulations confirm the decrease of the primary dendrite arm spacing with increasing gravity, nearly matching the experimental findings. In addition, the simulations show that above a critical magnitude of the gravity level dendrite tips display a characteristic splitting behavior, leading to highly branched microstructures. While tip-splitting can be periodic also without flow [1], the present results indicate that splitting events are closely coupled to the convection rolls between neighboring dendrites. The highly dynamic growth behavior however leads to an overall stable advancement of the average solidification front. The instabilities are discussed based on the imposed growth conditions and fluid flow velocities. The role of the anisotropy of the solid/liquid interface energy on the pattern dynamics will also be discussed.

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MECHANISMS OF TiAl ALLOYS ISOMORPHIC INOCULATION FROM CRYO-MILLED Ti-AL-Nb POWDERS

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Isomorphic inoculation has recently been introduced by the authors as a successful method to grain refine cast titanium aluminides [1]. Analyses of the cast grain size together with introduced particles size distributions revealed anomalously high grain refinement efficiency which was attributed to the particles breaking up during the holding stage prior to solidification [2]. In the present work, the microstructure of the inoculant powders is investigated in both the cryo-milled state and after simulated thermal cycles to reproduce their heating and holding in the melt. Results show that milling time does not impact the grain size in the particles, only their size distributions. Heat treatments between 1500 and 1600°C for short periods of time allowed the determination of the activation energy for grain growth and evaluation of the grain size evolution in the particles during the isomorphic inoculation process. Assuming that grain boundary melting is the predominant break up mechanism, a model to estimate dissolution of the powders is presented which includes diffusion and fluid flow. Despite its relative simplicity, the predicted number of particles remaining after heating and holding, which lead to grains in the as-cast structure, is it good agreement with the measured grain size. Finally the paper summarizes the main features and mechanism making isomorphic inoculation a promising route for grain refining as-cast alloys.
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EFFECTS OF STRAIN RATE ON HOT TEAR FORMATION IN Al-Si-Cu ALLOYS

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The alloy casting process is one of the major manufacturing processes to produce near net shape components. The casing process is prone to a wide variety of defects, with hot tear being one of the most detrimental. The two main factors generally recognized as the primary cause for formation of hot tears are the mechanical response of the mush (which effects its permeability), and the solidification range (solidification time). The response of the mushy zone under deformation is mainly affected by the solid fraction, strain rate and grain morphology. Even though the science behind the formation of hot tear is understood, there is no general criterion to quantify the hot tear formation under varying casting conditions . The d evelopment of ultra-fast X-ray

imaging has facilitated the means to quantify the effects of the critical parameters in-situ and develop better correlations for hot tear prediction. The in situ experiments will also provide insights into mush rheology, which has significant influence on hot tear formation. In this study, isothermal semi solid compression studies of Al-Si-Cu alloys were carried out using specially built thermo-mechanical rig. We studied the effects of the strain rate in the range of 4×10-4–0.04/s and solid fraction (˜0.6-0.9) on the mechanical response of the mushy zone. The sample were characterized before and after deformation using X-ray microtomography. The data was subjected to an image processing routine and the amount of porosity and hot tear was quantified. The stress-strain curve of the semisolid alloys showed a characteristic strain softening behavior for semi solid samples with ˜0.6-0.7 solid fraction, irrespective of loading rates, whereas the behavior at higher fractions were that of constant flow stress. Additionally, in situ compression experiments were carried out, wherein the liquid channel thickness at various strain values were measured. Isolated liquid channels were formed under loading, from where the hot tears were found to nucleate . Hot tear susceptibility was found to increase with increasing strain rate and rheology of the mush, which is dependent on solid fraction.

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THE USE OF ADVANCED ANALYTICS ON ENGINEERED FEATURES TO DETECT STICKER BREAKOUT IN CONTINUOUS CASTERS

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A method for detecting sticker breakouts in continuous casters is proposed based on extensive feature engineering and advanced analytical modelling. It is observed that the temperature patterns generated during a sticker breakout have a consistent signature, owing to the underlying physical processes involved. The aim of the present exercise is to capture this latent physical phenomenon in a reliable and robust way. The temperatures measured by thermocouples in the mold are used to extract features of physical significance and operational importance. The features were custom built iteratively to capture the difference between true and false patterns. These features are consequently used to develop a Gradient Boosting model to detect sticker breakout. The model is trained on previously raised sticker alarms that are manually tagged as true or false alarms for a time period of around 3 years (1500 alarm files). The sample space of the non-alarm (tagged 0) is increased by using data collected during normal operation. The GBM model shows an overall superior performance as compared to the existing in-place logic. While ensuring that no true alarms are missed, the GBM model reduces the false alarms by around 80%. The reduction in false alarms imply a huge production advantage while the feature engineering involved in the modelling process makes this a unique exercise in the realm of continuous casting research. The data used in the analysis was generated in continuous casters operating in Tata Steel Jamshedpur.

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THE EFFECT OF APPLIED MAGNETIC FIELD ON LASER ADDITIVE MANUFACTURING

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Vigorous fluid flow appears in laser additive manufacturing (LAM) weld pools, with strong thermal gradients introducing buoyancy and Marangoni forces. Applying an external static magnetic field to this process will introduce two key additional effects. The first is electromagnetic

damping that slows fluid motion across field lines, and the second is due to thermoelectric magnetohydrodynamics (TEMHD) driving solute flow along solid front interfaces. In the latter case, the large thermal gradients generate significant thermoelectric currents, which in the presence of a magnetic field drive the flow.
This paper focuses on the modelling of this coupled process using a bespoke numerical code that couples solidification, fluid flow and electromagnetism. Solidification is predicted using a cellular automata (CA) based method. The CA method is known to capture the larger length scales of microstructure simulation, typically formed in casting and directional solidification. Nevertheless, preliminary simulation results, show that this method has the potential to capture the entire LAM melt pool in 3-dimensions, while retaining many key microstructure features. This result compares favourably with benchmark cases. With hydrodynamics and electromagnetism already coupled to the numerical model, combined with a degree of parallelisation has provided the platform for investigating the magnetohydrodynamic effects on the melt pool shape and microstructure. These results will be validated by experiments.The ultimate goal is to use the magnetic field as an additional control mechanism to improve the quality of the microstructure.

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PARALLEL CELLULAR AUTOMATA, LATTICE BOLTZMANN METHOD FOR MULTIPHYSICS MICROSTRUCTURE SIMULATION

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TESA, Thermoelectric Solidification Algorithm, is a bespoke numerical code originally designed to capture the effect of Thermoelectric Magnetohydrodynamics in high undercooled growth. The code is actively being developed with parallelisation, a cellular automata method to capture micro-macroscale solidification and the Lattice Boltzmann method to resolve the hydrodynamics. This paper describes the general equation sets, discretisation and methods, focusing on parallelisation and coupling between the three key phenomena, solidification, fluid flow and electromagnetism. Examples of the fully coupled model are given for benchmarks and for cases where the code has been successfully used to predict scientifically interesting phenomena in a wide range of solidification conditions including: the formation of a screw structure in directional solidification, freckle formation in turbine blade casting, tip velocity dependency on a magnetic field in high undercooled growth and recently epitaxial growth in additive manufacturing. These methods were chosen to provide results that capture characteristic spatial and temporal evolution of the microstructure in a reasonable compromise between accuracy and computational time.

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NUCLEATION AND GROWTH TWINNING IN Al-Mn-Fe INTERMETALLIC SOLIDIFICATION IN Mg ALLOYS

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Al-Mn-Fe intermetallics are important for the corrosion resistance of cast Mg alloys but there have been few studies on their solidification mechanisms or microstructure development. Here EBSD, deep etching and FIB-tomography are combined to study the nucleation and equaixed growth crystallography of B2-Al(Mn,Fe), Al8Mn5, and Al11Mn4 in Mg-Al-Mn-based alloys. It is shown that twinning readily occurs during the solidification of all three compounds. In the case of rhombohedral Al8Mn5, the twinned particles consist of four orientations related by ˜90° rotations around three common [U+2329]1-102[U+232A], which is discussed in terms of the

pseudo-cubic <100> axes of the Al8Mn5 rhombohedral gamma brass. Under a wide range of solidification conditions, Al8Mn5 grew as equiaxed polyhedra that are explained by polyhedron models based on different combinations of {100}, {110} and {112} facets using a pseudo-cubic Al8Mn5 cell. It is shown that twinning also plays a role in the preferred orientation relationships that develop between the different Al-Mn-Fe compounds. Reproducible orientation relationships (ORs) and the lattice match between the phases are discussed in terms of the group-subgroup relationship between these phases. The role of solute rejection on the continuous nucleation of Al-Mn-Fe particles during cooling in a near-uniform thermal field and on the final number density of Al-Mn-Fe intermetallics is then discussed based on analysis of synchrotron radiogaraphy image sequences.

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COMPREHENSIVE IN-SITU OBSERVATION OF LIQUID/δ-FERRITE, δ-FERRITE/γ-AUSTENITE INTERFACES MOBILITY, AND ACICULAR FERRITE NUCLEATION AND GROWTH IN CARBON STEELS

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This work aims to provide a comprehensive in-situ observation from solidification to phase transformation in low alloy steels with different grades, and the analyses of their phenomena.
1) Liquid/δ-ferrite, δ-ferrite/γ-austenite interfaces mobility: In-situ kinetics of liquid/δ-ferrite and δ-ferrite/γ-austenite interfaces mobility during solidification and phase transformation are observed firstly by high temperature confocal laser scanning microscopy (HT-CLSM) in this work. Thereafter, the dihedral angles at triple points of high energy δ/δ grain boundary and two incoherent δ/γ interphase boundaries and measured, and the free energy of δ-ferrite/γ-austenite can be estimated based on the observations.
2) Acicular ferrite nucleation and growth: Subsequently, the intragranular acicular ferrite (IAF) nucleation and growth from non-metallic inclusion particles can be investigated. The effect of carbon content on the IAF formation and growth features, such as formation temperature of microstructure and phase fraction are quantitatively discussed. A modified classical nucleation model is applied here to predict the effective nuclei size as well as the effect of C content on the driving force of IAF formation. Finally, the IAF growth kinetics are directly measured by HT-CLSM, and the experimental data is compared with the empirical correlation calculation results. The Stereological issue on the IAF growth kinetics is also discussed.

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EFFECTS OF INTERPHASE BOUNDARY ANISOTROPY ON THE THREE-PHASE GROWTH DYNAMICS IN THE β(In) – In2Bi – γ(Sn) TERNARY-EUTECTIC SYSTEM

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We present an experimental investigation on the effects of the interphase energy anisotropy on the formation of three-phase growth microstructures during directional solidification (DS) of the β(In)–In2Bi–γ(Sn) ternary-eutectic system. Standard DS and rotating directional solidification

(RDS) were performed using thin alloy samples with real-time observation. We identified two main types of eutectic grains (EGs): (i) quasi-isotropic EGs within which the solidification dynamics do not exhibit any substantial anisotropy effect, and (ii) anisotropic EGs, within which RDS microstructures exhibit an alternation of locked and unlocked microstructures. EBSD analyses revealed (i) a strong tendency to an alignment of the In2Bi and γ(Sn) crystals (both hexagonal) with respect to the thin-sample walls, and (ii) the existence of special crystal orientation relationships (ORs) between the three solid phases in both quasiisotropic and anisotropic EGs. We initiate a discussion on the dominating locking effect of the In2Bi–β(In) interphase boundary during quasi steady-state solidification, and the existence of strong crystal selection mechanisms during early nucleation and growth stages.

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A NOVEL POWDER METALLURGY TECHNIQUE FOR INTRODUCING SYNTHETIC INCLUSIONS INTO LIQUID STEEL

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Previous studies have shown that it is extremely problematic to add synthetic inclusions successfully into liquid steel for clean steel experiments. Small micro-particles encapsulated in a metallic parcel are difficult to pass through the melt-gas interface and inclusions tend to agglomerate then float up to the liquid surface. In this study, powder metallurgy is used to distribute cerium oxide particles of a known size from 1μm to 14μm within a small-scale ingot. Carbonyl iron powder has been mixed with 0.1 wt% cerium oxide then sintered in an electrical furnace to produce sintered ingots of 500 grams. A series of induction furnace melting trials using a total of 400 grams of electrolytic iron and sintered ingot have been undertaken. The work has included extensive FE-SEM analysis using the INCA Feature® to characterise synthetic cerium oxide inclusions from both the sintered ingots and trial ingots. The INCA results showed that the size distribution and number of cerium oxide inclusions agreed well between the sintered ingot and trial ingot. The synthetic cerium oxide inclusions are homogeneously dispersed through the bottom, centre and top of the trial ingot with approximately 16 number counts/mm2. Analysis suggests that we recovered more than 95% CeO2 from the sintered ingot has been distributed throughout the trial ingot. The work has also been upscaled from 400 grams up to 1.5 kg and has been successful. The method developed will be useful for further studies into steel cleanness and grain refinement of high value alloyed steels.

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ANALYSIS OF THE IMPACT OF INLET INDUCED FORCED CONVECTION ON MACROSEGREGATION FORMATION IN DC CASTING OF ALUMINIUM SHEET INGOTS

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Macrosegregation refers to the inhomogeneous distribution of alloy elements at the macro scale in solidified castings. It is a common defect in direct chill (DC) casting of aluminium alloys. Since various transport phenomena contribute to the formation of macrosegregation, numerical

modelling is a valuable tool to assess their role and study their interplay with process parameters. One such parameter is inlet induced flow and consequently the effect of forced convection on liquid flow and moving solid grains. This complex and coupled flow phenomena cannot be addressed using a 2D simulation of sheet ingots. In this work, we conduct 3D modelling case studies on aluminium sheet ingots to analyze the inlet induced forced convection and its impact on macrosegregation formation. To carry out this investigation, we use a multiphase, multiscale solidification model also accounting for thermal-solutal convection, solidification shrinkage, and equiaxed grain nucleation, growth and transport. We show that forced convection alters significantly grain transport and sedimentation and that macrosegregation formation can be altered by varying the intensity of inlet flow.

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SOLIDIFICATION MODELING USING USER DEFINED FUNCTION IN ANSYS FLUENT

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The modelling of solidification processes in combination with fluid flow is one application of ANSYS Fluent. The solidification is modelled with the enthalpy porosity technique. Therefore, the fluid flow is damped similar to a flow through a porous media of dendrites. For the numerical simulation of remelting processes like electro slag remelting or vacuum arc remelting ANSYS Fluent is used due to the fast solvers and large implementation possibilities. In case of materials with large solidification ranges, like alloy 718, the built-in adjustment possibilities of ANSYS Fluent are often not adequate. The program postulates a simple dependency between liquid fraction and solidification enthalpy. To improve the simulation, the solidification was implemented by a user defined function (UDF). The principal modelling of fluid flow is based on the theory of ANSYS Fluent, but it is now possible to adjust the solidification enthalpy for each temperature exactly.

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MODELING OF EUTECTIC GROWTH KINETICS WITH THERMODYNAMIC COUPLINGS

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The formation of eutectic microstructures, composed of two phases or more, is often encountered during the solidification of industrial alloys. Fraction and characteristics of this structure have consequences on the subsequent phase transformations, mechanical strength and final end-use properties of metallic pieces. Consequently, estimation of eutectic growth kinetics is required in order to predict its development and internal scale during solidification processes.
However, most of existing eutectic growth models are within the frame of the primary Jackson-Hunt theory [1] and systematically use linear approximations for thermodynamic properties and solidification front curvature effects. These approximations limit their application to low growth rate. In addition, these models also neglect variations of densities between phases and advection of liquid phase induced by shrinkage effect.
An original model of directional growth for lamellar eutectics is presented. This model is based on the analysis and computation of thermodynamic equilibrium at the solidification front. Contrary to previous models, this new approach does not make use of linearization hypotheses for the alloy phase diagram. In addition this model considers variations of densities within phases along

with the influence of curvature on thermodynamic equilibrium at the solidification front. The numerical implementation is made possible through a coupling with a thermodynamic software based on the CALPHAD approach.
This new numerical model is applied to the Al-Al2Cu eutectic structure and compared to the Jackson-Hunt theory. Large differences between results of the present model and this theory are observed at high growth rate. Validations with experimental observations developed in a large range of growth velocities and reported in literature are also proposed. Analytical developments are finally provided in order to explain and estimate evolutions observed in eutectic microstructure evolution. The application of this model to multicomponent alloys will be discussed.
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DETERMINATION OF PATTERN ALLOWANCES FOR A STEEL CASTING USING AN INVERSE ELASTOPLASTIC DEFORMATION ANALYSIS

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In recent years, the development of computational models to predict casting distortions has led to improvements in efficiency and accuracy over traditional pattern design that relies on shrink rules. Unfortunately, the determination of pattern dimensions using simulation remains a trial-and-error process that requires several design iterations. In this study, the finite element inverse deformation method is utilized to calculate the pattern geometry in a single iteration for a plastically deformed (i.e., distorted) body. A simple bar is analyzed first to show proof of concept. Then, a simplified casting system is simulated to demonstrate the feasibility of the inverse method for production castings. For each case, an inverse simulation is performed first to calculate the pattern shape. This configuration is then used as the input geometry for a forward simulation, which is shown to successfully recover the original as-cast shape used for the inverse analysis. This sequence validates the inverse method and demonstrates its potential to be a powerful technique capable of accurately determining pattern dimensions with unprecedented efficiency.

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INFLUENCE OF COARSENING ON EUTECTIC MICROSTRUCTURE AND ULTIMATE TENSILE STRENGTH OF HYPOEUTECTIC Fe-C-Si ALLOYS

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Recent studies outlined the critical role of primary dendritic microstructure for the mechanical properties of perlitic lamellar graphite Fe-C-Si alloys (LGI). Previous models described ultimate tensile strength (UTS) as a function of the graphite microstructure, while this new approach uses Griffith's fracture model for brittle materials and the coarseness of the primary dendritic microstructure is the key parameter to describe UTS. This study investigates the effect of the coarsening of the primary dendritic microstructure on the UTS of a hypoeutectic compacted graphite Fe-C-Si alloy (CGI). The primary dendritic microstructure was isothermally coarsened for different times, and its influence on the UTS was studied. The primary austenite experiences significant morphological changes during coarsening, while the eutectic microstructure shows no relation to the coarseness of primary austenite in terms of number, size, and spatial distribution of eutectic cells. However, the UTS decreases with increasing coarseness of the primary austenite

microstructure. These results demonstrate the critical role of the coarseness of the primary dendritic microstructure on the mechanical properties of hypoeutectic Fe-C-Si alloys, independent of the eutectic microstructure.

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SENSITIVITY OF OSCILATORY GROWTH MODES TO MISORIENTATIONS OF THE CRYSTAL AXES

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Experiments performed in the International Space Station have evidenced oscillatory modes for the solidification of a succinonitrile-based transparent alloy. These oscillations have been studied by phase-field numerical simulations that allowed a better understanding of their origin [1-2].
A recent re-examination of the experimental data showed that, depending on the misorientation of the crystal axes with respect to the temperature gradient direction, the oscillations may be triggered or inhibited [3].
We present here new results of phase-field simulations that show a similar sensisitivity to the cystal axes misorientation. These results are analyzed and compared with the conclusions drawn from the experimental data. Combining both, a quantitative criterion for the inhibition of the oscillations is obtained.
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COMPARISON OF NUMERICAL MACROSCOPIC MODEL FOR SEGREGATION IN SOLIDIFICATION OF BINARY ALLOYS BASED ON A MESO-SCALE EQUIAXED SOLIDIFICATION

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Since last century, two and three-phase models are generally adopted for the meso-scale simulations of the growth of equiaxed grains in solidification of binary and ternary alloys [1]-[3]. Yet, as far as three-phase models are concerned, their implementation in the macro-scale model with the equiaxed grains transport can be realised in different ways. Indeed, since the solid fraction of a grain and its envelope are attached and transported together, they share the same velocity field. Furthermore, different implementation of the multiphase meso-scale models into macro-scale models implies different treatment of the fluid flow and the macroscale segregation. In the present work advantages and problems adherent to different models are discussed and some results obtained for macrosegregation are compared.
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HYPERBRANCHED DENDRITIC GROWTH IN 4D

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With the advent of high-energy X-ray sources, it is now possible to follow solidification processes in three dimensions and as a function of time. The ability to observe and quantify the solidification process in metals on sub-second time scales and micron spatial scales in three dimensions provide fundamentally new insights into this complex phase transformation. Additions of Zn to Al are known to have a significant effect on the anisotropy of the solid-liquid interfacial energy, changing the direction of dendrite growth from <110> to <110>. Here we examine the morphology of freely growing Al dendrites in Al-Zn alloys using X-ray tomography. We find hyperbranched morphologies that are qualitative consistent with phase field simulations. The morphology of these dendrites is characterized using Interfacial Shape Distributions (ISD), the probably of finding a patch of interface with a given pair of principle curvatures. Unlike the more classical Al dendrite morphologies wherein the dendrites grow in the <100> directions, by scaling the ISD with a time-dependent characteristic length we find that the morphology of these dendrites are approximately self-similar during growth. The reasons for this apparent self-similarity will be discussed

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IMPACT FORCE MEASUREMENT OF AN ATOMIZED FLUID USING PHASE DOPPLER INTERFEROMETRY

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When heating steel, its iron content interacts with the ambient oxygen, inevitably forming oxide scales on the steel surface. These scales negatively affect the steel's surface quality, physical properties, and appearance. In the production of high-quality hot-rolled products, it is imperative to remove these impurities from the metal surface.
High-pressure hydraulic nozzles are commonly used to blast the metal surface and remove oxide from the metal roll. To ensure both the quality of the final product and efficient operation, it is crucial that the nozzles maximize impact force, while minimizing water consumption. Increasing nozzle operating pressure serves to increase impact force as expected, but only to a limited extent. Excessive pressure introduces instabilities in the spray plume, thus decreasing impact. This decreased impact can occur due to reduced drop size, or a less directed spray trajectory, resulting from excessive atomization or droplet/turbulence interaction, respectively.

In this study, a novel method for measuring spray impact force using a Phase Doppler Interferometry (PDI) instrument is developed, and its results are compared against existing methods. The PDI is an optical instrument and therefore provides measurements in a non-intrusive manner, this allows testing to be conducted on spray fluids other than water, as well as characterization of in-flight fluids in a process environment. These advantages make it an attractive instrument to apply for this purpose, and testing, modeling and analytical results of this work provide the framework for this type of analysis. Additionally, spray distribution is a key element in any installation, and these impact measurements allow Virtual Overlap Analysis (VOA) multi-nozzle placement optimization tools to be used for volume distribution uniformity, or impact distribution on surfaces and walls

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MACROSEGREGATION IN 3D HORIZONTAL DIRECT CHILL CASTING SLABS

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A 3D model of equiaxed solidification is applied to horizontal direct chill casting (HDC) of Al-4.5 wt% Cu slabs. Unlike vertical direct chill casting, HDC can operate as a continuous process, allowing for increased productivity. The flow field and macrosegregation in HDC are asymmetric along the slab thickness due to the asymmetry in heat extraction and casting perpendicular to gravity. Previous investigations of HDC have been limited to 2D models, assuming the temperature and flow field gradients are insignificant across the width. The present study evaluates this assumption for various slab aspect ratios and shows that a 3-D model is necessary to predict the correct flow patterns in the sump and important macrosegregation features, such as highly enriched bottom corners. The area and aspect ratio of the inlet jet is varied to investigate the effect of inflow speed on the resulting flow field and macrosegregation.

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THREE-DIMENSIONAL STUDY OF NODULE CLUSTERING AND HETEROGENEOUS STRAIN LOCALIZATION FOR TAILORED MATERIAL PROPERTIES IN DUCTILE IRON

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Tailored heterogeneous distributions of microstructural features enable extraordinary material performance in biological and physiological structures as trees, the aortic arch, human teeth and dinosaur skulls. In ductile iron, a heterogeneous distribution in size and morphology of graphite nodules and variations of the fractions of ferrite and pearlite are created during solidification, and varies as a function of parameters such as local cooling rate, segregation and flow. In the current work, the size distribution as well as the orientation and relation between graphite nodules is obtained by a three-dimensional reconstruction of a ductile iron microstructure from X-ray tomography. The effect of the nodule morphology and clustering on the localization of plastic strains as well as absorption of strain energy in the microstructure is studied numerically using finite element analysis of the reconstructed microstructure. Real castings have a variation in geometry, solidification conditions and are subjected to variations in loads. Based on the current observations, a framework for optimized geometry and solidification conditions in order to design and deliver castings with tailored local material performance is proposed.

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AN INVESTIGATION OF THE SOLIDIFICATION OF A NEAR-EUTECTIC COMPACTED GRAPHITE IRON UNDER THREE COOLING RATES USING WATER QUENCHING

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Compacted graphite iron (CGI) is used in various complex automotive components due to its suitable combination of physical and mechanical properties. This study aims to investigate the solidification of CGI by employing a newly developed experimental technique. 400g specimens of spheroidal graphite iron are remelted in an Argon atmosphere and subsequently solidified as CGI by controlling the exposure to elevated temperatures. By ramping down the furnace temperature, specimens are allowed to solidify under three different cooling rates (0.16, 0.08 and 0.04 K/s). In a first series of experiments, cooling curves are recorded in two positions in the specimens, allowing for Fourier thermal analysis. In a second series, the solidification of the material is investigated by quenching the solidifying specimens in water at different times during solidification. The evolution of the microstructure through solidification is investigated qualitatively and quantitatively. The results of the investigation are expected to be useful for modeling the solidification kinetics and feeding behavior of CGI.

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MODELLING COLUMNAR AND EQUIAXED SOLIDIFICATION IN METAL ALLOY ADDITIVE MANUFACTURING

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Powder bed fusion processes in additive manufacture (AM) of metals typically involve solidification in high thermal gradients, leading to unwanted anisotropic columnar growth and high residual stress in as-printed components. Equiaxed solidification can alleviate such problems but is difficult to achieve due to the thermal fields naturally evolving in typical AM processes. Preheating of the powder bed in electron beam-based processes can reduce the thermal gradient and, together with grain refinement of the alloys, this encourages equiaxed solidification. However there is a material-dependent possibility of sintering of loose powders if this approach is taken which makes it more difficult to recycle un-used powder after print runs. The process is quite complicated, experimental trials are expensive and can be carried out only within limited ranges of specific machine parameters, and in-process experimental measurements are difficult. Computer simulation and modelling is therefore a key tool in investigating possible ways of creating conditions suitable for equiaxed solidification. A multi-scale modelling approach is presented which will predict columnar and equiaxed solidification and the columnar-to-equiaxed transition, using front-tracking at the scale of grains to simulate the non-equilibrium growth of dendritic fronts and grain envelopes, with phase field formulations for the micro-scale physics of dendritic growth. Preliminary results are outlined.

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THE EFFECT OF THE ANISOTROPY OF SURFACE ENERGY AND KINETIC ATTACHMENT ON SILICON SOLIDIFICATION

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Silicon is widely used in the industry of solar panels. During the manufacturing process, the molten silicon is solidified into ingots. These ingots are cut into very thin layers which are assembled into solar cells. It turns out that the solar cells efficiency depends on the solidification process and the final microstructure of the ingots. Several experimental studies of solidification showed that the growth shapes exhibit facets along the {111} directions because the growth rate of facets being much lower than that of rough surfaces, it thus controls the process. There seems to be an overall agreement on the fact that the facets appear because of the anisotropy of surface energy, kinetic attachment, or both. However, the experimental results do not allow a definite conclusion about which phenomenon is the most relevant and this question is still a challenge for the numerical methods. In this work, we developed a 3D phase-field code incorporating the two phenomena and that takes into account the experimental conditions described in [1,2]. The results of the simulations are compared to the experimental ones and conclusions are drawn out [3].

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THERMO-MECHANICAL MODELING OF ADDITIVE MANUFACTURING BY POWDER BED FUSION AT PART SCALE

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A thermo-mechanical model of powder bed fusion by laser beam is developed by the finite element method at the macro-scale. This approach focuses on the part construction, in which a level-set framework is adopted to track first the interface between the constructed part and the non-exposed powder, and second, the interface between gas and the successive powder bed layers. The accounting for the non-irradiated powder bed in the model allows an improved heat transfer resolution. In order to reach reasonable simulation time for industrial parts, the energy input and the formation of the additive deposit are simplified by considering them at the scale of fractions of layer, an entire layer or a so-called “super-layer”, that is a set of several layers. In each simulation strategy, the three stages of heating, cooling and the dwell time between two successive layers are included in the process modeling. In addition, the mechanical analysis following the thermal analysis is performed in each time step during all the stages of the construction process. At the end of the construction, the residual stress and distortion of the constructed part are presented. In all three strategies, mesh adaptation is employed, offering a good compromise between accuracy and sustainable computation time. Quantitative comparison between the three approaches will be presented and discussed.

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PHASE BOUNDARY ANISOTROPY IN LAMELLAR EUTECTICS: RESULTS FROM RECENT MICROGRAVITY EXPERIMENTS

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Directional solidification of eutectics has been extensively studied in systems which display regular coupled growth with the solid-liquid interfaces being non-faceted. The solid-solid phase boundaries however may be locked or loosely attached to planes with a low energy configuration being associated with a characteristic crystallographic orientation relationship (OR). The phase boundary energy landscape and its anisotropy can have a major impact on eutectic growth and we shall give an account of the current state of knowledge and of the most recent observations gained from bulk Al-Al2Cu eutectics during (i) the maze-to-lamellar transition, (ii) the steady state growth and (iii) the formation of eutectic cells. We refer to Al-Al2Cu eutectics for which the phase boundary energy anisotropy was estimated from molecular dynamic computations (MD). We shall give an outlook on future research tasks and discuss the ability to understand and control the orientation and defect density of an arbitrary lamellar eutectic.

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ADVANCED SOLIDIFICATION MODELS FOR THE SIMULATION OF MECHANICAL BONDING IN HYBRID LIGHT METAL STRUCTURES PRODUCED BY HIGH PRESSURE DIE CASTING

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In modern automotive structural components, metal sheets are combined with casting parts to enable a light and mechanical stable structure. In this study, the bonding between steel metal sheets and aluminum casting parts are achieved as part of the high pressure die casting (HPDC) process. In this way additional bonding steps like welding can be omitted.

Gas enclosure at the interface between metal sheet and casting part may hinder a strong bonding. This effect is supposed to be enlarged by the rapid solidification at the interface between sheet and casting, where hot melt hits a cold metal sheet. Cooling rates are in the range of 1000 K/s. Such a rapid solidification leads to a stop of the melt flow already during the filling process and can trap gas enclosure at the interface.

Coupled flow and solidification simulation is used to analyze the hybrid casting process with a focus on the wetting of the metal sheet by the melt and the formation of a strong bonding during solidification. Standard solidification models, based on a fraction solid curve, cannot describe essential phenomena of fast solidification, like undercooling of the melt. These phenomena may have a strong effect on the stopping of the melt flow and, hereby, the gas enclosure. Therefore, an advanced rate based solidification model is developed to address non-equilibrium aspects of the fast solidification and enable a more realistic simulation of the bonding process during solidification.

The solidification model is calibrated by microstructure simulations using the multiphase-field method. The simulation results are validated against experiments performed on a cold-chamber HPDC machine (Buehler H630-SC) using simplified test geometries.

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ANISOTROPY EFFECTS ON LAMELLAR-EUTECTIC SOLIDIFICATION MICROSTRUCTURES IN THIN Al-Al2Cu SAMPLES

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We present an in situ experimental study of crystallographic effects during lamellar- eutectic growth in thin Al-Al2Cu samples. The Al-Al2Cu alloy is known to form eutectic-grain dependent lamellar eutectic microstructures, and to present special, or heteroepitaxy orientation relationships (OR) between the eutectic crystals. The term crystallographic effects refers here to a marked dependence of the growth microstructure on the orientation of the two solid phases relative to each other, and the direction of growth. We prepared thin ($\approx$10 μm thick) metallic films by plasma sputtering on sapphire plates. The thin-sample geometry allows one to observe lamellar-growth patterns in real time without convection in the liquid, by using a long distance optical microscope (reflected-light mode) focusing the contact surface of the metallic film with one of the transparent substrates. We could identify both « floating » grains with a regular dynamic behavior in steady-state, and locked grains, within which the lamellae grow inclined, parallel to a fixed direction. We combined our optical observations with ex situ crystallographic analyses usign two methods, namely, x-ray diffraction and EBSD in order to determine the ORs in the different eutectic grains. We will comment on our results in the light of a recent work on the effect of an anisotropy of the surface free energy of the interphase boundaries on lamellar eutectics.

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SHAPE OF THE IN-SITU (Al,Zn)-Ti REINFORCING PARTICLES AND THEIR INFLUENCE ON STRUCTURE AND STRUCTURAL STABILITY OF SELECTED Zn-Al AND Al-Zn CAST ALLOYS

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The foundry engineering still needs new cast materials of improved properties. These can be achieved by elaborating completely new alloys and metal matrix composites or by elaborating the alloys/composites basing on the already very well-known matrixes. The good example of the latter solution are high-aluminium zinc (H-Al Zn) and high-zinc aluminium cast alloys (H-Al Zn). Both of these groups show good damping and strength properties but rather low ductility and insufficient structural (and dimensional) stability, caused by long term transformation of the Cu-containing bearing phases. The present paper summarizes the work of Cracow AGH University and Cambridge Department of Materials Science and Metallurgy performed over last several years [1-3]. The performed works were devoted, among others, to building composites of improved structural stability reinforced with ternary (Al,Zn)-Ti aluminides. The work was financially supported by the European (MTKD-CT-2006-042468) and Polish project (UMO-2017/25/B/ST8/00150) and laboratory facilities were provided by the both Institutions, which is kindly acknowledged. This paper is aimed at presenting the influence of the shape of the in-situ reinforcing particles on the mentioned properties, particularly the tribological and strength ones. The in-situ reinforcement was built by needle-shape ternary aluminides based on the DO22 TiAl3 binary phase introduced with AlTi-based master alloys or by compacted semi-globular ones based on the L12 Zn3Ti particles introduced with a ZnTi-based master alloy. The mentioned particles

substitute partly or totally for Cu-based bearing phase and the influence of this substitution on the structural stability and tribological properties is also discussed in the paper. REFERENCES 1. W.K. Krajewski, A.L. Greer, P.K. Krajewski, Trends in developments of high-aluminium zinc alloys of stable structure and properties, Archives of Metallurgy and Materials 58 (2013) 845-847. 2. W.K. Krajewski, J. Burać, P.K. Krajewski, A.L. Greer, K. Faerber, P. Schumacher, New developments of Al-Zn cast alloys, Materials Today: Proceedings 2 (2015) 4978 – 4983. 3. W.K. Krajewski, A.L. Greer, G. Piwowarski, P.K. Krajewski, Property enhancement by grain-refinement of zinc-aluminium foundry alloys, Proceedings of 4th International Conference in Advances of Solidification Processes (ICASP-4), IOP Conference Series: Materials Science and Engineering 117 (2016), paper No. 012004. DOI:10.1088/1757-899X/117/1/012004.

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EFFECT OF THE CORIOLIS FORCE ON THE MACROSEGREGATION OF ALUMINUM IN THE CENTRIFUGAL CASTING OF Ti-Al ALLOYS

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Ti-Al alloys have been studied for more than 20 years due to their low density and high resistance in high temperature environments, making them a good candidate for automotive and aerospace applications. However, their high reactivity in liquid state makes them difficult to cast because they need to be cast at very low superheat and at fast filling rates. Centrifugal casting enhances the mold filling speed but increases the magnitude of the liquid thermosolutal convection by the combined effect of the centrifugal and Coriolis accelerations.
Within the framework of the ESA's GRADECET project, experiments of directional solidification of cylindrical Ti-Al samples (8 mm diameter, 120 mm length) were performed in well controlled conditions. The experiments were performed in a centrifuge, with the apparent gravity (sum of centrifugal acceleration and terrestrial gravity) aligned with the cylinder centerline. Five levels of centrifugation, with an apparent gravity ranging from 1g to 20g (g: normal terrestrial gravity) were investigated.
We present 3D numerical simulations of the aluminum macrosegregation using a volume-averaging solidification model that accounts for the centrifugal and Coriolis accelerations in the non-inertial rotating reference frame. The model was implemented in the framework of the OpenFOAM finite-volume platform and was validated for the simulation of macrosegregation and for natural convection in rotating systems.
The results show that the Coriolis acceleration, although very weak, breaks the symmetry of the themosolutal liquid convection, having an important impact on the final macrosegregation pattern. The macrosegregation pattern is entirely modified in comparison with a sample solidified under terrestrial gravity conditions. Besides, as could be expected, the magnitude of the segregation of aluminum increases with the centrifugation level.

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AN INVESTIGATION OF THE CHILL-CASTING INTERFACE DYNAMICS IN PRODUCTION OF SAND-CAST A319 ENGINE BLOCKS

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In recent years, the automotive industry has been increasing the production of small, high-power gas engines as part of several strategies to achieve the new "Corporate Average Fuel Economy" (CAFE) standards. This trend requires an improvement in the thermal and mechanical fatigue durability of the aluminium alloys used in the production of the engine blocks. Conventionally, solid chills are employed in areas of these castings subject to high cyclic loading – i.e. in the main bearing bulkhead. A potential means of improving the efficacy of these chills is to incorporate water cooling. To assess the effectiveness of this method, a water-cooled chill was designed and installed in a bonded-sand engine block mould package (1/4 section). The moulds were instrumented with thermocouples, to measure the evolution of temperature at key locations in the casting, and "Linear Variable Displacement Transducers" (LVDTs), to measure the gap formation at the interface between the chill and the casting. A coupled thermal-stress mathematical model was developed in "ABAQUS 2016" to reproduce the experimental conditions and provide insight into interfacial heat transport and gap dynamics. This paper summarizes, at a high level, some of the findings of this work.

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INTERFACES AT INTERNAL CHILLS IN SOLIDIFYING STEEL SECTIONS

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Chills are used in the production of steel castings as a thermal aid to promote directional solidification in casted sections. This study will review microstructure and thermal circumstances of the internal chill interface where the chill is intended to be incorporated into the structure of the cast section. The conditions for interface coherency of cast steel sections from 25 to 50mm will be shown. Solidification proceeds away from the interface chill growing to a maximum thickness and then melting back to the original chill geometry. If the section solidifies before the internal chill entirely melts, then the interface will be coherent across the chill and cast sections for compatible steel alloys. A computer model of the heat transfer and interface evolution show the possibility of using the coherent interface of internal chills in the design of other cast components.

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VISUALISATION OF MELT FLOW EFFECTS ON DENDRITIC SOLIDIFICATION

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X-ray radioscopic studies have been performed to improve the understanding of the complex interrelation between melt flow and the evolution of dendritic structures during solidification of Ga-In alloys. Natural convection is caused by density variations within the solidifying alloys. Forced convection was produced by electromagnetic stirring. Within this work special interest was focused on dendrite fragmentation and segregation phenomena. Melt convection alters the solutal field near the solidification front, leading to different microstructures or even to the formation of freckle defects. Essential process parameters such as flow patterns, solute concentration, the mushy zone morphology and permeability, dendrite growth velocities were quantified by image

analysis. Particular attention is paid to the development of segregation structures and to the "self-healing" process of segregation zones. The observations indicate that if the local melt flow near the solidification front is destabilized, the Indium-rich melt flows inside the channel. The consequence is the "self-healing" process, i.e. the channel is filled in a short time by new dendrites and finally disappears. Eventual mechanisms that destabilize the channel formation are discussed so that the freckle defect can be eliminated by electromagnetic stirring on early stage of solidification. Moreover, our experiments demonstrate how the melt flow contributes to grain refinement, the CET (columnar to equiaxed transition) and dendrite fragments transport, which are discussed intensively in the literature.

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EFFECT OF STIRRING TIME AND COOLING RATE ON MICROSTRUTURE OF MRI230D ALLOY PROCESSED BY RHEOCASTING

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The semi-solid processing aimed to modify the solidification morphology, from dendritic to globular structure, turning this process interesting to improve the properties of magnesium alloys. This work aims to analyze the influence of the cooling rate and the stirring time on the microstructure of the MRI230D alloy submitted to the rheocasting process. The material was processed in the semi-solid state for modification of its solidification structure. The alloy was melted in a resistive furnace with inert atmosphere. Thermal analysis was performed to obtain liquidus and solidus temperatures of magnesium alloy studied. The mechanical stirring was applied for solid fraction between 0.2 to 0.5. The stirring times were 0, 1, 2, 4 and 8 minutes. For each stirring time, cylindrical samples with three different diameters (3, 6 and 9 mm) were extracted and quickly cooled into water to keep microstructural morphology of semi-solid in order to evaluate the influence of the cooling rate. The microstructure was analyzed by optical and scanning electron microscopy aiming to compare the morphology of the formed globules through the average grain size and shape factor. The initial results showed that for higher stirring times the globules become coarse, and for higher cooling rate the grain size decrease.

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RAPID SOLIDIFICATION OF Al-Cu DROPLETS OF NEAR EUTECTIC COMPOSITION

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Al-Cu droplets of eutectic composition with different purity levels, were rapidly solidified by Impulse Atomization. A wide range of microstructural scales was obtained at different cooling rates and undercoolings. The micrographs of the investigated microstructures revealed two distinct zones of different structural morphologies: An irregular eutectic morphology developed during recalescence following nucleation and a regular lamellar eutectic morphology resulting from the solidification of the remaining liquid. The volume fraction of each zone was measured as a function of the droplet size, and the nucleation undercooling was deduced using the hypercooling limit equation while the growth velocity and growth undercooling were determined using theoretical models. X-Ray Diffraction, Electron Backscatter Diffraction, Scanning and Transmission

Electronic Microscopy, Energy Dispersive Spectroscopy, Atom probe and Microhardness Tests were used to evaluate the microstructural scale/ composition, and mechanical properties. While microhardness measurements revealed exceptional properties for an aluminum-copper alloy, the microstructures analysis showed evidence of metastable phases.

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DENSITY VARIATION AT SOLIDIFICATION OF HYPOEUTECTIC LAMELLAR GRAPHITE IRON

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The main coexisting phases during solidification of lamellar graphite iron, the liquid phase, the precipitating austenite and graphite are interacting and causes a complex volume change pattern. In the present work the density of liquid iron and the austenite phase is investigated based on measurements with a push-rod dilatometer. The values of the densities have been calculated based on the assumption of isotropic behavior of the material during the measurement. The investigation covers the whole interval of industrial useful compositions of cast iron with carbon equivalent (CE) between 2,9 to 4,4 which is the broadest investigated interval with respect to the ones found in the literature. Likewise, the density at solidus temperature has been calculated as well as the slope of the density curves in the austenitic range. The obtained results are used to model the local density variation during solidification of lamellar graphite iron.

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POST-SOLIDICATION EFFECTS IN DIRECTIONALLY SOLIDIFIED TERNARY EUTECTIC Al-Al2Cu-Ag2Al

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During the solidification of ternary eutectics, three solid phases form simultaneously from the melt. One system often employed to study this complex multi-phase solidification behavior is ternary eutectic *Al-Al_2Cu-Ag_2Al*. In this system the solubility of silver in the α-Al phase decreases by approximately 50% in a range of less than 20 K below the ternary eutectic temperature. This diffusion-controlled solubility shift is obvious from a comparison of microstructure in a normally processed sample with microstructure from directly behind a quenched interface, in which the solubility shift did not have time to occur. There are differences not only in the phase fractions of the three solid phases, but also in the shape of the phase regions and the pattern itself. In order to study the evolution of the microstructure caused by this solubility shift, quenched samples of directionally solidified ternary eutectic *Al-Al_2Cu-Ag_2Al* were systematically annealed and the resulting post-solidification effects were studied with scanning electron microscopy for two different solidification patterns. The results show that the adjustment of the phase fractions takes place much faster than the rearrangement of the shape of the phases. This shape evolution is strongly influenced by the anisotropic interface energies, resulting in more straight solid-solid interface boundaries instead of the the competing curvature reduction. The outcomes of this work demonstrate that in order to obtain a more complete understanding of directionally solidified ternary eutectic *Al-Al_2Cu-Ag_2Al*, both the solidification and the subsequent post-solidification processes must be considered.

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THE FORMATION OF Al6 (Fe, Mn) PHASE IN DIE-CAST Al-Mg ALLOYS

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In aluminium alloys, iron is a common impurity as it is unavoidably picked up in practice. The excessive Fe is strongly prone to form various intermetallic phases. These intermetallics are generally brittle and act as stress raisers to weaken the coherence with Al matrix. Consequently, the cast components are degraded in terms of the elongation. However, Fe addition in Al-Mg alloys may be beneficial because of the improvement in the yield strength with the scarification of ductility of die-cast aluminium alloys. Therefore, the morphology of intermetallic phases has a vital effect on the properties of aluminium alloys. The addition of Mn in Al-Mg alloys can transform Al3Fe to Al6 (Fe, Mn). The increased cooling rate can also significantly refine the Al6(Fe, Mn) phase. Therefore, the present study aims to reveal the 3-D morphology and growth mechanism of Al6 (Fe, Mn) in Al-Mg-Mn alloys with different levels of Fe contents. The effect of Fe contents on the microstructure and the formation of Al6 (Fe, Mn) was studied in the die-cast Al-Mg-Mn alloys under as-cast condition is studied through crystal features and solidification behaviours.

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A STUDY OF THE MASS TRANSFER KINETICS DURING THE DISSOLUTION OF Ti-N PARTICLES IN LIQUID TITANIUM

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Abstract: The existence of local areas of high nitrogen concentration in titanium is highly problematic as they pose a risk of causing fatigue failure in aero-engine disc material. The particles responsible for these areas can come from various sources and can range in composition from a few weight percent up and including non-stoichiometric TiN particles. The challenge in removing these particles during primary ingot production is that they possess melting temperatures well above typical liquid metal processing temperatures. To meet this challenge, the titanium industry has adopted a number of strategies including the development of cold-hearth remelting technologies that aim to remove them by a process of chemical homogenization prior to entering the ingot mold. This paper summarizes the development of a computational fluid dynamics (CFD) model based on the commercial software package ANSYS-CFX which has been used to examine the kinetics of dissolution of a single stationary TiN particle surrounded by moving liquid titanium. The model accounts for diffusional mass transport in the solid particle, the formation of a two-phase solid/liquid boundary layer and both advective and diffusional transport to the bulk liquid. The purpose of the CFD model is also to estimate an effective mass transfer coefficient that may be applied in models based on the solid-state mass transport of nitrogen alone. The result shows that a correction is needed to the conventional Ranz-Marshall correlation to more accurately calculate the mass transfer coefficient during the TiN particle dissolution process.

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NUMERICAL SIMULATIONS OF ELECTROMAGNETIC COUNTERACTIONS TO MOLD FLUID FLOW ASYMMETRY DEVIATIONS

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Process stability during continuous casting is crucial in order to obtain homogeneous and constant conditions for the fluid steel to solidify evenly in the mold. In highly productive slab casters, the utilization of the submerged entry nozzle (SEN) feeding the molten steel into the casting mold is often maximized. Before the SEN is taken out of operation, it undergoes wear and erosion. Particularly in the last slabs before SEN exchange, clogging in the nozzle may be severe and inhomogeneous, leading to strongly asymmetric and biased molten steel flows in the upper portion of the mold. As a consequence of the asymmetric mold flow pattern, local mold powder entrainment or non-optimal inclusion seclusion may occur with deteriorated steel quality as a result. To avoid downgrades of steel quality in these slabs, it is vital to maintain stable and symmetric fluid flow conditions in the mold.
The FC Mold is a flexible electromagnetic device able to apply static and/or alternating electromagnetic fields in two levels in the mold to brake and stir the fluid flow near the meniscus region and below the SEN jets. The magnets can be configured to produce an asymmetric field distribution along the width of the mold, and in this way allow counteraction against e.g. biased mold flow or local excessive flow speeds.
A numerical computation model of the fluid steel flow in the strand, incorporating a magnetohydrodynamics coupling to the CFD equations, has been continuously developed and refined over the years. This model has been used to simulate a variation of casting conditions representative for a modern, dynamic slab caster, applying static and alternating electromagnetic fields to different extents depending on the flow intensity at hand. Simulations have been carried out to quantify the required fields to symmetrize biased flow scenarios caused by e.g. SEN clogging. In conjunction with steel plant trial feedback, the simulation results have been used to setup a control algorithm for the FC Mold.

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KINETICS OF RAPID CRYSTAL GROWTH: PHASE FIELD THEORY VERSUS ATOMISTIC SIMULATIONS

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Recent advancements in the phase field theory predict slow and fast regimes of crystal growth from melts and solutions [1]. We analyze kinetics of crystal interfaces invading undercooled melts using traveling wave solutions derived from phase field theory of fast phase transformations. These solutions are compared with data kinetics of molecular dynamics simulations [2-4] obtained for slow and rapid growth of crystals.
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Cerium containing inclusions: kinetic model and experimental results

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As nonmetallic inclusions (NMI) are unavoidable in steel production and commonly have a negative impact on product quality. Metallurgical research has always aimed at either the adjustment of inclusion morphology or inclusion separation to minimize their adverse effects. In the 1990s the conscious nucleation of particles to either promote or inhibit the subsequent growth of other phases became a new research issue. Today, inclusions are successfully used as grain refiner in the solidification of ferritic and austenitic steels providing that their size, number, morphology and chemical composition are precisely adjusted. Ce2O3 and AlCeO3 are considered active to trigger a fine grained solidification structure for many years now. Depending on the introduced amount of Ce the inclusion type present changes. To gain a better understanding for the conditions that lead to these favorable particles and evaluate the reliability of thermodynamic data, the following poster is presenting theoretical considerations based on results from a ChemApp–based kinetic inclusion prediction model that allows the quantification of the influence of chemistry taking into account microsegregation. These results are complemented by laboratory experiments in a vertical tube furnace, where Ce and Al were introduced simultaneously to a pure iron melt containing 80 ppm O and 40 ppm S. The comparison of simulation and experiment reveals that the simulation is fit to be used as guidance even if the agreement is not perfect. The deviations can mostly be attributed to the dissolution process of cerium. Nevertheless these results are invaluable for designing and performing future experiments with the goal of specific cerium inclusions and a refined primary solidification structure.

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ON ANALYTICAL CONCEPTS OF NOVEL MULTI-RESOLUTION CASTING SIMULATIONS

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One of the crucial ingredients of today's numerical simulation technologies is their cross-scale and cross-platform capabilities for material processes applications. Handling of simultaneous evolution paths at various scales\times (i.e., multi-scaling) during complex material processes where materials microstructure & microchemistry interacts with meso and macro events, is one of awkward challenges of computational material engineering. The material change of phase and also its thermal energy evolutions are also drastically increasing the complexity of the numerical simulation. The introduction of multi-resolution and multi-scale numerical schemes in recent years and their ground-breaking potentials for computational material applications has vividly raised the expectations for more resourceful future virtual tools. A crucial point in implementing these novel numerical techniques for simulation of material processes is their flexibility towards the modelling approach (i.e., discrete, continuous...) and also their compatibility with solver-independent platforms. The proposed multi-resolution framework herein, has been developed based on analytical \& numerical techniques built on sound physical and mathematical foundations developed during the last few decades. The combination of recently developed concepts of dynamic\textbackslash{}evolving domains along with cross-scale grid overlapping\textbackslash{}interfacing and sound parallel computing routines have been employed to address the multi-scale challenges of material processes simulations. Since many of industrial-scale material processes are inherently thermal-process (cyclic or monotonic) with cooling and also possible heat treatment events, the transient nature of thermal-mechanical histories has to be accurately considered. These transient histories shall be converted to a mathematically described data for scale bridging procedure to enable the cross-scale properties transport. The innovative potential of these physical-based and in the same time mathematically-oriented scheme is significant, since its biggest contribution relies in the balanced interaction between basic material science concept, advanced computational technologies and also fast scientific computing. It can promote a realistic short-cutting scheme with pragmatic industrial use cases for complex industrial processes. In the research work herein, analytical and computational aspects of multi-resolution simulation framework for dynamic casting processes (i.e., continuous and semi-continuous casting) has been presented and physical\textbackslash{}mathematical basis of the overlapping\textbackslash{}integrating grids, computational solidification module and also cross-scale bridging techniques are elaborated. Industrial applications of the techniques have also been envisaged using parallel-processing and fast computing facilities for full-scale casting application.

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ON MODELLING VISCOPLASTIC BEHAVIOUR OF THE SOLIDIFYING SHELL IN THE FUNNEL-TYPE CONTINUOUS CASTING MOLD

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As it was previously reported, a numerical model was applied to simulate the behaviour of the packed bed of equiaxed crystals [1]. At the high temperatures metals tend to follow a viscoplastic law according to Bellet et. al [2]. Thereby based on the authors developments a viscoplastic stress model was applied to the thin slab casting process. In this idea the solidifying shell represents a 'creeping solid'. Thus the Norton-Hoff stress model is formulated with the model parameters obtained experimentally. Since the strain rate is non-linearly introduced into the stress calculation, a coupling procedure is established to converge the non-linear terms.
The basic parameters of the model were selected from the previous studies [1-2]. A detailed study was performed for the stress model parameters influence on the solid velocities distribution and stress build-up in the solid shell. Next the model was applied for the simulation of the thin slab caster to improve previously developed one [3]. Instead of imposed solid shell velocities a viscoplastic rheology of the mush was applied to calculate the motion of the solidifying melt.
The results of the thin slab simulation showed, that the most deformations happen at the funnel part of the mould, causing highest strain rates. Viscoplastic 'apparent viscosity' drops at the region of the highest strain according to the Norton-Hoff law. Solid shell velocities are significantly uniform at the straight parts of the mould and strand but a slight acceleration of the shell is observed along the funnel surface. Strong compression / depression zones are detected at the funnel part, which could lead to defects formation. Solid shell thickness was successfully predicted as well and compared to the previous work by the authors [3].

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COMPARISON OF MICROSTRUCTURAL EVOLUTION OF AZ91 MAGNESIUM ALLOY PREPARED BY SIMA AND RHEOCASTING ROUTES

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The increasing tendency for near net shape production of industrial parts, taking advantage of costs reduction and quality improvement, is turning semi-solid processing into viable technologies. The Strain-Induced Melt Activation (SIMA) and the Rheocasting are the two semi-solid processing routes to produce feedstock with globular microstructure. In this work, the microstructure development in the semi-solid state of AZ91 magnesium alloy prepared by SIMA and Rheocasting were analyzed aiming to compare the morphology of the formed globules through the average grain size and shape factor. Thermal analysis was used to determine the solidus and liquidus temperatures of magnesium alloy studied. Semi-solid prepared by SIMA, was firstly preheated at 250°C for 30 min and rolled up to 6% predeformation, followed isothermal treatment helded at 570°C for 35 minutes. After, the samples were quickly quenched into water to keep microstructural morphology of semi-solid. By the Rheocasting route, the AZ91 alloy was heated up at resistance furnace with inert atmosphere and mechanical stirring was applied for 2 minutes at 550°C. Preliminary results show that the two processing routes in the semi-solid state can produce globular microstructures and the SIMA route presents globules with better shape factor.

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A MODEL FOR COUPLING PREDICTION OF INVERSE SEGREGATION AND POROSITY FOR UP-VERTICAL UNIDIRECTIONAL SOLIDIFICATION OF Al-Cu ALLOYS

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A mathematical model has been established to coupling predict the formation of inverse segregation and porosity for up-vertical unidirectional solidification of Al-Cu alloys. Based on the analysis on the redistribution behaviours of both gas element and the alloying elements in the mushy zone. The model first investigates the volume change during solidification intensively, including the specific mass variation and the solidification shrinkage both during the growth of primary phase and eutectic reaction, to derive the back flow needed. Then, the fraction of porosity is obtained by combing the effects of hydrogen segregation and the pressure depression associated with the feeding liquid flow through a porous media and being solved with Darcy's equation. Consequently, both the feeding flow and the well known 'local solute redistribution equation' are modified with the presence of porosity. Finally, the solute distribution is obtained by coupling a finite difference solidification model with the modified segregation model. Numerical results show that the overall back-flow, which is needed to compensate the volume shrinkage, decreases with an increasing initially dissolved hydrogen concentration. As a result, the inverse segregation, being induced mainly by back-flow which is generally rich in solute, decreases with an increasing amount of porosity. The calculating results are also compared with the experimental results reported in literatures, which shows rather good agreement. The model can be used to predict inverse segregation with the presence of porosity in vertically unidirectionally solidified Al-Cu alloys.

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IMPACT OF UNEQUAL PHASE BOUNDARY ENERGIES ON THE PERITECTIC REACTION STUDIED BY PHASE-FIELD SIMULATION

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Peritectic transitions - characterized by the formation of a secondary phase from decomposition of the primary phase and the melt - are very common in the solidification of metallic alloys. During the peritectic reaction, all three phases are in direct contact, thus forming a trijunction. Already in 1979, Hillert [1] emphasized the important role of the junction force balance in the peritectic reaction and pointed out that opposing capillarity forces are required to meet the local equilibrium conditions at the different boundaries in the vicinity of the junction. However, so far, little attention has been paid to the actual impact of the individual liquid-solid and solid-solid phase boundary energies, which cannot be expected to be equal in real materials. In this work, the multi-phase-field method was applied to study the impact of unequal phase boundary energies by the example of a peritectic TiAl alloy with negligible solid-state diffusion. Simulations were performed under isothermal conditions and systematic variation of the involved interfacial energies. Reaction rates, evaluated after reaching steady-state conditions, are discussed and correlated to the thickness of the peritectic layer. A major result of the case study is that two different growth modes can be distinguished a) when the triple junction is leading and rate-controlling and b) when the peritectic growth front is leading and its tip is rate-controlling. Which of these two growth modes is selected can be described by a critical ratio of the interfacial energies.
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CONTINUOUS CASTING OF HIGH CARBON STEEL: HOW DOES HARD COOLING INFLUENCE SOLIDIFICATION, MICRO- AND MACRO SEGREGATION?

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High-carbon steels used for the production of tire cord have rather simple steel chemistry with carbon being the main alloying element. They are however quite challenging to produce as segregation must be minimized and steel cleanness must be maximized. One technology that is often employed in continuous casting of high-carbon steels to minimize centre- (or macro) segregation is so-called hard secondary cooling: the strand is cooled with high intensity spray water so that the surface of the billet is cooled to temperatures of 300°C - 500°C in the secondary cooling zone after exiting the mould. Standard practice would be to cool the strand to 1000°C - 1150°C.
Investigations unanimously show, that hard cooling significantly reduces macro-segregation. On the down side, this technology is notoriously difficult to employ as the billets are very susceptible to internal reheating cracks, surface cracks, snaking of the billets, etc. In view of the importance and wide spread use of this technology, it is surprising to note, that there seems to be no consent in literature as to the mechanism by which macro-segregation is reduced by hard cooling.
In this paper various solidification simulations of the high carbon tire cord grade C80D, calculated using the Thermo-Calc software package and the diffusion add-on module DICTRA are compared. The calculations use the TCFE9 and MOBFE4 thermodynamic and mobility databases. These calculations clearly show, that for standard secondary cooling practices Scheil solidification simulations with carbon defined as a fast diffusing element agree reasonably well to solidification simulations that include the full phase transformation and diffusion kinetics calculated with DICTRA. For the faster cooling rates encountered in hard cooling however, Scheil simulations fail badly. It is further shown, that it is vitally important to consider the solidification kinetics when calculating the thermodynamic input data for process control software such as FEM solidification simulations, that are routinely used in modern steel-plants to define the optimal casting parameters. It is shown why hard cooling makes the billet more sensitive to internal cracks and finally a mechanism is proposed by which hard cooling leads to significantly reduced centre-segregation. These results can directly be used by steel-plants employing hard cooling to re-evaluate their casting parameters.

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A PARTITIONED SOLUTION ALGORITHM FOR FLUID FLOW AND STRESS-STRAIN COMPUTATIONS APPLIED TO CONTINUOUS CASTING

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The paper presents a partitioned resolution algorithm for concurrent simulation of fluid flow and solid mechanics with application to solidification processes. The general objective is to concurrently model liquid flow in the non-solidified regions and solid deformation in solidified regions. The scheme is developed to include partially solidified regions (i.e. mushy zone) as this is the locus for segregation and stress related defects such as hot tears. This should be achieved while simulating i filling of cast parts or ingots, ii cooling of products, with special emphasis on iii continuous casting of billets or slabs.

The solution algorithm for momentum conservation consists in a two-step resolution performed at each time increment. In the first step, a solid-oriented resolution deriving from an existing thermomechanical solidification model [1,2] is performed, in order to calculate stress and deformation fields in the regions containing solid. In the second step, a liquid-oriented resolution is derived, which addresses fluid flow in the bulk liquid, and in the mushy zone. Volume averaging and Darcy's law is used to model the interaction between solid and liquid phases in the mushy zone.

Both resolutions are formulated with 3D finite elements on the same domain which includes the metal (whatever its state: liquid, mushy, or solid), and a surrounding gas domain. The level-set method is used to track the motion of metal/air interface induced by hydrodynamics, solidification shrinkage, thermal dilatation and deformation phenomena. The algorithm is coupled with an existing non-linear energy solver to calculate the temperature field [3]. Validation is demonstrated by comparison with analytical solutions in the context of directional solidification. The paper will present and discuss its application to case studies approaching the complexity of industrial solidification processes.

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HIGH SHEAR TREATMENT ASSISTED FABRICATION OF METAL MATRIX PARTICULATE NANOCOMPOSITES

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Metal matrix composites (MMCs) can be tailored to produce various combinations of stiffness and strength and have found a wide range of applications where existing materials are not suitable for use in automotive and aerospace industries and many other areas. Stir casting is commonly used for fabricating large quantity of primary MMCs, in comparison to liquid metal infiltration and powder metallurgy, which are methods for making near net-shape MMC components or small quantity MMCs. Stir casting is cost-effective but suffers from severe particle

agglomeration, particularly when the size of reinforced particles is down to nanoscale. The present work was carried out to investigate the effect of high shear treatment on the distribution of reinforcing particles in the fabrication of magnesium and aluminium alloy matrix particulate nanocomposites. An Mg-2Zn-0.5Ca alloy and commercially pure aluminium was selected as the matrix. Hydroxyapatite nanoparticles (˜50nm, spherical, 1-5wt%) were added to the magnesium alloy as reinforcing elements and alumina nanoparticles (˜30nm, spherical, 1-3wt%) to aluminium. The high shear treatment was employed after the admission of reinforcing particles by mechanical stir and performed with a rotor-stator device at a speed of ˜5000rpm. Experimental results showed that the high shear treatment effectively reduced particle agglomeration for both Mg/HA and Al/Al2O3 nanocomposites, although the features of particle segregation are different, probably due to difference in wettability between the matrix and reinforcing elements in these two systems. The as-cast Mg/HA and Al/Al2O3 nanocomposites were deformed by hot extrusion and cold rolling respectively. The microstructure and mechanical properties of the material were characterized and the effect of processing parameters was studied.

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QUANTIFICATION OF MICROSTRUCTURE TO REVEAL THE SOLIDIFICATION PATH OF AN ALLOY

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This paper reports on the development of Solidification Continuous Cooling Transformation (SCCT) diagrams relating the solidification paths to the inherent microstructures of binary and ternary alloys. The methodology is based on the quantification of a solidified microstructure for its various phase fractions. This measured data is combined with well-established solidification models to yield undercooling temperatures of individual phases. The thermal history and undercooling of different phases in the solidified alloy are estimated for a wide range of cooling rates (from 0.5 K/min to 104 K/s). A detailed quantitative analysis of eutectic structures also reveals solidification conditions that yield optimum properties. To describe the methodology, dedicated samples of Al-Cu, Al-Cu-Sc alloys as well as Al-Si were solidified in a controlled manner under a wide range of cooling rates and undercoolings by Impulse Atomization, Electro-Magnetic Levitation, and Differential Scanning Calorimetry.

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OPTIMIZATION STRATEGIES FOR IDENTIFYING THE CONTROLLING MECHANISM FOR SOLID-STATE TRANSFORMATION IN FeCrNi DURING RAPID SOLIDIFICATION

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Ternary Fe-Cr-Ni steel alloys often exhibit a multi-step transformation known as double recalescence where primary ferrite converts to austenite during rapid solidification processes such as casting and welding. In addition to the volume free energy associated with undercooling between the phases, the free energy driving the transformation comes from two additional sources that are retained within the metastable solid – one from the primary phase undercooling and one from melt shear. A new physical model is proposed based on accumulation of defects, such as dislocations or tilt boundaries, and lattice strain. A dimensionless analysis technique shows that the free energy associated with metastable solidification is conserved and the contribution from melt shear can be predicted based on a modification of the Read-Shockley dislocation energy

equation. With these additional terms the incubation time between nucleation events becomes inversely proportional to the total free energy cubed for a grain boundary diffusion mechanism. In the case of the steel alloys studied, the grain boundary mechanism provides a better fit and when the model is applied the delay time behavior collapses to a single master-curve for the entire alloy family.

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NUMERICAL SIMULATIONS OF LIQUID STEEL ALLOYING IN THE THREE STRAND CONTINUOUS CASTING BLOOM TUNDISH

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The scientific aim of the present work is to obtain fundamental information on chemical homogenisation process of liquid steel with alloy additions in the tundish. For alloy feeding to liquid steel pulse step alloying method was applied. Author checked the effect of hydrodynamic conditions occurs in the internal working space of tundish on the process of alloy mixing with liquid steel. Within the work basic and proposed tundish equipments were considered. Numerical modeling technique was employed to demonstrate the process of alloy addition mixing during liquid steel flowed through the three strand bloom tundish. Ansys-Fluent computer program was used for numerical simulation. For particular continuous casting strand time mixing was calculated.

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TUNING MECHANISM FOR HETEROGENEOUS NUCLEATION OF METALLIC CRYSTALS

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For liquid metal, heterogeneous nucleation is main channel towards the formation of solid crystal. Fine tuning of nucleation means an optimized solidification structure, and consequently promises tailored properties for application. There are a few extensively used industrial practices for nucleation tuning, as AlTiB catalyzed grain refining in Al alloys, silicon modification for AlSi alloys, spheroidization of graphite in cast iron, and so on. In new energy storage area, the nucleation control is also important for high energy lithium-ion batteries. An unexpected nucleation of lithium leads to infinite relative volume expansion presenting low cycling efficiency and even safety hazards in batteries with lithium metal electrodes. The nucleation potential of a new crystal on substrate was believe to be a function of lattice misfit between new crystal and substrate as stated by conventional nucleation theory. But as we understood, solidification is a liquid/solid transition rather than solid/solid transition, thus the lattice misfit between two crystals are hardly to elaborate the real scenario of nucleation process. The state-of-the-art analytical techniques offer the opportunities tracking the atomic structural evolution adjacent to solid-liquid interface which makes the in situ observation on heterogeneous nucleation possible. Here we report up-to-date results on in situ observed heterogeneous nucleation of a few metals on different substrates. The results indicates that the nearest neighbor distance of liquid atoms and their coordination number can be tuned by the alloying element or substrate. The prenucleated ordering structures in the liquid have a tendency to be aligned in a preferred orientation, which is templated by the lattice structure of the substrate. This prenucleated ordering structure with preferred orientation will match the atomic structure of the substrate forming new crystals. That's the reason why the lattice mismatching, a parameter describing the matching of new crystal with substrate, is still able to predict the nucleation potential of the substrate in a given liquid. The alloying element can be used to tune the lattice mismatching at the interface through interfacial structural tuning to enhance heterogeneous nucleation in the liquid. This findings will extend the understanding on heterogeneous nucleation leading to more effective nucleation tuning

approaches in casting foundries, epitaxial growth of functional metal film or even more extensive application as energy storage area.

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DESTABILIZATION OF EUTECTIC LAMELLAE UPON RAPID SOLIDIFICATION OF UNDERCOOLED EUTECTIC Ni-Sn ALLOY: EXPERIMENTS AND MODELING

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Achieving a high undercooling prior to solidification ([U+25B3]T) is expected to be an effective strategy to significantly reduce lamellar spacing of bulk eutectic alloys which will be of great benefit to either mechanical or functional properties of eutectic alloys. However, the undercooled eutectic alloys usually exhibit coarse anomalous eutectic structure when [U+25B3]T exceeds a critical value. The formation mechanism of the anomalous eutectic structure has been a controversial issue and aroused intensive investigations since it was observed. In this work, we proposed that the formation of anomalous eutectic structure in undercooled bulk eutectic alloys is caused by the destabilization of eutectic lamellae during post-recalescence upon rapid solidification using a Ni-Sn system as example. First, we demonstrated that the lamellar structure is preserved by solidifying the undercooled alloy melt in a copper mould. Then, the destabilizing process of the as-preserved lamellar structure was observed in situ in a high-temperature laser scanning confocal microscopy which showed clearly that the non-equilibrium lamellar structure will subject to a rapid disintegration and granulation in semi-solid state at a temperature well below the melting temperature. On this basis, an analytical model within the framework of Rayleigh instability was established to analyzing the destabilization of the lamellar structure under this specific condition. It is indicated that the destabilization of the eutectic lamellae is driving by the interfacial energy and solute supersaturation and its kinetics is controlled by atomic diffusion along the interface. The present work is fundamentally helpful in understanding the formation of anomalous eutectic structure and tailoring microstructures of eutectic alloys.

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A NOVEL TECHNOLOGY TO PRODUCE HOMOGENIZED STEEL BY FORGING SOLIDIFYING METAL

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The manufacturing of special steel forgings normally follows the basic technical process from casting, homogenization annealing, pre-heating, forging and post-heat treatment after forging. Such treatment obviouly is high-cost, energy dissipation and long manufacturing cycle. In terms of the formation mechanism of internal casting defects such as macrosegregation, shrinkage cavity and coarse grains in large steel ingot, this study proposes a novel casting-forging integrated technology (CFIT), in which the solidifying ingot is forged before its complete solidification. It was found that composition and microstructure were both inhomogeneous when deformed by CFIT with a higher liquid fraction above 0.5, and even A circle-like C, Cr, Mo and V macrosegregation band appeared in the forging. In contrast, a uniform microstructure and mechanical properties were obtained at the liquid fraction of 0.3. Further, to obtain the appropriate liquid fraction of 0.2 before forging and the time period of individual step, the plant-wide numerical simulations of CFIT by the arbitrary Lagrangian-Eulerian method and three-dimensional thermo-mechanical analysis were carried out when foring the 19t 16Mn thread tightening ring in industry. It shows that the forging by CFIT has slightly higher strength and hardness, and comparable impact energy and plasticity compared with the traditional processes. More significantly, the current technology

presents highly economic, energy-conservation and short-period advantages in producing special steel forgings.

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STEPS IN BUILDING THE FOUNDATIONS OF MODERN SOLIDIFICATION SCIENCE BEFORE 1953

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The aim of this talk is to present the evolution of the important concepts that led to the modelling of solidification, before the landmark paper by Tiller, Jackson, Rutter and Chalmers in 1953 on constitutional supercooling, and how they influenced our present-day models. Before the relevant research on solidification could start it required the development of essential basic concepts. Important theoretical contributions during the 19th century were; on contact angle, capillary pressure, heat and solute diffusion, statistical mechanics, equilibrium thermodynamics, and solidification as a free boundary value problem. The most important experimental developments were; the optical microscope and observations of solidification of transparent organics, followed by the methods of directional solidification, the discovery of X-rays and their diffraction in crystals, the electron microscope, and the microprobe. On the ground of these developments some 25 scientists, mainly during the first half of the 20th century, created the foundations of solidification science, a field that will be presented in six topics. **Nucleation** theories began with condensation of a supersaturated vapour and were later applied to nucleation in metals. **Crystal growth** was analysed and the energetics of attachment evaluated. Non-equilibrium solute distribution (**segregation**) was modelled. **Morphological stability** was described, first qualitatively and later the concept of "diffusional undercooling" developed. Observations of growth of transparent salt **dendrites** led to the conclusion of a parabolic tip with side branches that ripen during solidification. The diffusion equation for the tip was solved in parabolic coordinates. **Eutectic** growth forms were examined and growth rates of transparent organics as a function of undercooling determined. A solution of the diffusion equation for coupled eutectoid growth was given. Finally Zener presented in his highly original 1946 paper a first complete theory for single-phase (plates) and two-phase (eutectoid) structure formation using a new criterion of growth at extremum in combination with approximate solutions of the diffusion problems. Zener's extremum criterion has been used during the following three decades before it was replaced by marginal stability. - Scientific research is done by people. The most influential authors in the field of solidification science before 1953 were, in order of the year of their contributions; Gibbs, Tammann, Volmer, Papapetrou, Scheil, Zener, Ivantsov, Turnbull. They all influenced in one or other way our modelling capabilities - the theories of Gibbs, Ivantsov and Turnbull being used still today.

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PREDICTION OF SOLIDIFICATION STRUCTURES IN A 9.8 TON STEEL INGOT

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The control of the carbon macrosegregation level in steel ingots is important for the structural integrity of the final component. Previous studies using the SOLID® multiscale modelling software [1] have shown that in order to obtain predictive results for the macrosegregation and the grain structure (CET, grain morphology) in steel ingots, a model needs to account for fragmentation of columnar dendrites as a source of equiaxed grains.
The goal of the present study is to determine constitutive fragmentation laws that can be used in process scale models of ingot casting. These laws give the flux of fragments from the columnar zone. The fragments are generated at the surface of columnar structure and are then swept into

the bulk liquid, where they can grow or remelt depending on local conditions. The surviving fragments then become equiaxed grains that settle on the bottom of the casting, leading to the columnar to equiaxed transition. The fragmentation laws were determined with the help of experimental data from four heavy steel ingots cast by ArcelorMittal Industeel, with weights from 9.8 to 179 metric tons. The macrosegregation and the grain structure observed on the cast ingots were used to identify the fragmentation laws. With the appropriate fragmentation laws, the model can then be used to explain the formation of the observed structures. For example, we show that the structural transitions, first from columnar to equiaxed globular and then to equiaxed dendritic at the bottom of the ingots are a consequence of the concurrent transport and growth of the dendrite fragments from the columnar zone.
References

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PRIMARY DENDRITE TRUNK DIAMETER IN Al-7wt% ALLOY DIRECTIONALLY SOLIDIFIED ABOARD THE INTERNATIONAL SPACE STATION

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Under a NASA-ESA (European Space Agency) collaborative research project, MICAST (Microstructure formation in casting of technical alloys under a diffusive and magnetically controlled convection conditions), three Al-7wt% Si samples (MICAST-6, MICAST-7 and MICAST 2-12) were directionally solidified aboard the International Space Station to determine the effect of mitigating convection on the primary dendrite array. About 25-cm long 7.8-mm diameter cylinders, machined from [100] oriented terrestrially grown dendritic Al-7Si samples, were inserted into alumina ampoules kept within the Sample Cartridge Assembly (SCA) inserts of the Low Gradient Furnace (LGF) for MICAST-6 and MICAST-7 and in the Specimen Quench Furnace (SQF) for MICAST2-12. The feed rods were partially re-melted in space and directionally solidified by withdrawing the furnace with respect to the SCA; their un-melted solid portions at one end acting as [100] oriented seed. For MICAST-6 the withdrawal speed was 5 um s-1 for 3.75-cm, and then 50 um s-1 for rest of the 11.2 cm long melt. For MICAST-7 it was 20 um s-1 for 8.5 cm and then 10 um s-1 for the rest 9 cm. For MICAST2-12 it was 40 um s-1 along its entire 11 cm long melt column. The thermal gradient at the liquidus temperatures varied from 22 to 14 K cm-1 during growth of MICAST-6, from 26 to 24 K cm-1 for MICAST-7, and from 33 to 31 K cm-1 for MICAST2-12. Microstructures on the transverse sections along the sample length have been analyzed to examine the growth-speed dependence of the trunk-diameters of the primary dendrite arrays during steady-state growth, and also during the transients following the speed changes. The observed primary dendrite trunk diameters during steady-state growth of MICAST samples show a good agreement with predictions from a coarsening based model developed by the authors. The MICAST samples grown at 10, 20, 40 and 50[U+F06D]um s-1 did not show the radial macrosegregation observed in the terrestrial grown MICAST equivalent Al-7Si samples. The trunk diameters in the terrestrial grown equivalent samples were larger than those predicted from the model. This suggest that “steepling” type thermosolutal convection increases the trunk diameter of primary dendrites, perhaps by increasing their tip radius.

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STUDY ON MICROSTRUCTURES, GROWTH ORIENTATION AND MECHANICAL PROPERTIES OF DIRECTIONALLY SOLIDIFIED Mg-14.61Gd ALLOY

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Microstructures, growth orientation and the room temperature mechanical properties of Mg-14.61Gd alloy were investigated by using directional solidification technology and CAFE simulation method under G=30K/mm and v=10-200μm/s. The experimental alloys were mainly consisted of primary α-Mg phase and (α-Mg+Mg5Gd) eutectic phase under all the growth conditions, which is consistent with the calculated results by Scheil model. It was found that α-Mg primary phase presented unidirectional dendritic morphologies on longitudinal cross-section, the growth interface appearance of α-Mg changed from the protruding forward growth to the flat growth gradually and the dendritic arm spacing decreased gradually with the increasing v. When v increased from 10 μm/s to 100 μm/s, the main growth orientation of α-Mg changed from <11-20> and <10-10> to <11-20> , and the deviation angle (ϑ) from solidification heat flow direction reduced from 11.070° to 5.711°, the reason for this lied mainly in the change of the heat flux. Further increasing v up to 200 μm/s, the main growth direction of α-Mg was still in <11-20>, but the value of ϑ increased to 10.620°, and the anisotropy of the crystal was the dominant factor then. It was proved that the CAFE numerical simulation model could predict the grain structure and growth orientation reasonably for Mg-alloy. In addition, the intrinsic mechanism between microstructures, growth orientation and mechanical properties was also discussed. KEY WORDS Mg-Gd alloy, directional solidification, CAFE model, growth orientation, mechanical properties

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LEVEL-SET MODELLING OF LASER BEAM MELTING PROCESS APPLIED ONTO CERAMIC MATERIALS - COMPARISON WITH EXPERIMENTAL RESULTS

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In recent years, significant progress has been achieved in additive manufacturing processes. Among these technologies, large attention has been generated for Laser Beam Melting (LBM). This process provides the possibility to develop parts of complex geometries with well-suited mechanical strengths. It is also able to develop pieces on a wide range of metallic and non-metallic materials and meets the needs of industries in many applications. Consequently, an interest appears in recent years for its application on ceramic for aeronautical applications due to the well-known creep strength of these materials at large temperature.

However, porosities and cracks may also develop on such materials depending of process parameters. Theses defects and theirs consequences limit the progress in LBM technology and highlight the need to propose optimized manufacturing strategy. In this approach, a level-set modelling is developed and applied on alumina powders in order to simulate tracks development [1]. Thermo-mechanical evolution of material is investigated in both liquid and dense domains. Fluid flow evolutions in the melt pool are also presented considering the effects of surface tension and Marangoni forces [2]. The same resolution gives access to the velocity field at the liquid/gas interface to estimate track shape. In addition the mechanical resolution is also achieved considering a well-suited constitutive law depending from local temperature in the solidified domain. The influence of laser

power, scanning velocity and physical properties of materials on track development is investigated and discussed.
As a complementary part, experimental observations are presented [3]. The volumetric heat source parameters used in simulations are calibrated with an analytical model also considering original reflectance measurements. Comparisons of melt pool dimensions and shapes between simulations and experiments validate the model. A coherent evolution of the track morphology when varying the heat source parameters or material properties is shown. Balling effect is also highlighted when scanning speed is increased and explained through the simulations.
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MACROSEGREGATION FORMATION AND CONTROL IN BEARING STEEL VIA NUMERICAL SIMULATION AND EXPERIMENTAL CHARACTERIZATION

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Chemical inhomogeneity and inclusions are the most severe defect types in bearing steel which have great influences on the ingot quality and final product properties. Based on a series of full-dissections of steel ingots varying with composition and weight, numerous experimental characterizations by SEM, EPMA, TEM, ASPEX and 3D Micro-CT techniques and multi-scale simulations, a new driving force, inclusion flotation, has been discovered to drive the formation of solutal macrosegregation, especially channel segregation. Sufficient populations of light oxide-based inclusions with appropriate size are able to alter the local flow pattern and destabilize the mushy zone, consequently dominating the channel segregation formation. Accordingly, a significant concept to control the macrosegregation in practice is the low-oxygen purifying treatment of the melt and inclusion modification, such as via Rare earth addition. Actually, even with a highly low proportional of RE's additions in industrial-level 100Cr6 bearing steel ingots, inclusions can be effectively modified into smaller and much more compatible RE-O-S type with Fe matrix, and over 60% large-size inclusions beyond 5 μm disappear, avoiding the growth of large-size MnS/Al2O3. In addition, the small density contrast between RE-O-S inclusions and steels also leads to a slow flowing among inter-dendritic regions. These two factors reduce and even eliminate channel segregation, and also lower the global macrosegregation extent significantly. The magic of RE treatment on segregation control has been widely verified and applied in other special steels of mould, gear and nuclear power component. Besides, the appropriate casting process and optimized ingot design are also significant factors to reduce macrosegregation in bearing steel. For instance, the higher superheat degree above 40 oC induces the longer solidification time and stronger interdendritic natural convection; meanwhile the decrease of the local cooling rate coarsens the dendrite arm, consequently elevating the mushy zone permeability. Obviously, both the large density difference and coarse microstructure provoke the severity of macrosegregation. On the other hand, the larger height, narrower shoulder width and the smaller taper in the riser are beneficial to shifting the hot spot and the maximum segregation value from the ingot body towards the riser top. In summary, the current study highlights the importance to produce super-homogenized bearing steel by jointly purifying the steel melt, modifying the inclusions, lowering superheat degree and ideal hot-top design.

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MULTISCALE MATHEMATICAL SIMULATION STUDIES ON THE 3-D MORPHOLOGY AND ORIENTATION

SELECTION MECHANISM OF MAGNESIUM ALLOY DENDRITE

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The 3-D morphology, orientation selection and behind mechanism of magnesium alloy dendrite were investigated by performing multiscale mathematical simulations. The results showed that the α-Mg dendrite prefers to grow along <11-20> basal direction and <11-23> nonbasal direction, and the resultant 3-D dendritic morphology exhibits a typical 18-primary branch pattern. Such dendritic microstructure formation was found to be associated with the surface energy anisotropy in light of the hexagonal-close-packed (hcp) lattice structure of the α-Mg dendrite. An anisotropic function model describing the α-Mg dendrite growth was developed by combining the observed 3-D growth pattern, the spherical harmonics, and the calculated anisotropic strength via DFT-based atomistic simulations. Accordingly, the dendritic growth behavior and morphological evolution were further investigated by coupling the anisotropy function with the phase-field model. The simulated results on the 3-D dendritic morphology agreed well with those reconstructed from X-ray tomography experiment. Our investigations provides a deep understanding on the growth behavior of magnesium alloy dendrite from phenomenological descriptive picture to a more intrinsic predictive way.

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LARGE-SCALE MULTI-PHASE-FIELD SIMULATION OF POLYCRYSTALLINE GRAIN GROWTH WITH ANISOTROPIC GRAIN BOUNDARY PROPERTIES

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Grain growth, a competitive growth of crystal grains that occurs after or simultaneously with solidification, is one of the most important phenomena in controlling the microstructure of polycrystalline materials. The fundamental process underlying grain growth is the migration of grain boundaries; thus, the growth behavior is largely dominated by the properties (energy and mobility) of grain boundaries. In real materials, these properties usually exhibit strong anisotropies depending on the boundary structures. Over the past few decades, many researchers have attempted to elucidate the effects of the anisotropies of the boundary properties on grain growth by performing numerical simulations. However, conclusive knowledge is not yet established especially for three-dimensional systems, mainly due to the limitations in the computational accuracy of the grain growth models and computer resources that have been employed so far. To address the above issues, based on the multi-phase-field (MPF) grain growth model [I. Steinbach and F. Pezzolla, Physica D (1999) 385], this study proposes a novel numerical scheme to accurately handle the anisotropic grain boundary properties. Furthermore, the MPF simulations are drastically accelerated by parallelizing multiple graphics processing units (GPUs) on a GPU-rich supercomputer. Using these techniques, we perform a series of large-scale simulations on anisotropic grain growth, through which the effects of the anisotropic grain boundary properties on the growth behaviors are elucidated in detail.

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MULTISCALE MODELING OF DENDRITIC GROWTH USING THE DENDRITIC NEEDLE NETWORK APPROACH: RECENT DEVELOPMENTS AND FUTURE DIRECTIONS

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In this talk, we will review recent developments using the multiscale Dendritic Needle Network (DNN) approach for dendritic growth, with a particular emphasis on its application to convective transport in the liquid phase. The DNN method was developed for the modeling of dendritic growth of hierarchical needle-like dendritic crystals, which typically form at low solute supersaturation or undercooling that are common to a host of solidification processes. It retains a good accuracy for a numerical space discretization about one order of magnitude larger than what is typically required in phase field simulations. By not tracking complex morphological details of the solid-liquid interface, the DNN method allows a scaling-up of phase-field with quantitative simulations orders of magnitude faster, while still tracking the transient growth competition of individual dendritic branches in each grain at the larger scale of heat and mass transport.
After briefly summarizing key aspects of the method, we will illustrate validations of the model in 2D and 3D, including quantitative predictions of microstructural features measured in directional solidification experiments, and critical quantitative comparisons with other multiscale approaches for dendritic growth. We will demonstrate the applicability of the model for fluid flow in the liquid phase. We will show that quantitative predictions comparable to those from phase-field simulations can be achieved, hence opening the way to macro-scale simulations with experimental/processing relevant transport conditions, e.g. accounting for gravity-driven buoyancy. We will offer a critical assessment of the DNN approach, of the investigations it makes possible, of its current limitations, and of the resulting next developments in order to address more complex mechanisms in dendritic growth. We will present ongoing work, challenges, and perspectives on the effect of buoyancy in constrained directional solidification, and on further coupling with micro-mechanical modeling, i.e. crystal plasticity, in order to link processing, microstructures, and properties.

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PHASE FIELD STUDY OF SPACING EVOLUTION DURING WIRE AND LASER ADDITIVE MANUFACTURING UNDER TRANSIENT CONDITIONS

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Wire and laser additive manufacturing (WLAM) is a potentially disruptive manufacturing technique in which large metallic materials can be fabricated layer by layer. Understanding the dynamic evolution of primary cellular/dendritic spacing in the laser melt pool is significant from a technological viewpoint because primary spacing is one of the foremost parameters that control the final mechanical properties of additive manufactured products. In this work, a multi-scale computational framework that couples FEM and a developed quantitative phase field method is employed to simulate the evolution of microstructure and primary spacing of a nickel-based superalloy during WLAM solidification. Transient conditions in the laser melt pool are considered in which both temperature gradient G and pulling speed V are made time-dependent. Through the use of this model, the dendrite morphology, tip velocity and spacing evolution during the solidification are investigated to provide the relationship between the laser processing parameters and the final spacing. The spacing evolution under transient conditions is related to the instantaneous interface velocity. According to the tip velocity field, the cellular/dendrite growth can be divided into three stages: the planar growth stage, the initial competition stage and the short-term stable stage. The simulated average primary spacings display a gradual transition period from one spacing range to another in the short-term stable stage which is consistent with the experimental work conducted by Losert et.al. In addition, effects of the laser processing

parameters on the primary spacing are investigated. Results show that when the same laser scan speed is given by 10 mm/s and the laser power ranges from 1.5 KW to 3 KW, the primary spacing increases with increasing the laser power. While when the same laser power is given by 2 KW and the laser scan speed ranges from 4 mm/s to 10 mm/s, the primary spacing decreases with increasing the laser scan speed. Moreover, primary cellular/dendritic spacing predicted by this multi-scale model agrees well with experimental results. This work provides meaningful understanding of spacing evolution in nickel-based superalloy and demonstrates the potential of controlling the complex microstructure morphologies and final primary spacing during wire and laser additive manufacturing.

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EFFECT OF COOLING RATE ON THE POROSITY DEFECT IN THE THICK ALUMINUM CASTING BY 3D COMPUTED TOMOGRAPHY ANALYSIS

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In the present study, effect of cooling rate on the formation of the porosity in the thick aluminum sand casting was investigated. Nowadays large scale thick aluminum casting replaces steel frame for vacuum chamber compartments in the semiconductor factory, with the consideration of weight and cost reduction. Aluminum casting specimens and real large castings were manufactured using chill with temperature measurements. The castings were inspected by using 3D computed tomography in order to quantify the porosity defect density in the castings. Effect of the thickness of the chill on the porosity defect density were also discussed.

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SEMI-GRAND CANONICAL MONTE CARLO SIMULATION FOR DERIVATION OF THERMODYNAMIC PROPERTIES OF BINARY ALLOY

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Solid-liquid interfacial properties of Fe-Cr alloy are investigated by molecular dynamics simulation using an EAM potential. First, solidus and liquidus compositions with respect to temperature were estimated as follows. The solid-liquid coexisting system with the same concentration as the initial state was relaxed under the constant pressure and temperature (NPT) condition. Calculations were carried out until the propagation of the solid-liquid interface due to solidification and solute partition did not proceed. It is considered that converged concentrations in solid and liquid phases correspond to the equilibrium concentration at the set temperature. Therefore, the same calculations were performed for various temperatures. By connecting solidus and liquidus concentrations with respect to temperature, the phase diagram for the Fe-Cr alloy for the EAM potential was successfully derived. Next, a solid-liquid coexisting system with equilibrium concentrations in the obtained phase diagram are relaxed at various temperatures to investigate the temperature dependence of the velocity of the solid-liquid interface. The interfacial velocity became very slow near the equilibrium temperature due to the solute drag effect, whereas the interfacial velocity increased rapidly at the temperature far from the equilibrium one by the solute trapping effect. From the slope of the interfacial velocity with respect to temperature, the kinetic coefficients were estimated for both regions of solute drag and solute trapping. Moreover,

a solid-liquid coexisting system with equilibrium concentrations in the obtained phase diagram are relaxed at various temperatures and the atomistic configuration of the solid-liquid interface are obtained. Using these atomistic configurations, the dependence of Cr concentrations on the solid-liquid interfacial energy are investigated by the capillary fluctuation technique. It is significant in this study to reveal the solid-liquid interfacial properties including the effect of solute redistribution at the interface.

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MOLECULAR DYNAMICS SIMULATION OF THE HETEROGENEOUS NUCLEATION VIA GRAIN REFINER INOCULATED IN ALUMINIUM MELT

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Since many of metallic materials are formed through solidification from the undercooled melt, it is indispensable to control the nucleation at the initial stage of solidification. In actual material production processes, heterogeneous nucleation is often promoted by inoculating grain-refiners in the melt. In this study, the effect of grain-refiners of Ti and Ti3Al solid particles on the heterogeneous nucleation of the Al melt with are investigated by the molecular dynamics method simulation.
It was confirmed from the simulation that the nucleation conditions were correlated with the size of grain-refiner and the degree of undercooling. That is, the larger the size of refiner added, the smaller undercooling was for the threshold of the nucleation. The effect of surface orientation for the grain-refiner on the nucleation was also examined. The FCC phase of Al was nucleated from the (0001) plane of the grain-refiner, which is the same as the (111) plane of the FCC phase. On the other hand, a small amount of HCP phase of Al was nucleation on the other planes: (10-10) and (11-20) planes. Then, previously nucleation FCC Al on the (0001) plane went around in front of the HCP Al on (10-10) and (11-20), and, eventually the FCC became dominant in the entire system. In order to discuss this phenomena, the kinetic coefficient of Al was derived from the temperature dependency of the solid-liquid interfacial velocity. The kinetic coefficient of Al at the (0001) plane was larger than the other planes.

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STUDY OF NUCLEATION AND GROWTH IN RAPIDLY SOLIDIFYING Al-Ni ALLOYS

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Experiments on the International Space Station (ISS) lead to the idea of a special growth mechanism in Al-rich Al-Ni melts. Previous analyses of dendrite growth velocity as a function of undercooling in these alloys showed anomalous behaviour, particularly a decreasing velocity for increasing undercoolings [1]. The experiments on the ISS reproduced the results obtained on earth but with an unprecedented clarity. During rapid solidification, the visible growth front does not consist of dendrite tips that grow along the surface of the sample, but is formed by a sequence of nucleation events propagating perpendicularly to the actual dendrite growth direction. The front progression is thus a superposition of growth of existing surface nuclei and

new nucleation events in the vicinity of the existing nuclei. Microstructure analysis strongly supports the theory of this growth mechanism. It shows dendrites growing towards the sample centre and provides clear evidence of nucleation at the sample surface. However, the question concerning the anomalous behaviour (slower apparent growth with higher undercoolings) is not yet fully answered by the nucleation mechanism. For this, a time resolved analysis of nucleation and surface growth is presented to investigate the relation between the nucleation rate, front propagation and undercooling.

Acknowledgements

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OBJECTS INTERACTING WITH SOLIDIFICATION FRONTS: FROM MATERIALS SCIENCE TO GEOPHYSICS AND BIOLOGY

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The ice-templating of porous materials has received a great deal of attention during the past few years. This simple process, where a material suspension is simply frozen and then sublimated, provides materials with unique porous architectures, where the porosity is almost a direct replica of the frozen solvent crystals. The basic principle of ice-templating is the assembly of a second phase, usually particles, triggered by their progressive concentration increase in the inter-crystal space. This concentration mechanism can be used to induce ordering or self-assembly of various types of building blocks between the ice crystals, providing thus materials with an increasingly elaborate architecture with improved functional properties. I will present first a few examples of such materials and phenomena investigated in our group.
The interaction of objects with a moving solidification front is however a common feature of many industrial and natural processes such as metal processing, the growth of single-crystals for photovoltaics and microelectronics, the cryo-preservation of cells, the formation of sea ice, or the preparation of frozen food. Solidification fronts interact with objects with different outcomes, from the total rejection to the complete engulfment of objects. Being able to understand and control the solidification dynamics and microstructure is of primary importance in these domains. I will discuss how the recent developments in the lab with cryoconfocal microscopy may help us make progresses in these domains and revisit some of these old but still relevant problems.

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INFLUENCE OF SIDE ARCS ON THE SOLIDIFICATION OF A VAR INGOT

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Secondary metallurgical processes such as Vacuum arc remelting (VAR) are extensively used for production of metal ingots with superior quality. The complex VAR process involves a wide range of physical phenomena including heat transfer with phase change (solidification/melting), Plasma arc, and the interplay between flow and electromagnetic field known as magnetohydrodynamics (MHD). The spatial and temporal distribution of the arc has a significant influence on the energy and electric current supplied to the ingot top surface. Thus, the evolution of the ingot is to a great extent controlled by the behavior of the arc. During the process, a notable fraction of current (˜ 50%) in the vacuum region is transferred directly between the electrode and mold without flowing through the ingot known as "side-arcing". The latter influences the electric current path in the whole system that in turn determines the hydrodynamics in the molten pool. Of note, the flow in the molten pool is driven by buoyancy, and self-induced electromagnetic force. Therefore, the amount of current which flows through the molten pool impacts the strength of the electromagnetic force that in turn determines the quality of the final ingot. Most often, the quality of the ingot is characterized by the shape of melt pool, i.e., the depth and thickness of mushy zone. The desired outcome of the VAR is a shallow melt pool that promotes unidirectional (upwards) solidification of the ingot and consequently formation of segregation-minimal alloy. The degree of macrosegregation is dependent on the slope of the solidus/ liquidus isotherms that in turn is related to the mushy zone depth. In fact, deep mushy zone results in a severe macrosegregation and subsequently inadequate mechanical properties, cleanliness, and yield. Therefore, the melt pool profile is often used as an indicator of the internal quality of the ingot. Generally, experimental analysis and measurements are quite difficult during the operation at the elevated temperature (˜ 2000 K) of the process. Therefore, simulation tools can be applied to obtain a deeper knowledge of the VAR process. In this paper, a numerical study is performed to investigate the effect of "side arcs" on the pool profile of the VAR ingot. A series of simulations are performed considering different amount of "side arcs" (e.g. 20%, 50%, and 70%). Details of the analysis of the electric current, flow, and thermal/solidification fields are presented.

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THERMO-ELASTO-VISCOPLASTIC CONSTITUTIVE LAWS FOR SEMI-SOLID ALLOYS DURING THEIR SOLIDIFICATION

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During solidification metallic alloys undergo a continuous transition from the liquid to the solid state. At first, solid dendrites growth and are free to move in the liquid matrix. In this case, the alloy can be considered as a suspension. As solidification progresses, interactions between dendrites occur and the mush develops shear strength due to dendrite entanglement. For higher solid fractions, dendrites interlock, solid skeletons are built and the mush reaches mechanical coherence. At that state, the solid skeleton densifies under external pressure (expelling liquid) or dilates under tensile loading (draining liquid). Toward the end of solidification, solid grains starts to coalescence and liquid feeding drops drastically. The complexity of the solid-liquid interactions at the micro-scale at each solidification state makes their characterization and rheological modeling difficult and delicate. Our aim is to develop for each semi-solid regime (coherent and non-coherent) a specific constitutive law depending on microstructural features like fraction solid and grain size, which are extracted from a coupled multi-phase field simulation of the microstructure evolution [1]. This way, equiaxed solidification can be distinguished from directional one. These simulations show also that, due to undercooling and recalescence phenomena, the temperature is not unique in the mushy regime and thus the developed constitutive laws have to be formulated in function of fraction solid instead of the temperature. The effective thermoelastic properties of the mushy zone are derived by homogenization of the simulated microstructures [1]. In addition, the nonlinear behaviour of the coherent semi-solid phase on the macro-scale is described by an original single surface viscoplastic flow potential that includes micro-structural parameters and takes the internal cohesion of the solid skeleton into account. The variation of the cohesion with the fraction solid is described either by a simple law or by a loading dependent evolution law [2]. The proposed

viscoplastic potential takes the effect of isotropic and kinematic hardening, pressure dependence of yielding and the strength difference in tension and compression of the coherent semi-solid state into account. For the non-coherent mushy state, presenting some shear resistance, a simplified viscoplastic potential is adopted. It neglects kinematic hardening and pressure effects on the solid dendrites and describes large plastic flow under shear loading. The continuity condition at mechanical coherence allows us to reduce the additional microstructure parameters for the non-coherent regime to one. The developed constitutive laws are then implemented in a finite element casting simulation tool, which allows us to identify the model parameters for an A356 aluminium alloy by simulating uniaxial tension, compression or pure shear experiments [3].
The financial support from the DFG in the framework of the collaborated research center SFB1120 is gratefully acknowledged.
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ON THE IMPROVING OF HOMOGENEITIES ON HEAVY INGOTS

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The inhomogeneity in large ingots not only decides the final properties of the product, but also restricts downstream hot working processing severely. It is very important to improve the homogeneity of ingots for saving energy, improving material utilization ratio, increasing performance of component, and the construction of key equipment.
In this research, the evolutions of general inhomogeneity problem in large ingots, such as macrosegregation, inclusion, shrinkage porosity, and large crystal in the subsequent hot working processing have been discussed, based on which the concept of homogeneity window for large ingots has been proposed.
Three fundamental reasons triggered the inhomogeneity of ingots were concluded, i.e. the uneven cooling rate, the uncontrollable multiphase flow, and the solute redistribution during solidification. Aiming at these three fundamental reasons, casting method called Layer Casting (LC), which has been proposed recently by our team, was introduced to modify the serious inhomogeneity problem in large ingots. In this method, molten alloy was poured into the mold separately and layer upon layer. As soon as the poured molten alloy solidified to a critical volume fraction range, the next layer amount of molten alloy was poured into the mold. For each layer, the mass, composition, and pouring temperature of poured molten alloy could be artificially designed and controlled. A comprehensive control model has been established, which can design the optimal casting parameters, including pouring temperature, time, composition, and mass for each layer, based on the target homogeneity requirement. Both experiment and numerical simulated results shown that LC method can significantly decrease the uncontrollable multiphase flow, uniform the cooling rate, and improve the solute redistribution, subsequently, improve the homogeneity of ingots. Its wide application prospect for high quality large ingots is expected.

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PHASE-FIELD SIMULATIONS ON MORPHOLOGICAL CHANGE OF DENDRITE WITH DIFFERENT PREFERRED GROWTH DIRECTIONS

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The preferred growth direction of crystal in solidification of metallic materials is mainly determined by anisotropy of solid-liquid interface energy, g(n), where n represent the crystallographic orientation normal to the solid-liquid interface. The anisotropy of g(n) is described by anisotropy parameters e1 and e2 that characterize <100> and <110> growth, respectively. Effect of e1 has been considered in most of phase-field simulations for dendritic growth in metallic alloys which have a cubic crystal such as fcc and bcc, because the preferred growth orientation in cubic crystals has been supposed to be <100>. However, it was reported that the preferred growth direction of Al-Zn alloy, which has fcc structure, changes from <100> to <110> with an increase in Zn concentration [T. Haxhimali, A. Karma, F. Gonzales and M. Rappaz, Nat. Mater., 2006(5), 660.]. This phenomenon implies that anisotropy parameters depend on solute concentration. The morphological change of dendritic structures with transition in the growth direction of Al-Zn alloy was investigated in detail by phase-field simulations [J.A. Dantzig, P.D. Napoli, J. Friedli and M. Rappaz, Metall. Mater. Trans. A, 2013(44), 5532.] and several important findings were reported in the early work. A further investigation should be aimed at investigating effects of solidification conditions and type of alloy systems on the morphological change. Therefore, in this study, we conducted quantitative phase-field simulations to clarify the morphology of dendrites for different sets of e1 and e2 systematically. Also, effects of several factors such as degree of undercooling and temperature gradient in different alloy systems were investigated.

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ELEMENTAL ADSORPTION AT THE LIQUID/OXIDE INTERFACE IN ALUMINIUM ALLOYS

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Grain refinement of aluminium alloys has always been desirable in foundries. It is a common practice to add grain refiners into the alloy melt to promote heterogeneous nucleation and hence achieve effective grain refinement. However, the efficiency of commercial grain refiners is extremely low as less than approximately 1% of the added particles initiate aluminium grains during solidification while the rest remain inactive and stay in the final castings. These particles become inclusions when the castings are recycled and the effect accumulates with repeated recycling. Recently, it has been demonstrated that the native oxide particles can be utilised for effective grain refinement in aluminium alloys. This holds great promise to achieve grain refinement without the addition of grain refiners and provides a solution to produce closed-loop recyclable aluminium alloys. Nevertheless, further investigation is still needed for commercial aluminium alloys, which normally contain certain levels of alloying and impurity elements. One of the major reasons is that it is unclear how these solute elements affect heterogeneous nucleation, particularly the potency of nucleation substrates. Most recently, it has been found that the adsorption of solute elements onto the surface of nucleant particles plays a significant role in affecting the effectiveness of these particles acting as nucleation sites for aluminium grains. Therefore, it is intriguing to study the potential elemental adsorption on the surface of native oxide particles in aluminium alloys. In the present work, the potential element adsorption onto the surface of native oxide particles has been investigated by analytical transmission electron microscopy on samples prepared using a melt filtration technique. Using selected area diffraction and high-resolution imaging, the crystal structure and the habit plane of the native oxide particles has been firstly determined. Furthermore, the potential elemental adsorption at the interface between oxide particles and Al grain matrix has been studied by using super scanning transmission electron microscopy combined with electron energy loss spectroscopy. Based on the experimental results, the nature of the elemental adsorption in terms of composition and structure has been

analysed using a simple lattice matching model. Finally, the effect of elemental adsorption on the nucleation potency of oxide particles and hence on their role in solidification will be discussed.

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THE EFFECT OF NUCLEANT PARTICLE AGGLOMERATION ON THE EFFECTIVENESS OF GRAIN REFINEMENT BY A CELLULAR AUTOMATON APPROACH

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Grain refinement of metallic alloys is of critical importance to minimize the risk of solidification defects and obtain the desired mechanical properties. The effectiveness of grain refinement depends strongly on the interplay between potency of nucleant particles for heterogeneous nucleation and their ability for grain initiation. For a given alloy, the former is an inherent property of the nucleant particle while the latter is strongly dependant on the size, size distribution and spatial distribution of the nucleant particles. Through analytical and numerical modelling, it has been shown recently that agglomeration of the nucleant particles has a strong influence on their grain initiation behaviour, and is largely responsible for the discrepancy in grain size between theoretical predictions and experimental measurements. In this work, a cellular automaton model is used to investigate the effect of nucleant particle agglomeration on the effectiveness of grain refinement. The spatial distribution of nucleant particles is modelled by a log-normal distribution and the mean particle spacing is used to represent different levels of particle agglomeration. Other variables include alloy composition, particle size, size distribution and number density.

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MICROSTRUCTURAL EVOLUTION DURING MULTICOMPONENT EUTECTIC SOLIDIFICATION IN THE Al-Cu-Si-Mg SYSTEM

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Our comprehensive understanding of binary eutectic solidification is largely due to years of extensive studies of many metallic and non-metallic systems. Recently, there has been increasing effort to understand ternary eutectic solidification due to the potential for refinement of microstructure resulting from increased number of co-existing crystalline phases during the solidification of multicomponent alloy systems. So far, our understanding of quaternary eutectic solidification is very limited. Recent research work at BCAST has revealed the existence of nanostructured anomalous eutectic regions within intercellular colonies of the lamellar eutectic mixture found in suction cast Al-28%Cu-6%Si-2.2%Mg (wt%) quaternary eutectic alloy, characterised by a combination of EDX, high resolution SEM and TEM techniques. This contribution presents detailed studies of the microstructure and chemistry of the cellular colonies of lamellar eutectic and nanostructured anomalous eutectic regions in the as-cast Al-28%Cu-6%Si-2.2%Mg (wt%) alloy, together with a description of the quaternary eutectic solidification behaviour in the Al-Cu-Si-Mg multicomponent alloy system.

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MULTI-GPU ACCELERATION OF THREE-DIMENSIONAL PHASE-FILED COMPUTATION FOR DENDRITE GROWTH WITH THERMAL-SOLUTAL CONVECTION

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Thermal-solutal convection necessary occurs during the terrestrial solidification of alloys. Thanks to the recent progress in the in-situ observation technique using X-ray radiography, the direct observation of dendrite growth under high temperature has been made possible. In the in-situ observation, however, it is difficult to see the liquid flow during the dendrite solidification. In order to clarify the physics occurred in the images obtained in the in-situ observation, it is essential to reproduce the same phenomenon by the numerical simulation. Although a phase-field method is the most powerful numerical tool to simulate the dendrite growth, the high computational cost is a drawback. Moreover, the computational cost of the phase-field simulation coupled with thermal diffusion, solute diffusion, and melt convection is quite expensive. Therefore, the most phase-field simulations of dendrite growth performed so far are limited to a single dendrite growth or dendrites growth in two-dimension. In this study, we develop a high performance computing scheme of the three-dimensional phase-field simulation for the dendrites growth with thermo-solutal convection. The computations are accelerated by a multi-GPU parallel computation in a GPU supercomputer, TSUBAME3.0 at Tokyo Institute of Technology. Then, we introduce the large-scale phase-field simulations of dendrite growth taking into account the thermal-solutal convection.

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NUMERICAL SIMULATIONS OF SOLIDIFICATION STRUCTURES AND MACROSEGREGATION BY A CELLULAR AUTOMATON MODEL COUPLED WITH FLOW CALCULATION

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A numerical model was developed to predict solidification grain structures and macrosegregation based on a three-dimensional cellular automaton finite different method coupled with flow calculation of natural convection and shrinkage flow. Direct simulations of grain growth and macrosegregation were performed using the numerical model. First, in order to confirm the effect of natural convection, simulations of unidirectional solidification cooled on the bottom surface of mold were performed at Al -10wt.%Mg alloy. Columnar grain structures have formed from the bottom to the top in alloy melt. During solidification, Mg-rich plumes rising in the melt were seen due to a subsequent upward flow, which caused by the thermosolutal buoyant force. Once the plume occurred in the melt above the mushy zone, the morphology of columnar grains varied and the grains became coarse. Mg-rich channels forming in the mushy zone were observed. Such region could delay solidification inside liquid-rich channels and results in a freckle defect. Examined the average Mg concentration profiles of the cross section from the bottom to the top, the negative segregation occurred in the middle of solidification and the positive segregation occurred at the end of solidification. From these results, it was confirmed that the proposed model was effective to predict the macrosegregation coupling with the grain structure formation. Next, in order to confirm the effect of shrinkage flow, the simulations in the condition formed the bridging of columnar grains like continuous casting were performed at Al-10wt.%Cu alloy. In the simulations, the bridging of columnar grains formed in the center of ingot during solidification, and then the positive segregation was generated in the region below the bridging. On the other hand, the negative segregation was generated in the region above the bridging. The primary factor of this macrosegregation was the shrinkage flow with the formation of bridging, and the degree of positive and negative segregation was enlarged by the presence of natural convection. As the results, it was confirmed that the shrinkage and the bridging of solidification structures played an important role for the formation of macrosegregation.

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MICROSEGREGATION AT GRAIN BOUNDARY IN A BINARY ALLOY BICRYSTAL ANALYZED BY PHASE-FIELD SIMULATIONS

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Microsegregation has a great influence on properties of materials such as mechanical and corrosive properties and it entirely depends on size and morphology of solidification microstructure. Although a number of efforts have been devoted to understanding and controlling of microsegregation in alloy systems, little has been clarified about microsegregation behavior at grain boundaries formed by growth of differently-oriented dendrites. Quantitative phase-field simulations have become one of the most powerful approaches for studying solidification phenomena and they have recently been employed in studies on competitive growth of dendrites in bi-crystal systems. Importantly, it is possible to analyze detail of microsegregation behavior using a quantitative phase-field model for two-sided asymmetric diffusion. In this study, therefore, we investigate microsegregation behavior at grain boundaries by means of two-dimensional quantitative phase-field simulations of directional solidification in bi-crystal systems. Our focus is placed on grain boundaries which are formed by two columnar dendrites; one is favorably-oriented (FO) dendrite and the other is unfavorably-orientated (UO) dendrites against the direction of temperature gradient. The microsegregation at the grain boundaries are investigated by changing the inclination angles of UO dendrite against the temperature gradient. The simulations are accelerated by using parallel computing on graphics processing unit (GPU) and by using moving frame scheme.

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THE EFFECTS OF TiC NANOPARTICLES AND COOLING RATE ON THE MICROSTRUCTURE OF Al-Cu AND Al-Mg-Si ALLOYS

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At present, the strength and toughness of Al alloys are still far from meeting the rapid development of the aerospace and automotive industries. Adding ceramic nanoparticles or increasing cooling rate can significantly refine the microstructure of Al alloys and improve the mechanical properties. In our work, an Al-TiC master alloy containing TiC nanoparticles was synthesized by combustion reaction, which was added into Al melt prior to permanent mold casting. Scanning electron microscopy was used to study the grain structure and constituent particles. The solidification process of Al-Cu alloys with/without nanoparticles was observed by in situ X-ray radiography. Results show that TiC nanoparticles could refine grains and constituent particles, promoting nucleation of α-Al and reducing the nucleation undercooling. The effect of cooling rate on the dendrite structure of Al alloy has also been studied. We found that the increase of cooling rate reduced the primary dendritic size and dendritic tortuosity. When the cooling rate was reduced, the coarsening of primary dendrites and secondary dendrites was significantly enhanced.

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PHASE-FIELD SIMULATIONS OF SOLID/LIQUID INTERFACE MORPHOLOGY AND THERMODYNAMIC PARAMETERS EVALUATION IN PERITECTIC STEELS

FOR THE CONCENTRIC SOLIDIFICATION TECHNIQUE USING HIGH TEMPERATURE LASER SCANNING CONFOCAL MICROSCOPE (HTLSCM)

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We have used high temperature laser-scanning confocal microscopy by utilizing a concentric solidification technique to observe in-situ and in real time solidification events and high-temperature microstructural development, with a special emphasis on high temperature phase transformations. However, the solidification and subsequent solid-state transformation kinetics, on both heating and cooling, are largely determined by the axi-symmetric and dynamically changing temperature profile within the cylindrical specimen, thereby hindering quantitative analysis. We have experimentally determined the temperature distribution and created a simulation domain whereby we can replicate almost exactly the concentric configuration. This combination of thermal analysis with numerical simulations assistance with 3D modeling has enabled us to develop a powerful technique to convert in situ observations into quantitative analysis. We are now able to characterize by numeric modelling, the pertaining solute distribution at different stages of solidification incorporating grain boundary diffusion and maintaining the same solute boundary layer thickness as in the experimental set-up. In the present study, we have carefully defined the domain prior to the solidification, and then compared the numerically calculated solid/liquid interface velocities with the experimental determined values in Fe-0.18C and Fe-4.2Ni alloys at cooling rates that varied from 2K/min to 200K/min. Peritectic reaction kinetics are compared with experimental results for the developed solute profiles at the solid/liquid interface and optimized mobility coefficient between δ/γ . Because we have experimentally determined the pertaining thermal gradients, it is possible to assess thermodynamic parameters at the solid/liquid interface and at triple points using Thermo-Calc. The agreement we obtained between simulation and experimental results, provided us with confidence that the technique can be extended to the quantitative prediction (calculation) of the fundamental thermodynamic parameters pertaining to the concentric solidification platform.
Keywords: Phase-Field simulations, peritectic reaction, solute segregation, interface kinetics

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MOLECULAR DYNAMICS SIMULATION OF NUCLEATION AND SOLIDIFICATION FOR ALLOY SYSTEMS

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We have performed the large-scale molecular dynamics simulations for nucleation, solidification and microstructure formation [1] and found various new insights such as the heterogeneity in homogeneous nucleation [2] and decrease of the averaged grain boundary mobility during the grain growth [3]. Although these studies were performed using pure metallic system for simplicity, the most of practical structural materials consists of alloys. Therefore, nucleation and solidification processes for various alloy systems are investigated by molecular dynamics simulation in this study. Regarding the homogeneous nucleation from undercooled melt of Ni-Al alloy, the B2 structure is directly nucleated from the undercooled melt of Ni-50mol%Al, whereas no specific compound is not nucleated but mixture of bcc and fcc phases appeared from Ni-25mol%Al. The heterogeneous nucleation in Al melt inoculated with Ti and Ti3Al particles as grain refiners are performed and the relationship between the particle size and the undercooled temperature needed

for the heterogeneous nucleation are discussed. The preferential facet of the hcp Ti surface for the heterogeneous nucleation of Al melt is also investigated. Moreover, interfacial properties such as the solid-liquid interfacial energy and the kinetic coefficient are closely examined for Fe-Cr system by focusing on the concentration dependence. Our cutting-edge results will be introduced in the presentation. [1] Y. Shibuta, et al. JOM 67 (2015) 1793. [2] Y. Shibuta, et al, Nature Comm. 8 (2017) 10. [3] S. Okita, et al., Acta Mater. 153 (2018) 108

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ESTIMATION OF PROPERTIES OF SOLID-LIQUID INTERFACE BASED ON DATA ASSIMILATION

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Computational simulations of solidification microstructures have contributed to understanding of time evolutions of complex morphologies of crystals in a variety of solidification processes. A phase-field method is an effective method in simulating the solidification microstructures such as a dendrite structure, a typical morphology of growing solid in solidification of metals. Importantly, accuracy of phase-field simulations is entirely determined by accuracy of input parameters for the simulations. In particular, accuracy of parameters for solid-liquid interfacial properties such as interfacial energy and its anisotropy strength are very important because such parameters directly affect the morphology of growing solids. However, it is not straightforward to determine interfacial properties with high accuracy by means of experimental methods. Methods such as capillary fluctuation method and cleaving technique have been developed to calculate the interfacial properties based on molecular dynamics simulations. Although these methods are very effective, these methods are applicable only to calculation of the equilibrium properties of solid-liquid interface. Since little has been clarified about non-equilibrium properties of interface, it is necessary to develop a method that can be applied to estimation of non-equilibrium interfacial properties as well as equilibrium one. In addition, it is highly desirable to develop a simple but accurate method for estimating the interfacial properties. In this study, data assimilation is applied to the estimation of interfacial properties at the solid/liquid interface during solidification of metals. The twin experiment was performed in order to investigate the effectiveness of data assimilation to the estimation of interfacial properties.

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PHASE-FIELD SIMULATION OF ABNORMAL GRAIN GROWTH IN CARBON STEEL

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After solidification, grain growth occurs in the metallic materials, in general. It is very important to understand grain growth as well as solidification in order to control the mechanical properties of metallic materials. Abnormal grain growth(AGG), in which some grains preferentially grow to be extremely large, often occurs during cooling and isothermal holding at high temperatures after the solidification. AGG is related to non-uniformity of secondary phase particles and/or change in their distribution with time. Since AGG degrades mechanical properties, it is necessary to elucidate the mechanism and condition for occurrence of AGG. The precipitates in matrix and also remaining liquid in solidification serve as the second phases associated with AGG and the size of such pinning particles is often much smaller than the grain size of the matrix. Phase-field models have been utilized for simulating pinning effects on grain growth. However, early models

cannot be applied to analysis of pinning effect and AGG when the pinning particle is very small compared with the grain size of matrix. This is because the pinning particles are explicitly described in the early models and hence the simulation of grain growth with very fine particles requires huge computational cost. Therefore, in this study, the pinning effects of particles are introduced in the phase-field model based on a mean-field approximation. The present model can reproduce the curvature driven motion of grain boundary with pinning force. Using this model, we investigate occurrence of AGG in carbon steels under various heat treatments.

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OBSERVATION OF BUBBLE AND INTERMETALLIC COMPOUND BEHAVIORS DURING HEATING Al-Mn ALLOY BY SYNCHROTRON RADIOGRAPHY

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We provide direct visualization of the microstructural evolution during heating Al-Mn alloy by synchrotron radiography. The bubbles vary gradually from irregular to subglobose and finally deform into spherical shape with increasing temperature. And some bubbles grow, while some others gradually became small or even all of them disappear during heating. There are two different reasons for bubble growth, bubbles aggregation and the hydrogen distribution around bubbles, while bubble annexation and hydrogen bubble dissolution result in reduction of bubble radius. Also, a logistic model can be used to describe the variation in the IMCs area with the time during heating.

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HETEROGENEOUS NUCLEATION BY STRUCTURAL TEMPLATING

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It has been recently realized that atomic ordering in the liquid adjacent to the substrate (i.e., prenucleation) has a significant implication on the subsequent heterogeneous nucleation process. In this paper, we report an atomistic mechanism of heterogeneous nucleation through structural templating. Using molecular dynamics (MD) simulation, we investigated the process of heterogeneous nucleation in a model system consisting of liquid Al and fcc substrates with <111> surface orientation and varied lattice misfit. We found that heterogeneous nucleation occurs at a critical undercooling, proceeds layer-by-layer through a structural templating mechanism and finishes by creating a template (i.e., a crystal plane), which permits further growth of the new solid phase. In most cases, Shockley partial dislocations with predominant screw component are generated in the second layer, leading to a twist of the new phase relative to the substrate. Our study indicates that the energy barrier is dependent on the density of the dislocation network, which is directly related to the lattice misfit. Further, we calculated interfacial energy of the liquid/substrate interface, which increases with increasing lattice misfit. We show that potency of a nucleant particle is directly relevant to the structural property, chemical nature and surface condition of the substrate.

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COMPOSITIONAL TEMPLATING FOR HETEROGENEOUS NUCLEATION OF INTERMETALLIC COMPOUNDS

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The understanding of heterogeneous nucleation of intermetallic compounds (IMCs) during solidification of engineering alloys is of both scientific and technological importance, and is particularly relevant to recycling. However, effective refinement of IMCs is currently limited by our poor understanding of their heterogeneous nucleation. In this contribution, we present out latest advance in the understanding of heterogeneous nucleation of Fe-containing IMCs in Al-alloys. First we demonstrate that heterogeneous nucleation of IMCs is difficult and therefore requires large nucleation undercooling. Our differential scanning calorimetry (DSC) measurements show that under normal solidification conditions the undercooling required for heterogeneous nucleation of IMCs is in the order of tens of Kelvin, and that the undercooling increases with increasing complexity of the stoichiometry of the IMCs. This is because nucleation of IMCs needs to create not only the correct crystal structure but also the correct elemental compositions. We then present our new approach to enhancing heterogeneous nucleation of IMCs by both structural templating and compositional templating. We show that chemical segregation of selected elements at the liquid/TiB2 interface can lead to significant reduction of nucleation undercooling and hence refinement of MMCs in Al-alloys.

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PRENUCLEATION ON OXIDE PARTICLES IN Al- AND Mg-ALLOYS FROM AB INITIO MOLECULAR DYNAMICS SIMULATIONS

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Prenucleation refers to the phenomenon of atomic ordering in the liquid adjacent to the liquid/substrate interface at temperatures above the nucleation temperature, which becomes the precursor for the subsequent heterogeneous nucleation process through structural templating. Understanding of prenucleation is therefore of both scientific and technological importance. Based on recent investigations of the effects of lattice misfit and chemical interactions on prenucleation, in this work we study atomic ordering adjacent to the surfaces of native oxides (alumina, magnesia) in Al and Mg melts, using a parameter-free ab initio molecular dynamics simulation (MD) technique based on the density-functional theory (DFT). Our modelling reveals that in liquid, the oxide surfaces exhibit a rich variety of 2D ordered structures containing various structural defects, depending on the structural nature of the substrate and chemical interactions between the substrate and the liquid metal. Formation of atomically rough substrate surfaces was observed on the oxide particles in both Mg and Al melts during the ab initio MD simulations. This atomic roughness of the substrate surface weakens prenucleation and reduces significantly the potency of oxide particles as substrates for heterogeneous nucleation.

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MACRO-MICRO COUPLED SIMULATION OF SOLIDIFICATION MICROSTRUCTURE DURING LASER ADDITIVE MANUFACTURING PROCESS

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Laser metal deposition is an additive manufacturing technique for fabricating complex metal components layer by layer. The complex thermal behavior during this process results in the complex microstructure evolution, which directly affects the final mechanical properties of the

products. Numerical modeling offers a cost efficient way to better understand the related complex physics in laser metal deposition process. It helps to reveal the effects of processing parameters on the desired characteristics of deposition parts. In this work, a heat transfer finite element model is coupled with a multi-phase-field model to predict the thermal behavior and solidification microstructure evolution during laser metal deposition process. The thermal behavior during single-track and multi-track deposition process was simulated numerically by using a three-dimensional transient finite-element model, where deposition of material was modeled through activation of a new set of elements within each solution step. The deposition geometry was well predicted without assuming a prior shape. The influences of the scanning speed and laser power on the morphology and dimensions of molten pool were investigated. It is found that the molten pool height decreases with the increase in the scanning speed, while the increase of laser power results in the increase of molten pool size. The temperature history extracted from the macro simulation was then transferred to a micro region inside the mushy zone of the molten pool, where dendrite growth during solidification was simulated by the multi-phase-field model. The effects of several process parameters on the solidification microstructures were investigated. Directional dendritic growth from the bottom of the pool was observed with various dendrite arm spacing and orientation depending on the location in the pool. The microstructure and the value of dendrite arm spacing obtained in simulation agree well with previous experimental observation.

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CHARACTERIZATION OF DENDRITIC GROWTH IN Fe-C SYSTEM BY USING TIME-RESOLVED X-RAY TOMOGRAPHY AND PHYSICS-BASED FILTERING

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This paper demonstrates time-resolved and in-situ tomography using synchrotron radiation X-rays in SPring-8. Voxel size of reconstructed image was approximately 6.5 μm x 6.5μm x 6.5μm and time resolution was 0.5s - 4s (2rps - 0.25rps). Convolution back-projection (CBP) image reconstruction was typically performed using 200 transmission images. The technique was applied to observe dendritic structure in Fe-C alloys. Dimension of specimen was approximately 1mm in diameter and 5mm in length. The specimen was once melted in a vacuum chamber (0.1-1Pa) and was cooled at a constant cooling rate (5-30K/min). Dendrites was reconstructed even without image processing. However, it was rather difficult to trace S/L interface precisely and to evaluate interface area and curvature, because difference in X-ray transmission between solid and liquid phases was relatively small, comparing to that in Al-Cu alloys. A physics-based filtering method significantly improved the evaluation of interface area and curvature. For example, S/L interface area were quantitatively measured as a function of solid fraction. Average curvature gradually decreased and became zero at a solid fraction of 0.8. The evaluation of dendrite shape will be beneficial for modeling and simulation of solidification phenomena.

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NUMERICAL OPTIMIZATION OF THE MELT CONDITIONED DIRECT-CHILL (MC-DC) CASTING PROCESS

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Melt conditioning, i.e. shearing of liquid metal using a rotor-stator device, refines the grain structure without the need for grain refiners. Melt conditioning as applied to direct-chill (DC)

casting, forming the MC-DC process, has recently been demonstrated to be an effective method of producing high quality light alloy billets. The optimisation of melt conditioning parameters through experiments is expensive and difficult due to the large variability in DC casting and melt-conditioning parameters, diameters of billets, and compositions of the treated alloy melt. In this contribution, we present a new numerical model of melt conditioned direct-chill (MC-DC) casting that considers grain motion and use this model to determine the position of the mixer inside the sump that maximises the temperature gradient across the mushy zone. This numerical model is implemented using the OpenFOAM library. The model is based upon a continuum formulation that avoids the need for tracking phase interfaces, thereby making the model computationally affordable and attractive for optimization studies. The model is validated using temperature and sump profile measurements in conventional DC casting from the literature and in-house measurements in MC-DC cast billets. Turbulence is handled using a Large Eddy Simulation (LES) to accurately resolve the effect of turbulence on grain redistribution; this flow model has been validated using particle image velocimetry (PIV) measurements in a water tank. The optimization search is performed over the global design space using an Evolutionary Algorithm (EA). Melt shearing results in an increased temperature gradient across a shortened slurry zone and a shallower sump, consistent with previous experiments in both Mg and Al alloys. The consequent uniform cooling rate in the slurry zone contributes to a finer, more uniform grain structure in the as-cast billet. The optimization study will be extended to other design parameters (rotation speed, rotor-stator geometry, operating temperature, alloy composition etc.)

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NUMERICAL SIMULATION OF FLUID FLOW, SOLIDIFICATION AND DEFECTS IN HIGH PRESSURE DIE CASTING (HPDC) PROCESS

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Complex part geometries and the high injection speed during the high pressure die casting (HPDC) process cause non-equilibrium solidification and vigorous fluid flow with free surface fragmentation and splashing. This results in a high probability of forming defects, in particular porosity. Defects tend to distribute very randomly and irregularly, which leads to a substantial variability in the mechanical properties and poor repeatability between casting cycles. This is a major drawback to achieving weight reduction through lighter design. Numerical simulation is a powerful and cost-effective tool to address this topic, as it gives access to quantities that are difficult to obtain experimentally. In this contribution, a numerical simulation approach based on the finite element casting software ProCAST is presented. The model is used to study fluid flow, solidification and defect formation during each stage of the HPDC process: pouring, injection and cooling. To better describe the flow and heat transfer at the melt/sleeve and melt/die interfaces, two important factors are considered in the model: i) the effects of die coating, oxides and surface roughness of the sleeve and die walls on melt flow; and ii) the effects of residual air in the sleeve and die, turbulence and phase. Air entrapment and porosity distribution in the cast part are predicted. The model is applied to the HPDC process to produce tensile test samples of two different aluminium alloys. Comparisons with temperature measurements, porosity observations and solid distribution in the sleeve prior to injection will be presented. The mechanisms responsible for the variability of mechanical properties will be discussed in light of these new results.

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INVESTIGATION OF MASSIVE-LIKE TRANSFORMATION FROM δ TO γ DURING AND AFTER δ-SOLIDIFICATION IN CARBON STEELS BY 4D-CT

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In Fe-C alloys (<0.5mass%C), it has been considered that the solidification of δ phase (BCC) was followed by the peritectic reaction (L+δ -> γ). Radiography proved that delta phase transformed to gamma phase in the solid state (massive-like transformation). Recently, time-resolved tomography (4D-CT) has been developed by different groups. This technique allows us to perform 3D observation of solidification structure. In addition, this technique can be used to measure volume change due to solidification / transformation and to analyze crystallographic orientation relationship. This paper presents the massive-like transformation observed by the 4D-CT. According to the observations of Fe-C (0.05, 0.18 and 0.45mass%C) alloys, fine γ grains are formed even in a single δ grain. δ grains and γ grains have a certain crystallographic orientation relationship. For example, the close-packed plane (110)δ tended to agree with the close-packed plane (111)γ. The massive-like transformation caused approximately 0.6% volume shrinkage. Coarsening of γ grains occurred immediately after the massive-like transformation. The coarsening often completed within several seconds. The fine γ grains which contain strain and defects induced by the volume shrinkage can contribute to the rapid coarsening. Thus, the grain structure of autunite can be influenced by the massive-like transformation.

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GRAIN INITIATION BEHAVIOUR AND ITS EFFECT ON GRAIN REFINEMENT

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Effective grain refinement strongly depends on the interplay between nucleation potency of nucleant particles (measured by nucleation undercooling), grain initiation behaviour (affected by size, size distribution, spatial distribution and number density of nucleant particles) and solidification conditions (specified by alloy concentrations and cooling rate). Recently, we have made good progress in understanding grain initiation behaviour, and developed the concepts of progressive grain initiation and explosive grain initiation. We found that the most effective grain refinement can be achieved by impeding nucleation using nucleant particles of least potency, which is in direct contrast to the traditional approach to grain refinement, in which the most potent nucleant particles are used to enhance heterogeneous nucleation. In this contribution we present our latest understanding of effective grain refinement though analytical and numerical modelling of solidification processes. We will show that grain initiation behaviour can be best represented by a grain initiation map, which can be used as a practical guide for effective grain refinement.

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SOLIDIFICATION BEHAVIOUR OF HYPOEUTECTIC QUATERNARY Al-Cu-Si-Mg BASED HPDC ALLOYS

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Traditional aluminium casting alloys are based on binary eutectic systems with additions of minor alloying elements for improved castability and mechanical properties. The increasing demand for high strength aluminium casting alloys has led to several studies of ternary eutectic aluminium alloy systems, such as Al-Si-X (X = Sn, Ge, Cu) for the formation of bulk nano/ultrafine composite microstructures. Recent research at BCAST has led to the development of a hypoeutectic quaternary Al-xCu-2.2Si-1.1Mg (x = 5, 6.6, 10.6) (wt%) alloy for high pressure die casting (HPDC), with a good combination of strength (e.g. yield strength between 219 and 276 MPa) and ductility (e.g. elongation between 3 and 7%). The resultant as-cast microstructure of these multicomponent HPDC aluminium alloys, characterised by optical microscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM) and X-ray diffraction (XRD), consisted of a hierarchical composite of ductile, micron-sized, dendritic [U+F061]-Al phase and a hard nanocrystalline eutectic mixture. This contribution presents a detailed study of the solidification behaviour of Al-Cu-Si-Mg multicomponent hypoeutectic HPDC alloys, with an emphasis on the size/morphology/volume fraction/chemical composition of each phase as a function of Cu content.

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A MESOSCOPIC MODEL FOR SOLIDIFICATION OF SYSTEMS OF LARGE NUMBER OF COLUMNAR DENDRITES

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The last decade has witnessed the development of various solidification models based on volume averaging methods. To reduce the calculations cost, the averaging reduces information contained within the mushy zone to a single variable, the solid volume fraction. The solidification rate and the permeability are then calculated with the help of closure laws often based on some semi-empirical correlations. In the present paper it will be shown that beyond the need of sub-grid correlations, some essential mesoscopic features lakes these models.
During solidification, natural convection arises from the temperature and concentration gradients. Concentration gradients are caused by the preferential incorporation or rejection of solute element at the solid-liquid interface. In order to catch the smallest solute plumes scale the solidification model simulates directly the envelope of the columnar dendrites with a cellular automaton model. The mushy interior of the dendrite is modelled with a volume averaging method. The dendrites tips are assumed to growth with a modified LGK model to account for the effect of the magnitude and the direction of the flow. Secondary arms are allowed to transform into a primary arm if the curvature of the envelop exceeds a critical value. The competition between grains is well reproduced by the variation between dendrite tips velocities. This model allows the study of the effect of both the grains, and the primary arm spacing on the hydrodynamics. The results given by this model (with primary arms) are compared with the ones predicted with a model using a full volume averaging method (primary arms invisible).

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INTERACTION BETWEEN FLOW AND FACETED CRYSTAL GROWTH

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The growth of faceted crystals occurs often in nature and industry, involving always the presence of flow. Insulin, silicon, pyrite, quartz, gallium are only few examples of faceted crystals. The present paper presents a numerical model for the simulation of facetted crystal growth, taken into account the incidence of flow. The growth in facetted crystals is the results of interface kinetics and flow hydrodynamics. This model was applied to the Fe2Al5 faceted crystal, presenting a hexagonal crystal shape. These facetted crystals (Fe2Al5), so called top dross particles are

forming during the production of Zn coated steel sheets (Galvanizing industry). In the galvanizing industry their occurrence is a problem and therefore it should be limited. Comparison was made between simulation and experimental observation of crystal shape. The growth was found to be the result of the coupling between the interfacial kinetic and the hydrodynamic induced kinetics.

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SOLIDIFICATION PROCESSING OF SCRAP Al-ALLOYS CONTAINING HIGH LEVELS OF Fe

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The accumulation of iron in molten aluminium alloy scrap is one of the main concerns for the recycling and casting industries because it can lead to the formation of Fe rich intermetallic compounds which are detrimental to mechanical properties. Existing methods to reduce accumulated iron may be effective, but they all suffer from poor efficiency. Hence, if downgrading secondary aluminium to low quality products or dilution with primary aluminium is to be avoided, more efficient methods to minimize the effect of high levels of iron in the melt before casting have to be found. The aim of this study is to investigate the solidification of different aluminium alloys with varied levels of Fe and to evaluate the nucleation and growth of the Fe rich intermetallic phases under different solidification processing conditions, using both thermodynamic predictions and experimental results. The effect of the addition of other elements, such as Mn, and the use of physical melt treatment processing technologies, based on intensive high shearing, have also been evaluated. We present a detailed microstructural analysis showing that the type, size and morphology of the Fe rich intermetallic compounds are not only dependent on the processing parameters such as temperature, holding time and cooling rate but also on the melt treatment processing before solidification. It has been found that chemical melt treatment by element addition leads to the formation of larger but more compact intermetallic particles; meanwhile physical melt treatment enhances their nucleation and initial growth resulting in an increased number density as well as reduced particle size. It is therefore possible to have a better control of the formation, type, morphology and size of the intermetallic particles as well as their distribution along the casting, something that has direct impact on the mechanical properties as well as benefits for the recyclability of scrap aluminium alloys as it allows the transformation of low grade material into a low cost and low carbon feedstock for high quality castings.

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Si POISONING OF TiB2 BASED GRAIN REFINERS FOR Al-ALLOYS

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Inoculation with exogenous particles has been widely used in industry to grain refine various alloys during solidification. Among a series of Al-Ti-B based grain refiners developed for Al-alloys, the Al-5Ti-1B master alloy, which contains potent TiB2 particles for enhancing heterogeneous nucleation of α-Al grains, has been most widely used for decades. However, it has been reported that, in the presence of certain alloying or impurity elements in Al-alloys, the effectiveness of Al-Ti-B master alloys for grain refinement can be dramatically reduced, resulting in a coarse and columnar grain structure in some cases. This adverse effect on grain refinement is often referred to as “poisoning” in the literature. When its content exceeds 2-3 wt.%, Si is one such element that poisons the Al-Ti-B based grain refiner. So far, the exact mechanisms for Si poisoning have not

been fully understood, although significant research effort on the subject has been made. In this work, state-of-the-art electron microscopy, including aberration (Cs)-corrected high resolution STEM, has been carried out focusing on the Al/TiB2 interface at the atomic scale, in order to reveal any possible modification of TiB2 substrates caused by interaction between Si and TiB2 at the interface. In this contribution, we present the mechanism underlying Si poisoning in the context of Si segregation at the Al/TiB2 interface and its consequence on the potency of TiB2 particles as substrates for heterogeneous nucleation of Al.

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MULTISCALE MODELLING OF THE TWIN ROLL CASTING PROCESS

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Twin roll casting (TRC) is an energy efficient way of producing Mg alloy sheet for lightweight applications. However, unfavourable microstructural features, such as columnar grains and centreline segregation, are present in the as-cast alloy sheet. By modelling the effects of casting parameters, melt conditioning and material parameters on microstructure development, feedback can be provided to optimise the TRC process to improve the quality of TRC strip. A multiscale model is used to simulate the evolution of microstructure during TRC, in which the process of grain growth in fluid flow is modelled via phase field simulation coupled with a lattice Boltzmann model, and a Lagrangian macroscale model is applied for heat transfer analysis, which provides the boundary conditions for the microscale grain growth model. Results from the macroscale model can be used to deduce the upper bound casting speed, thus allowing manufacturing efficiency to be improved, and the deformation zone to be reduced, which is particularly favourable in TRC of Mg alloys.

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ON THE FORMATION OF INCLUSION AND MACROSEGREGATION BY AN INCLUSION-COMBINED MACROSEGREGATION MODEL

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The endogenous inclusion during solidification may generate from the combination of solute and non-metallic element, i.e, O, S, therefore the formation of such inclusion would take effect to global macrosegregation. To legitimately examine the interaction between endogenous inclusion and macrosgregation, an inclusion-combined macrosegregation model, which coupling the inclusion growth theory with the multicomponent solidification model, has been developed. Here solidification of a ternary alloy (Fe–0.45 wt.%C–1.06 wt.%Mn) is considered and MnS is the only generated inclusion. Spherical granular morphology is assumed for MnS which is treated as another continuous phase, apart from liquid, columnar and equiaxed crystals. Thermodynamic-controlled classical nucleation theory and diffusion-governed growth model are applied to calculate its precipitation process. The mixed solidification model principally takes some features into account as follows: growth of columnar dendrite trunks; nucleation, growth and sedimentation of dendrite equiaxed crystals; thermosolutal convection of the melt; solute transport by both convection and grains(equiaxed and inclusion) floatation; and the columnar-to-equiaxed transition (CET). This inclusion-combined macrosegregation model had been employed to study the formation of macrosegregation and inclusion in a 2.45-ton ingot. The final segregation pattern are in qualitative agreement with the reported experimental results. The formation mechanism of inclusion in such an ingot, and its influence in macrosegreation have been also discussed.

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RECENT ADVANCES IN UNDERSTANDING THE EARLY STAGES OF SOLIDIFICATION

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Recent Advances in Understanding the Early Stages of Solidification
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Solidification of single phase alloys occurs in a number of distinctive stages during the cooling process. For isothermal solidification these may include prenucleation (atomic ordering in the liquid adjacent to the liquid/substrate interface), heterogeneous nucleation, grain initiation, spherical growth, morphological instability, dendritic growth and grain impingement. Here, we define the early stages of solidification as the process between prenucleation and the point of morphological instability. Since the majority of historic research has concentrated on dendritic growth, our current understanding on the early stages of solidification has been very limited despite it contributing predominantly to the formation of the solidified microstructure. In recent years, we have been devoting our research effort to understanding the early stages of solidification and have made good progress. In this contribution we present an overview of the recent advances in understanding the early stages solidification, focusing on heterogeneous nucleation, grain initiation and their effect on grain refinement. We will demonstrate both theoretically and experimentally the following key conclusions: • The current grain refining approach (take Al-5Ti-1B grain refiner as an example) has reached a saturation point; it is difficult to achieve any further grain refinement; • More significant grain refinement can be achieved by impeding heterogeneous nucleation using less potent nucleant particles (larger nucleation undercooling), which is in contrast to the conventional approach to grain refinement by enhancing heterogeneous nucleation on the most potent nucleant particles. • Al- and Mg-alloys do not need grain refiners since they contain sufficient native solid particles to achieve grain refinement once they are made available by appropriate melt treatment, for example, by intensive melt shearing.

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SOLIDIFICATION MICROSTRUCTURE DURING SELECTIVE LASER MELTING OF Ni BASED SUPPERALLOY: EXPERIMENT AND MESOSCOPIC MODELING

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Selective laser melting (SLM) is a commonly-used additive manufacturing technique, which generally consists of the melting of the powder and of the solidification of the molten pool. The SLM process is being widely investigated using both experimental and modeling methods. Until now, the focus has been on the heat transfer and liquid flow in the molten pool, on defects and on the properties of the final product. However, there is a lack of studies on the formation of the solidification microstructure during SLM, which is crucial for controlling the grain texture, the segregation, and ultimately the material properties. The solidification during SLM is a highly complex process and is significantly affected by various conditions, such as the spot size, the power and the velocity of the laser, as well as the powder-bed. Therefore, it is necessary to elucidate the effects of these conditions on the solidification microstructure.
In this study, a set of SLM experiments was performed on a same IN718 plate under varying laser power and velocity, both with and without a single-layer powder. The original microstructure of this plate was characterized as the equiaxed grains structure without any texture. After the SLM

process, the morphologies of the molten pool, as well as the new solidified grains in both cross- and longitudinal sections of the melting path were characterized by SEM (Scanning Electron Microscope). Moreover, the EBSD (Electron Backscattered Diffraction) was used to characterize the orientations and the origins of the grains to analyze the selection of the grain growth in the molten pool. The results were compared to evaluate the impact of the laser parameters as well as the powder on the solidification features during SLM, especially on the orientation selection of the grain growth as the first step of the solidification. Additionally, the mesoscopic envelope model was used to analyze the solidification process and the grain selection during SLM.

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APPLICATION OF CLASSICAL NUCLEATION THEORY TO THE HETEROGENEOUS NUCLEATION OF PRIMARY SILICON IN HYPEREUTECTIC Al-Si ALLOYS

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The applicability of the classical heterogeneous nucleation theory for an inoculated Al-18.6Si (wt%) alloy was investigated. In this work, nucleation models (surface-dependant and volume-dependant) proposed by Perepezko were used to study the heterogeneous nucleation of primary silicon in phosphorus-inoculated alloys. For this metallic system, the nucleation temperature was found to be the most crucial variable in both models.
If a spherical-cap model is assumed for heterogeneous nucleation, then the contact angle changes only by the interfacial energy. However, the data applied to Perepezko's model showed it changed by undercooling. Therefore, it is suggested that the Perepezko's nucleation model is not applicable for analysing data in inoculated hypereutectic Al-Si alloy. This work also suggests a new modelling approach to predict the size of inoculated primary silicon particles after solidification. The approach uses the basis of "Free Growth" nucleation model developed by Greer, which was introduced initially for nucleation of primary aluminium. Results from the numerical modelling based on the new approach was in reasonable agreement with the measured data.

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COARSE PARTICLES FORMED DURING THE DC CASTING OF Al-Mn-Ti-Fe-Si ALLOYS

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The formation of coarse Fe and Mn containing intermetallic particles during the DC casting of Al-Mn-Ti-Fe-Si alloys is detrimental to the alloys' cracking susceptibility, formability and even final mechanical/corrosion properties. In this talk, SEM/TEM are employed to reveal the microstructural features of the particles including composition, size distributions and morphologies. These experimental measurements are then compared with the predictions from Phase field method and Frequency Distribution Function method (implemented in our in-house software PreciMS). The combination of modeling and experimental approaches is able to shed some lights on the origins of these coarse particles. It is expected that this work is useful for the heat exchanger alloys composition design and casting parameters optimization.

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THE PREDICTION OF CASTING DEFECTS: FROM MACROSEGREGATION TO MULTI-DEFECTS MODELLING

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The formation of casting defects, including macrosegregation, shrinkage cavity, porosity, and inclusion, which resulting from the combined action of multi-physics filed, is a complex process. This process including the nucleation, growth, floating (or settling) of both inclusion and equiaxed crystals; growth and fragmentation of dendritic crystals; solidification shrinkage; solute redistribution and migration; etc. Therefore, it is a big challenge to predict these defects together in one model.

Based on the dendritic-equiaxed & columnar macrosegregation model, a four-phase solidification model that further consider the gas phase, which supplement the volume reduction of solidification shrinkage, has been established to realize the prediction of shrinkage cavity in metal solidification process. For the prediction of inclusion, in order to distinguish the difference between exogenous and endogenous inclusions, two models had been established respectively: 1) for exogenous inclusions, the coupling of Discrete Phase Model (DPM) and four-phase solidification has been considered, which has the possibility to track the moving of inclusion particle; 2) for endogenous inclusions, inclusion-combined macrosegregation model, which coupling the inclusion growth theory with the multicomponent four-phase solidification model, has been established.

The formation process of defects in steel ingots had been investigated by these multi-defects models, which provide reasonable results by compared with experiment results. The interaction behaviors and its mechanisms between shrinkage cavity, inclusion and macrosegregation had been deeply studied.

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MICROSTRUCTURE EVOLUTION IN AN Al-Si PISTON ALLOY UNDER ULTRASONIC MELT PROCESSING

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Piston Al-Si eutectic alloys are used to produce direct-chill cast billets for subsequent forging. Because of a very complex composition and multi-phase heterogeneous structure, it is necessary to control the formation of primary and eutectic compounds either through alloying or casting conditions (or both). In this study we used ultrasonic melt processing above of across the liquidus line to affect the occurrence and size distribution of primary Si as well as morphology of primary Al dendrites and high-temperature eutectic phases. The refinement of these particles has potential benefit for mechanical properties and formability during forging. In addition the role of Cu and rare earth additions in the phase composition of the alloy is discussed.

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NUMERICAL MODELLING OF INFILTRATION OF Al INTO ADDITIVE MANUFACTURED Fe PREFORMS IN ORDER TO OBTAIN Fe-Al INTERMETALLICS

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The current work, describes a numerical methodology to obtain deeper understanding of the kinetics of solidification, the formation of intermetallic phases and the dynamics of Al melt infiltration into porous iron preforms. The model was calibrated against test cases from infiltration experiments performed using the centrifugal casting process with liquid Al on additively manufactured SLM Fe-preforms with channels, with the goal to obtain fine-grained Fe-Al intermetallics. First macro-simulations performed using STAR-Cast, on the casting process, provided temperature history, which served as thermal boundary conditions to perform microstructure simulations using MICRESS. Comparisons against experiments (test cases) carried out using different initial temperatures of preform and melt provided insights into the formation of Fe-Al intermetallics. The channel sizes and process parameters affecting infiltration and solidification is discussed. Next, this simulation methodology is applied into design and development of complex structured preforms from metal injection moulding and other methods. This work was performed under project EQUINOX supported by Horizon 2020, European Union's Research and Innovation framework, under Grant Agreement No. 689510 and a patent application by Kochanek, and co-workers, on EQUINOX manufacturing process is underway.

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PHASE FIELD CRYSTAL AND MOLECULAR DYNAMIC MODELING OF NUCLEATION DURING SOLIDIFICATION ON THE ATOMIC SCALE

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Nucleation of crystalline materials, the starting point for crystal formation from melts, has long been an important issue in condensed matter physics and materials science. Nucleation plays a key role in determining the microstructures and mechanical properties of crystalline materials; therefore, controlling nucleation is a very effective way for regulating the macrostructures of materials for specific applications. As nucleation occurs at atomic length scales and diffusional time scale, it is still hard to investigate such kind of multiple scale issue with regular methods. Classical nucleation theory (CNT) can descript nucleation issues well, however, it does not take the lattice structure transition during nucleation into consideration, which makes CNT can't descript crystal nucleation quantitatively. Further, more and more investigations reported that nucleation often pass through some intermediate states, and the properties of the intermediate phases has significant influence on nucleation pathways. This kinds of nucleation often calls two-step nucleation (TS), however, the atomistic pathways of TS still unknown. A deeper understanding of nucleation process requires experimental or numerical work to provide atomistic visualizations and images of nucleation. In this dissertation, both the Phase field crystal model and Molecular dynamic method are employed to study the nucleation pathways and pathway selection mechanisms on atomistic scales for both single phase and binary alloy solidification.

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ANALYSIS OF COLUMNAR-TO-EQUIAXED TRANSITION EXPERIMENT IN LAB SCALE STEEL CASTING BY A MULTIPHASE MODEL

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Correct prediction of composition heterogeneities and grain structure across a steel ingot is critical in optimizing the industrial processing parameters for enhanced performance. Previous studies using the SOLID® software have been able to predict the grain structure, grain density, grain morphology and macrosegregation pattern in industrial scale ingots by incorporating fragmentation and heterogeneous nucleation. Columnar to equiaxed transition (CET) affects the mechanical properties of the final product along with the macrosegregation patterns. Larger equiaxed regions are preferred for most industrial applications. CET is significantly affected by the number density of equiaxed grains and by the nucleation undercooling. These parameters can be controlled by addition of different nucleating agents to the molten steel. 8 kg 42CrMo4 alloy steel ingots (240 cm x 60 cm x 60 cm) were cast without inoculants and with different inoculant additions in order to promote the equiaxed zone. The cast structure was characterized by ASCOMETAL. The experiments were simulated with a multi-phase process-scale model of solidification that incorporates a multi-scale description of the microstructure formation. The goal of the present study is to show the capabilities of such a process-scale solidification model to explain the observed structure distributions (extent of the columnar and equiaxed zones, equiaxed to columnar transition).

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FORMATION AND GROWTH MECHANISMS OF INTERMETALLIC COMPOUNDS AT THE LIQUID Al/SOLID Ni INTERFACE USING SYNCHROTRON RADIOGRAPHY

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Due to the excellent performance in oxidation resistance and creep strength of intermetallic compounds (IMCs), the IMCs formation and growth behavior at the liquid Al/solid Ni interface is of great interest in the technological applications of liquid-metal infiltration, hot dipping coating, diffusion brazing, and transient liquid-phase bonding. However, there is no consistent conclusion on formation and growth mechanisms of IMCs. In this paper, the microstructural evolution at the liquid Al/solid Ni interface with different Al amounts were observed through synchrotron radiography. The IMCs formation and growth mechanisms at the interface were analyzed. For the Al plate of dimensions 10 mm × 10 mm × 0.5 mm, the Al3Ni2 layered phase first formed during cooling, then partially reacted with liquid Al to forming Al3Ni phase through peritectic reation. The growth of Al3Ni2 layer was divided into four different stages, the growth behavior at stage I and stage III was mainly controlled by diffusion mechanism. The growth of peritectic Al3Ni phase was governed by the melting of small grains accompanied by the growth of adjacent large grains and coalescence of grains near the tips. For the Al plate of dimensions 10 mm × 0.5 mm × 0.5 mm, the Al3Ni2 layer first formed during holding, followed by the formation of scallop-type Al3Ni phase. The growth of Al3Ni2 layer contained four different stages, accompanied by the mechanism changing from reaction to bulk diffusion. The scallop-type Al3Ni grew through the cost of adjacent small grains to change the morphology from scallop to hemisphere, which was governed by the fluxes of repening and interfacial reactions.
Key words: liquid/solid interface, synchrotron radiography, solidification, formation and growth mechanisms

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SEGREGATION OF Ca AT THE Mg/MgO INTERFACE AND ITS EFFECT ON GRAIN REFINEMENT OF Mg ALLOYS

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Grain refinement of Mg alloys is usually achieved through enhanced heterogeneous nucleation by chemical inoculation. Albeit the most commonly used grain refiner for Mg alloys, Mg-Zr master alloy works only for Al-free Mg alloys and suffers from high material cost and low alloying efficiency. Recently, our research demonstrates that the native oxide particles in Mg-alloy melts can be harnessed for promoting heterogeneous nucleation, resulting in significant grain refinement. However, commercial Mg alloys contain various alloying elements that are essential to promote the performance of the alloys. Alloying elements are expected to affect the potency of the native oxide particles for heterogeneous nucleation and consequently effectiveness of grain refinement. Therefore there is a need to understand the surface condition of oxides in Mg-alloy melts in terms of nucleation potency. In this work, heterogeneous nucleation and grain refinement have been studied in Mg-Ca alloys. Advanced electron microscopy, including aberration corrected STEM, was used to investigate the effect of Ca addition on the nature of the oxide particles in the Mg-Ca alloys. TEM/STEM investigation revealed that Ca segregates to the surface of the MgO particles, which have either {1 1 1} or {1 0 0} surface terminations. The mechanism underlying the heterogeneous nucleation of Mg by the native MgO particles is discussed in terms of the Ca segregation and crystallographic match at the Mg/MgO interface.

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ELECTROMAGNETIC EFFECTS OF MELT AND DENDRITE GROWTH WITH PULSED MAGNETIC FIELD

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Electromagnetic effect produced in alloy melt and dendrite growth under the action of a pulsed magnetic field are researched by experimental and simulation. Simulation results show that alternating gradient electromagnetic forces act on the melt in front of the interface of the growing dendrites and the maximum electromagnetic force appears near the front of the solid/liquid interface, which forms a local electromagnetic oscillation and a strong disturbing effect on dendrite growth. Experimental observation shows that the stable growth of dendrites was disturbed, which led to occurrence of columnar to equiaxed transition (CET) and refinement of solidified grains. In addition, the pulsed magnetic field also produces electromagnetic convection in the melt which promotes the CET. As the results, the dendrites are observably refined even to spheroidal grains with the pulsed magnetic field. The CA-FD calculation shows that the electromagnetic convection causes the primary dendrite to rotate in solidification process. Because of the interface front is subjected to the action of multi-directional melt flow, the optimal growth of crystal is inhibited, which leads to the formation of spheroidal grains solidification.

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THREE-DIMENSIONAL MESOSCOPIC MODELING OF EQUIAXED DENDRITIC SOLIDIFICATION IN A THIN SAMPLE: EFFECT OF CONVECTION FLOW

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A mesoscopic envelope model is used to numerically simulate the equiaxed solidification of an Al-20 wt%Cu thin sample under isothermal and constant cooling rate conditions in the presence of gravity. The solute rejection from the grains to the melt yields composition gradients in the latter. This results in a non-uniform density of the melt which triggers the melt natural convection when gravity is present. The shape of each equiaxed dendritic grain is described by an envelope that joins its active secondary-arm tips. The grain envelopes evolve according to an analytical microscopic model of the dendrite tip growth kinetics. It is based on Ivantsov's solution for a parabolic tip that relates the tip growth velocity with the solute concentration field ahead of it. A hydraulic boundary layer much larger than that of the solute concentration field is assumed which is valid for our case of investigation where the Schmidt number is $o(10^2)$. The thin sample has L_x, L_y, and L_z dimensions of 1000, 1000, and 200 μm, respectively. The case of study consists of a single fixed grain, the centroid of which is located at the centroid of the sample, with the primary arms aligned along the sample sides. Depending on the orientation of the sample with respect to gravity, the melt flow might play an important role on the grain growth. In case that the sample is oriented in such a way that the thin sample side is aligned with gravity, the flow plays a negligible effect on the growth kinetics of the primary branches aligned along x and y sample sides. Along the thin dimension, the grain develops attached to the top wall whereas the solute-enriched melt flows to the lower region. In the case that the sample is oriented in such a way that the thin sample side is perpendicular to gravity, the growth kinetics of the primary branches aligned along x and y sample sides are highly affected by the flow. The branch pointing at the top grows over 1.8 times faster than without flow convection whereas the that pointing at the lower region grows over 4.4 slower than without flow convection.

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THREE-DIMENSIONAL PHASE-FIELD LATTICE-BOLTZMANN MODELING ON DENDRITIC AND EUTECTIC GROWTH WITH COUPLED THERMAL-SOLUTE-CONVECTION FIELDS

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The interaction between the capillarity and the thermal-solute-convection fields determines the microstructure evolution during solidification, which significantly influences the eventual mechanical properties of materials. However, to achieve the coupled thermal-solute-convection microstructure evolution with a realistic Lewis number (Le ˜ 104) and Prandtl number (Pr ˜ 10-2), the computing overhead is gigantic. In this work, the multi-physical microstructure evolution was simulated via a phase-filed lattice-Boltzmann approach, which enhanced the time step by 2-3 orders of magnitude in comparison with the explicit finite difference method. A parallel and adaptive mesh refinement algorithm was developed to further improve the computational efficiency. Accordingly, the fully coupled 3-D thermal-solute-convection dendritic and eutectic growth for Al-Cu alloys was first reproduced with a realistic Lewis number and Prandtl number. It was confirmed that the domain temperature and the presence of convection have significant influence on the final morphology. The simulated results agree well with the experimental findings.

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IN SITU AND OPERANDO SYNCHROTRON QUANTIFICATION OF PRIMARY SOLIDIFICATION IN IN713C DURING ADDITIVE MANUFACTURING

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Laser Additive Manufacturing (LAM) can directly produce near-net-shape metallic components using commercial alloy powders. However, primary solidification during LAM is far from equilibrium due to the ultra-fast laser-powder interaction (<50 ms), mixing of solutes during melting and micro-segregation upon rapid solidification. Our understanding of these phenomena and the resultant microstructural features formed cannot be fully elucidated using traditional a posteriori characterization, necessitating in situ and operando characterization. We have developed a LAM Process Replicator (LAMPR) that allows real and reciprocal space synchrotron imaging of LAM. The X-ray diffraction study presented exploits the quasi-steady-state and layer-wise AM to enable the detection of the primary solidification of tracks under conditions distant from the near equilibrium transformations observed from conventional processing. This is complemented with in situ and operando x-ray imaging of the same process. The results can be used to help design new alloys and guide the optimisation of processing parameters to exploit the full potential of LAM.

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SOLID-LIQUID INTERFACIAL ENERGY OF SOLID Alα SOLITION IN EQUILIBRIUM WITH AlZn LIQUID

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The grain boundary groove method has been successfully used to measure solid-liquid interfacial energies, σsl, experimentally for binary eutectic, peritectic systems, multi-component systems as well as pure materials, for opaquate materials as well as transparent materials. It was shown that the grain boundary groove method can be use to obtain, σsl, for any alloy system provided that the prepared alloy sample can be hold at the evaluated temperature for a long enough time with a very stable temperature gradient.
In order to show the applicability of the groove method to any system, a part of the Al-Zn phase diagram was chosen. Equilibrated grain boundary groove shapes for solid Alα solution (Al-5wt%Zn) in equilibrium with AlZn liquid (Al-10wt%Zn) have been directly observed with a radial heat flow apparatus. The Gibbs-Thomson coefficient, Γ, was determined with a numerical method using observed groove shapes. The measured thermal conductivities of the solid Alα solution and AlZn liquid phases and the temperature gradient in the solid phase at the solid-liquid interface were used for the calculation of Γ and then σsl was determined using the Gibbs-Thomson equation. The grain boundary energy for the same system was also obtained from the observed groove shapes. The results of the work were compared with the results of the related experimental works. The results of the work were compared with the results of the related experimental works.

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EFFECT OF Mn/S RELATIONSHIP IN PRECIPITATION SEQUENCE OF THE MnS IN A HYPOEUTECTIC GRAY IRON

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Deleterious effect of sulphur excess in gray iron is shortened by Mn addition. The suitable Mn addition according to sulphur in the metal is preformed according to the different addition rules available in open literature. With Mn addition is intended to avoid FeS formation by MnS precipitation that also prevents the undesirable effect of sulphur dissolved in the melt in the morphology of graphite flakes. To achieve the latter effect, it is thinking that MnS precipitation must occurs before eutectic reaction were flakes of graphite are formed. In order to get more basis for the choice of the rule of Mn addition, this study was focused to provide experimental evidence of MnS precipitation sequence in a hypoeutectic gray iron; Fe-3.3%C-2%Si-0.012P with 6 different Mn/S ratios: 28, 16, 4, 4.6, 2.6 and 0.7. Partially solidified samples of these alloys were obtained using a Bridgman furnace with quenching capabilities. Experimental evidence shown that the temperature of precipitation of MnS is in a reasonable agreement with the temperatures that could be calculated using thermodynamic data extrapolated from 1600 °C.

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CAPTURING RAPID SOLIDIFICATION DURING LASER ADDITIVE MANUFACTURING USING SYNCHROTRON IMAGING

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Solidification phenomena during laser additive manufacturing (LAM) occur under rapid solidification conditions, with the entire melting and solidification process occurring in a few milli-seconds. New characterisation techniques are required to capture the powder-melting, weld pool formation, together with the subsequent solidification phenomena including defect formation. To enable this, a laser additive manufacturing process replicator (LAMPR) was designed and commissioned that performs full LAM builds in situ and operando on a synchrotron beamline. This enables imaging of the process in real and reciprocal space at ultra-fast speeds (up to 50,000 frames per second) and high resolutions (ca. 1 microns). Dozens of layers can be built with hatching in each layer, whilst capturing the laser-powder interactions, including melting and the formation of spatter caused by combined metal vaporisation and argon gas heating. During track formation, we observe the mechanisms by which contiguous track is formed, and when beading occurs and why. The different types of porosity formation are also observed and quantified, suggesting ways of avoiding their formation. Finally, the processing space is explored for an SS316 powder, and a mechanistic processing map is produced which not only quantifies the processing window, but also shows the mechanisms which limit operation to within this window, and hence how the window can be expanded to produce higher strength components more efficiently.

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PHASE-FIELD MODELLING OF NON-EQUILIBRIUM SOLIDIFICATION BY THE THERMODYNAMIC EXTREMAL PRINCIPLE

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Modelling of non-equilibrium solidification is of singular importance in microstructure control, which however owing to the complex systems with complex additional constraints is still an open problem. In this work, the thermodynamic extremal principle was applied to solve the complex additional constraints self-consistently in thermodynamics for both binary and multi-component alloys. Consequently, short-range solute redistribution and long-range solute diffusion that share the same mobility are integrated naturally into the solute diffusion equations, thus avoiding the introduction of additional kinetic coefficients (e.g. interface permeability) to describe solute redistribution. Under non-equilibrium conditions, solute trapping as well as solute drag happens and at the critical interface velocity that is equal to the maximal solute diffusion velocity in liquid, abruptly concurrent occurrence of diffusionless solidification and absence of solute drag happens, thanks to the adoption of effective mobilities for non-equilibrium solute diffusion. Under equilibrium conditions, the interface and bulk contributions are completely decoupled, indicating that the current model might be preferred for simulations not only because of its simplest form of evolution equations but also its feasibility to increase the simulation efficiency by the "thin interface limit" analysis.

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INSTABILITY PATTERN FORMATION AND MAGNETISM OF LIQUID METALS BY USING LIQUID-LIQUID PHASE SEPARATION UNDER HIGH MAGNETIC FIELD

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Supercooled liquids may offer fascinating phenomena as compared with the normal state. In the case of supercooled paramagnetic liquids, completely different phenomena in high magnetic fields have be observed thanks to the high undercooling leading to higher magnetization and very strong magnetic coupling in the liquids. However, due to the restriction of the magnetic field intensity and maximum undercooling, the instability evolution in uniform magnetic field and magnetic field liquid are still not directly evidenced. In this study, high static magnetic field up to 25 T is applied to the metastable miscibility gap of Co-Cu alloys which owns liquid-phase separation at undercooled state, leading to the formation of α Co liquid phase at lower temperature that very close to the Curie temperature. With the application of strong magnetic field, the undercooled liquid are highly magnetized and Rosensweig instability with different shape and patterns are evidenced. The size distribution, volume fraction and instability pattern are strongly influenced both by the undercooling and field intensity. The mechanism of magnetic field on instability pattern formation and magnetism of liquid metals are discussed.

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SOLIDIFICATION BEHAVIOR AND MICROSTRUCTURE EVOLUTION OF γ-TiAl ALLOYS

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γ-TiAl alloys are regarded as promising candidates in aero and automobile industry due to their superior properties including low density, high specific strength, excellent oxidation resistance

and creep strength. However, the application of these alloys is limited by the problems such as micro-segregations, inhomogeneous microstructure, texture and severe cracking tendency. In the article, the effect of thermal cycling in the mushy zone and solidification rates on the microstructure of Ti-48Al-2Cr-2Nb alloy and Ti-45Al-8.5Nb-(W,B,Y) alloy were firstly discussed. Then, the phase transformation behaviors and microstructure evolution of Ti-45Al-8.5Nb-(W,B,Y) alloy was investigated. And based on phase transition sequence, a novel multi-step isothermal treatment (TIT) during solidification process was proposed to control the microstructure of Ti-45Al-8.5Nb-(W,B,Y) alloy and the influence of TIT on lamellar structure, homogeneity, texture and cracking was analyzed.

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REVEALING THE TEMPERATURE GRADIENT INFLUENCE ON THE HETEROGENEOUS NUCLEATION BEHAVIOR OF GRAINS IN INOCULATED Al ALLOYS

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An in-situ study on the directional solidification of an inoculated Al-20 wt%Cu alloy under well controlled constant cooling rates and temperature gradients has been carried out using a microfocus X-radiography set-up. The influences of temperature gradient and cooling rate on the heterogeneous nucleation rate and growth kinetics of equiaxed grains have been studied quantitatively. It is shown that under the same cooling rate, the nucleation rate of grains decreases with increasing temperature gradient. A high temperature gradient also promotes preferential growth of dendrite arms along the temperature gradient direction, and therefore the formation of elongated grains. However, the temperature effects on nucleation and grain growth decrease with increasing cooling rate. It is revealed that the propagation velocity of the nucleation front in directional solidification castings is approximately equal to the ratio between cooling rate $\dot{T}$ and temperature gradient G. Based on the experimental observations, a grain size prediction model has been developed, in which the temperature gradient effect on the nucleation kinetics was rigorously treated by introducing two new concepts termed as 'inhibited nucleation zone' (INZ) and 'active nucleation zone' (ANZ). The model has been applied to simulate the present in-situ solidification experiments. A good agreement was achieved between the predicted grain number density and the experimental measurements. Furthermore, such a model can be used to predict the temperature gradient necessary for the transition from equiaxed to columnar grain growth.

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REVEALING THE NUCLEATION AND GROWTH BEHAVIOR OF PRIMARY Si DURING SOLIDIFICATION OF HYPEREUTECTIC Al-Si ALLOYS

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The nucleation and Growth behaviors of primary Si particles in hypereutectic Al-Si-Cu alloys solidified under near-isothermal melt and constant cooling rate condition, have been studied by

in-situ X-radiography. The influences of cooling rate and addition level of P on the nucleation temperature, maximum nucleation undercooling, nucleation rate, growth velocity and morphology development of primary Si particles were quantitatively studied. In addition, thermal analysis and ex-situ characterization of the TP-1 type solidification samples by SEM were performed. The in-situ experimental results were compared with TP-1 type solidification samples. An EBSD study has been conducted on the as-solidified in-situ X-radiographic samples to reveal the Growth crystallogrphy of the Si particles. The effect of P on the nucleation and growth of primary Si has been discussed based on experimental results and modeling results.

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DETECTION AND SIMULATION OF INCLUSION DISTRIBUTION IN A CONTINUOUS CASTING SLAB

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Controlling of steel cleanliness has always been an issue of great concern for the metallurgists, because the bubbles/inclusions in[U+FB02]uence directly the mechanical properties of the slab, lead to internal cracks, slivers, and blisters in the [U+FB01]nal rolled product. Two studies concern inclusion distribution in the slab have been carried out in the current work. First, the three-dimensional inclusion distribution map in the actual continuous-casting slab was detected through a fast-detection platform. The inclusion size, morphology and spatial distribution have been given. Then a coupled computational model is developed to simulate the transient [U+FB02]uid [U+FB02]ow, solidi[U+FB01]cation, and inclusion transport processes in the continuous-casting mold. A criterion is developed using the user-de[U+FB01]ned functions to model the motion and entrapment of inclusion based on the Lagrangian approach. The predicted results are compared with the experimental measurements of the fast-detection platform. The results are helpful to understanding the final distribution of inclusion in the continuous casting slab and the entrapment mechanism by the solidified shell.

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THERMO-MECHANICAL SIMULATION OF TRACK DEVELOPMENT IN THE LBM PROCESSES - EFFECT OF LASER-METAL INTERACTION

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Interest has recently emerged for the manufacture of aeronautical parts by Laser Beam Melting (LBM) additive process. Indeed, this energy efficient process can for instance be used to build complex geometries, which cannot be built with traditional processes. However, complex phenomena occur in the early stages of powder melting and track development: vaporisation phenomena influence laser-matter interaction by creating metal vapours which are responsible for the reduction of absorbing energy. In addition, the recoil pressure generated by the vaporisation counteracts the surface tension between the melt pool and the inert gas also inducing liquid instabilities. Therefore, the study of laser-matter interaction and induced phenomena can help understand the origin of defects such as porosities or cracks. In this approach, a level-set modelling of the LBM process at a mesoscopic scale is proposed to follow melt pool evolution and track

development during scanning. A volume heat source model is used for powder considering the material absorption coefficient. A surface heat source is used to take into account the high laser energy absorption by dense metal alloys. An energy solver is coupled with thermodynamic database and pre-determined solidification path. Shrinkage during consolidation from powder to liquid and compact medium is modelled by a compressible Newtonian constitutive law. An automatic remeshing adaptation is also used to save time and avoid high computational cost. This model is compared with experimental observations in the context of a benchmark focused on a laser shooting. The present work will be then used for modelling multiple beads with the resolution of mechanical equations to be able to predict the occurrence of cracks.

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FORMATION CONDITION AND PATTERN EVOLUTION OF TWINNED DENDRITES IN Al-4.5%Cu ALLOY DURING BRIDGMAN SOLIDIFICATION

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Feathery grains have attracted considerable research interest since they were first observed in semi-continuous casting of industrial aluminum alloys about 70 years ago. Different from the regular columnar or equiaxed morphologies observed in alloy castings, this special crystal structure exhibits the alternant twinned and untwinned lamellae morphology. Previous studies focus on the analysis and characterization of the twinned dendrite growth appearing in direct-chill (DC) or similar semi-continuous casting processes. And the twinned dendrite growth during these solidification processes is believed to occur when the following solidification conditions are met: (i) a relatively high thermal gradient (typically 100 K/cm); (ii) a large growth speed (at least 1 mm/s); (iii) the presence of convection in the melt. In this work, we first successfully produced twinned dendrites in Al-4.5 wt.% Cu alloys during Bridgman solidification. Based on the twin planes already formed at 3000μm/s, by introducing an abrupt decrease in growth speed, the twinned growth could be produced till the end of solidification after abruptly decreasing the growth speed to 100, 50, 20, 10, 5, 3, 1 and 0.3 μm/s, respectively. The twinned patterns in aluminum alloys are richer than previously expected during a wide range of solidification processes. The corresponding pattern selection map was further revealed. Besides, an interesting orientation rotation phenomenon was verified by EBSD on either side of the coherent twin boundary during twinned cell growth. In high-resolution transmission electron microscopy (HRTEM) views, successive stacking faults (SFs) occurred nearby the twin boundaries (TBs) at 1μm/s, while the distortion around the TBs at 3000μm/s was quite slight. Importantly, distinct SF structures directly connecting two adjacent TBs, with a spacing of about 221nm, provides a direct experimental evidence for the close correlation between the SFs and the twinned dendrite growth in aluminum alloys.

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INNOVATIONS AND IMPLICATIONS OF NEAR NET SHAPE CASTING ON THE MICROSTRUCTURE OF MODERN STEELS

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Belt casting as a technology has been suggested as a potential casting method for steels for decades. However it has been hindered by technological capabilities and investment. The potential draw of > 3GJ/tonne reduction in energy this process has on conventional continuous casting has meant that this technology has always shown great potential. With recent improvements and the active mill in Salzgitter then the number mechanical limitations of this process are quickly being reduced, leaving metallurgical implications or potential areas of exploitation. The work presented here focuses on some of the implication belt casting has on the microstructure

of the cast product. This includes, cast grain size, segregation and precipitation. Whilst also highlighting the further benefits of this techniques with regards to castability of advanced high strength steel, low density steels etc, as well as the opportunities it offers. Through a range of lab based experimentation, including high temperature confocal microscopy, small scale lab casts and full casting XRF and EBSD, a large amount of information has been gained about the implication and possible exploitations of belt casting.

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MICROSTRUCTURE IN A356/AA6xxx AFTER COMPOUND CASTING WITH FLUX COATING

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Great efforts have been paid by the automotive industry towards producing lightweight vehicles. Aluminum alloys, with high strength-to-weight ratio, has been one of the main materials in achieving these weight demands. This work focuses on compound casting between A356 alloy melt and profiles of AA6xxx wrought aluminum alloys through a gravity casting process. With the incorporation of a wrought alloy insert, it is possible to obtain improved mechanical properties in the overall casting. However, combining two aluminum alloys is difficult due to the thermodynamically stable aluminum oxide present on the surface of the aluminum inserts. The oxide layer strongly reduces the wettability between aluminum melt and solid metal, which will prevent diffusion and formation of a metallurgical bond. In order to obtain sound metallic bonding between the two alloys, different surface treatments, including coating and chemical treatments of the profiles have been tested. The influences of preheating temperature and melt flow modes on the quality of the compound casting have been addressed. Hardness measurements and tensile tests have been applied to characterize the strength of the obtained metallurgical bond. Based on a detailed microstructure characterization of the bonding layer in the casting, by using Optical Microscopy (OM), Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDS), the solidification structure development has been discussed.

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ANALYSIS AND MODELING OF DENDRITE FRAGMENTATION IN DIRECTIONAL SOLIDIFICATION

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The quantitative prediction of dendrite fragmentation has remained a major issue in the modeling of solidification processes. A systematic approach to this issue is presented that consists of two parts. First, a thorough analysis is carried out of existing and new experimental data. A suite of different image processing techniques is developed that allows for obtaining robust statistics of the complex history of dendrite fragments, ranging from the growth conditions of sidearms through their detachment to the buoyant motion as free dendrites. Second, an analytical model is proposed that incorporates local solidification conditions of the sidebranches as well as the dynamics of the pinch-off process, which has been characterized in a previous numerical study. The predictive potential of this model is discussed in the context of the columnar-to-equiaxed transition and formation of single-crystal defects.

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EVALUATION OF AHSS CONCEPTS WITH A FOCUS ON THE PRODUCT PROPERTIES AND APPROPRIATE CASTING CHARACTERISTICS OF ARVEDI ESP THIN SLAB CASTERS

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The Arvedi ESP process and a variety of produced materials have been continuously developed since the opening of the Arvedi ESP plant in Cremona in 2009 to meet market demands for more sophisticated steel grades. The development of grades for more advanced applications such as advanced high strength steels and multiphase grades is of interest. Dual phase grades such as DP600 are already produced through an ESP line on an industrial scale; additional multi-phase grades such as TRIP are under development. High-strength steels for the automotive industry have especially high demands on material properties. In addition to the mechanical material properties, an excellent surface quality is required. The fundamental basis for such material properties on rolled coils needs to be provided from continuous casting. This paper deals with the classification of different – either Si- or Al-based – alloying concepts for TRIP steels with respect to their prospective behaviour in a thin slab caster. The investigated alloys are characterized by means of experiments, measurements, thermodynamics and phase transformation kinetics. The phase transformation sequence during solidification, the tendency towards internal and surface defect formation, the expected inclusion population and the presumed interaction with mould fluxes are considered. In addition to the selection of suitable alloying concepts, the process stability regarding high mass flow rate for good temperature guidance, consequent product homogeneity, minimum inclusion content and stable mould level for the highest surface quality are of outstanding importance. The high technical and economic potential of the Arvedi-ESP process to produce AHSS steel grades indicates significantly expanding production in the future.

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PERMEABILITY PREDICTION IN ANY DIRECTION OF COLUMNAR DENDRITE BY PHASE-FIELD AND LATTICE BOLTZMANN METHODS

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Permeability for flow of interdendritic liquid is a very important parameter in a macrosegregation prediction during alloy solidification. For systematical permeability prediction in various solidification conditions, a numerical simulation coupling a phase-field method and computational fluid dynamics would be the most promising approach. In our previous study, we have developed a permeability prediction method by large-scale simulations of phase-field and lattice Boltzmann methods [Takaki et al., (2018) submitted]. In the study, we have concluded that the permeability normal to a columnar dendrite in a regular hexagonal array can express one of the multiple columnar dendrites [Takaki et al., Acta Mater. 118 (2016) 230-243]. In addition, one advantage of the developed permeability prediction method is that we can use a periodic boundary condition for the single columnar dendrite. This means that we can apply the liquid flow in any direction to the single columnar dendrite. In this study, using the permeability prediction method developed in our previous study, we compute the permeability in various directions of a columnar dendrite. And, we investigate the direction dependent permeability of columnar dendrite in detail. Through the detail investigation, we attempt to develop a permeability tensor of the columnar dendrite.

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MULTI-PHASE-FIELD LATTICE BOLTZMANN SIMULATIONS DURING FORMATION PROCESS OF EQUIAXED STRUCTURE CONSIDERING DENDRITE MOTION

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Formation process of equiaxed structure is quite complicated phenomenon. The most difficult point in the modeling of the equiaxed structure formation process would be a motion of dendrites. In our previous study, we succeeded in expressing the growth of a single dendrite accompanying the motion by coupling phase-field method, lattice Boltzmann method, and equations of motion [R. Rojas, T. Takaki, M. Ohno, J. Comp. Phys. 298 (2015) 29-40]. After that, we have extended the model to the polycrystalline solidification, where we expressed the multiple dendrite growth with motion, collision, and coalescence and subsequent grain growth occurred after the formation of grain boundaries [T. Takaki, R. Sato, R. Rojas, M. Ohno, Y. Shibuta, Comp. Mater. Sci. 147 (2018) 124–131]. In the model, we assumed the same energy and mobility for all solid-liquid interfaces and grain boundaries. In this study, we improve the accuracy of our previous polycrystalline solidification model by employing a multi-phase-field model [I. Steinbach, F. Pezzolla, Physica D 134 (1999) 385-393], and accelerate the simulation by employing the APT (active parameter tracking) algorism for multiple phase-field variables and the multi-GPU (graphical processing unit) parallel computation. Finally, we introduce some simulation examples, such as the formation processes of the sediment bed [C. Beckermann, C.Y. Wang, Metal. Mater. Trans. A 27 (1996) 2784-2795] and the equiaxed structure through dendrite fragmentation [L. Arnberg, R.H. Mathiesen, JOM 59 (2007) 20-26].

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FORMATION OF MICRO-PLUMES AT A PLANAR SOLID/LIQUI INTERFACE IN A TEMPERATURE GRADIENT

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For directional solidification experiments with low withdrawal rates near and even below the constitutional undercooling limit of the corresponding alloy, a sample is needed which reveals an homogeneous concentration along the sample axis. As stirring in longish samples is diffi-cult, homogenization by rapid solidification is very common. Hereby, the liquid sample is rapidly moved from hot to cold and thus fine and long dendrites with segregated interdendritic liquid forms. By subsequently melting and holding the sample in rest within a given temperature gradient, diffusion in the liquid and enhanced diffusion in the hot solid diminishes local concentration differences. In this paper, we report about homogenization experiences with transparent organic model alloys of TRIS-NPG. During one hour of homogenization we observed (i) formation of a coarse grain structure, (ii) droplet migration by TGZM and (iii) formation and eventually disappearing of liquid channels. For liquid channels that revealed a connection to the solid/liquid interface, we occasionally found liquid that rose in the channel and thus formed micro-plumes at the planar solid/liquid interface. This upwards motion is explained by solutal buoyancy of NPG-rich liquid and a feeding possibility through an interconnected network of channels.

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ON THE MODELLING OF MACROSEGREGATION DURING TWIN-ROLL CASTING

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Solidification during twin-roll casting happens by cooling of the melt between two counter-rotating rolls, where the molten alloy is constantly fed in. For an inoculated Al-melt, nucleation and growth of grains lead to a gradual increase of solid fraction, so that a coherent solid network forms. Depending on the process condition this solid network might then be subjected to compression within the gap between the two rolls. By using a two-phase Eulerian-Eulerian volume averaging model that accounts for (i) transport and growth of spherical grains within a flowing melt, (ii) the formation of a coherent solid network above a specific solid fraction and (iii) the viscoplastic flow of the solid network with the interstitial melt during casting and compression, the process is numerically analyzed. It is found that an optimum process with minimum centerline macrosegregation can be achieved for conditions where the kissing point of the two viscoplastic semi-solid shells nearly coincide with the roll nip. It is demonstrated how casting speed, cooling intensity and strand thickness must be related to hit the optimum process window.

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EFFECT OF DIFFERENT PROCESS PARAMETERS ON NON-METALLIC INCLUSIONS DURING ELECTO-SLAG REMELTING OF A TEMPERING STEEL

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The remelting behavior of the tempering steel 50CrMo4, was investigated with several experimental melts on a lab-scale ESR-plant. The investigated parameters included a variation of the slag compositions and the use of a protective nitrogen atmosphere. Variations of the slag composition comprised slags with different contents of CaF2, CaO and Al2O3 as well as a variation of the SiO2-content in the slag. The remelted ingots were forged and analyzed regarding their chemical composition as well as their distribution and composition of the non-metallic inclusions (NMI) by automated SEM-EDX method. The chemical composition of the slag after remelting was analyzed as well. The results clearly show a relationship mainly of Si and Al in the steel with the process parameters. NMI changed in their total amount, type and size distribution. The protective atmosphere reduced the Si-losses during remelting. The majority of the NMI were of the Al2O3- & MnS-type. Higher SiO2-contents and reduced Al2O3- and CaO-contents in the remelting slag led to some SiO2-type inclusions. In general, remelting lead to an almost complete removal of sulfides, a reduction of oxisulfides and a shift towards more oxides. The total amount of NMI was most strongly reduced by the high CaF2-containing remelting slag.

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THE EFFECT OF Cu AND Si CONTENTS ON THE HOT-TEARING SENSITIVITY OF 3xxx HEAT-EXCHANGER ALLOYS

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Al-Mn alloys (3003) alloys are the preferred alloy series for brazed heat-exchangers for applications in the automotive industry. Cu, Si and other alloying elements are added in different amounts to improve alloy properties and achieve excellent thermal efficiency, high strength and corrosion resistance. Addition of Cu and Si results in longer solidification intervals which makes the alloys susceptible to hot-tearing and hard to cast. To investigate the influence of Cu and Si on the hot-tearing susceptibility, different amounts of these alloying elements were added to commercial alloys and a series of hot-tearing experiments were performed. Analysis of the experimental results were combined with theoretical analysis including hot-tearing indicators and microstructural simulations. An increase in the Cu and Si contents lead to increase in the hot-tearing tendency until a maximum was reached. A further increase decreased the hot-tearing tendency. The maximum is found at different concentrations for the alloys investigated and depend on the interplay between all alloying elements as well as the cooling rate.

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SOLIDIFYING SHELL WAVINESS DURING CONTINUOUS CASTING OF AHSS SLABS

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Transverse cracking of continuously cast products has been encountered at almost every caster operation. Enormous efforts have been carried out in the past aiming at identifying the cause and reducing the problem, especially on steel grades with peritectic chemistries. So far, however, there is still no cost-effective solution with good trade-off for internal quality and productivity. In this study, a new cracking formation mechanism is proposed based on observations of equally spaced crack pattern and the undulation (shell thinning pattern) observed on the inside and/or outside (surface depression) of the breakout shell with similar spacing. This wavy solidification shell forms at initial solidification stage and induces the local shell thinning and reheating which in turn causes the local "Blown grains" inside the solidification shell. As observed on slab surfaces, these blown grains are closely related to transverse cracking problem.

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RECENT ADVANCES IN THE UNDERSTANDING OF THE ROLE OF VANADIUM CARBONITRIDE PRECIPITATION TO IMPROVE SURFACE EDGE CRACKING ON CONTINUOUS CASTING OF BLOOMS

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This study aimed in combining the material properties and numerical modelling techniques through practical application to provide understanding of surface edge cracking caused by V(CN) precipitation to optimize and enhance the yield of the continuous bloom caster at ArcelorMittal Ruhrort. The investigation for this work is carried out on three different micro-alloyed steel grades; one of them being the most crack sensitive 20MnV6. A process model was used which calculates the solidification process of the strand to design an optimum cooling strategy. Therefore, two cooling patterns are employed for the steel grade 20MnV6. Reduction of area values of the steel grades 20MnV6, 27MnSiVS6 and 38MnSiVS5 from the hot tensile tests using a Gleeble simulator has been used as an indication in assessing steel's cracking behavior. Further precipitates have been analyzed by SEM at ArcelorMittal. These laboratory results suggested that precipitation kinetics of V(CN) influences the crack sensitivity of the micro-alloyed steel. The software MatCalc® is used for simulating the different process parameters of continuously cast blooms at Arcelor Mittal

Ruhrort as well as the parameters of the Gleeble experiments. From these simulations the Zener pinning force (ZPF) resulting from V(CN)-particles on grain boundaries, was evaluated which can be used as a measure for the crack sensitivity. Using the values of the ZPF it was possible to identify the set of casting parameters of the steel grade 20MnV6 which lead to the minimum crack intensity on the surface of the blooms. Moreover it was possible to make a ranking list with respect to the ductility drop occurring in the Gleeble experiments for the analyzed steel grades. The proposed statement is an issue for a continuing investigation of precipitation modelling.

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EXPERIMENTAL AND NUMERICAL INVESTIGATION OF THE EFFECTS OF FILLING DYNAMICS IN LOW PRESSURE SAND CASTING

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In Low Pressure casting (LPC), the filling stage is led by gradually increasing the gas pressure above the liquid metal, which is pushed through the pipe and into the mould cavity. In opposite to gravity casting, the LPC filling stage however does not only depend on the filling system and part geometries. By smartly choosing the pressure casting ramp, one could control the filling flow and thus avoid the filling induced defects. To avoid defects when considering the filling stage, it is necessary to simultaneously fill the mould cavity fast enough to avoid misrun and sufficient slowly to avoid oxides defects in the part. Indeed, when filling too fast, the oxides forming at the metal front are more susceptible to entrapment into the bulk [1], leading to poorer final mechanical properties. The relationship between the imposed gas pressure ramp, the system geometry and the induced metal filling dynamics needs to be investigated. Moreover, several oxides entrapment risk criteria were proposed in the literature [2][3][4] without reaching consensus. Filling flow criteria adapted to LPC should be defined. In this work, the filling dynamics induced by the geometry and LPC process parameters is investigated. An experimental setup developed at the semi-industrial scale permits to track the metal front during filling using electrical contacts. The experimental results are compared to commercial software fluid flow simulations and to a new proposed analytical model. Combining those three techniques, the link between process parameters, geometry and filling dynamics is quantitatively determined. Moreover, experiments with different process conditions are analysed in order to link the filling flow to the final mechanical properties of the parts. Eventually, new design rules adapted to LP can be proposed.

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DOUBLE DENDRITE GROWTH OF Al-Cu ALLOY DURING DIRECTIONAL SOLIDIFICATION: A PHASE-FIELD STUDY

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Double dendrite growth of an aluminum alloy was observed in directional solidification under certain thermal conditions. However, the underlying mechanisms of double dendrite growth remain unclear. Using the simulation of two-dimensional phase-field implemented on a cluster of parallel computers, double dendrite growth of Al-Cu alloy during the directional solidification was investigated. Using Al-4.5wt% Cu at different pulling rate (0.2, 2, 4.25, 10, 50mm/s) at high temperature gradient, it was found that the double dendrite forms only at a certain speed range. Our simulation also showed that the selection of double dendrite depends strongly on the

intensity of anisotropy, which is associated with the initial concentration. The formation of double dendrite can be attributed to tip-splitting or meeting of two adjacent side branches. In addition, the simulation results indicated that double dendrites have the significant growth advantage over regular ones, and this is primarily because of the greater constitutional and curvature supercooling at the tip of double dendrites. These results are consistent with previous experiments.

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APPLICATION OF A CONCENTRIC SOLIDIFICATION TECHNIQUE TO STUDY EARLY SOLIDIFICATION PHENOMENA PERTINENT TO THE CONTINUOUS CASTING OF STEEL

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We have used a concentric solidification technique to study events occurring in the early stages of solidification during the continuous casting of steel. We have found that the major factors contributing to crack susceptibility are the fraction of δ-phase present prior to the occurrence of the peritectic reaction; the rate at which the δ-to-γ interface propagates and the extent of undercooling. In addition, we have studied the δ-to-γ solid-state phase transition in low-carbon iron alloys of non-peritectic compositon and have shown that at cooling rates pertinent to continuous casting, a massive-type of δ-to-γ phase transformation can occur. We shall present and discuss important aspects of the concentric solidification technique and present selected studies in more detail. More recently, we have developed and will discuss, a differential thermal analysis technique, which combines synchronically in-situ observations with thermal analyses, thereby making it possible to correlate bulk behavior with in-situ observations.

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SOLIDIFICATION CRACKING DURING WELDING OF STEEL: IN SITU X-RAY OBSERVATION

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Solidification cracking is a key phenomenon associated with defect formation during welding, casting and some of the additive manufacturing process. To elucidate the failure mechanisms, solidification cracking during arc welding of steel are investigated in situ with high-speed, high energy, synchrotron X-ray radiography approach. Ex situ tomography is then implemented to rebuild and analyse the 3D crack network. Analysis of the in situ radiography sequence revealed the solidification cracking initiates in the weld sub-surface trailing the welding electrode at relatively low true strain of about 3.1% in the form of micro-cavities. The initial micro-cavities, with sizes from 10 × 10−6 m to 27 × 10−6 m, are mostly formed in isolation as revealed by synchrotron X-ray micro-tomography. The growth of micro-cavities is driven by increasing strain induced to the solidifying steel. Cavities grow through coalescence of micro-cavities to form micro-cracks first and then through the propagation of microcracks. Cracks propagate from the core of the weld towards the free surface along the solidifying grain boundaries at a speed of between 2.2 -3.2 × 10−3 m s−1. In addition, a three-stage mechanistic model for solidification cracking during welding of steel is proposed.

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SOLIDIFICATION OF NIOBIUM-SILICIDE-BASED ALLOYS DURING LASER ADDITIVE MANUFACTURING PROCESS

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Niobium silicide-based composites, in the application of gas turbine blades, promise significant efficiency improvements compared to current Ni-based alloys. The higher temperature capability would allow the engine to run at a higher temperature than that of current alloys, increasing engine efficiency. Nb-Si based composites possess a lower density, due to the presence of ceramic phases such as Nb5Si3 and/or Nb3Si. This would reduce the weight of the rotating blades. However, improvements in certain properties, such as ductility, room temperature toughness and oxidation resistance are needed. The alloy must also be cost effective to manufacture if niobium silicide systems are to reach their full potential.
This study focuses on the manufacturability aspect of the powder feeding laser additive manufacturing (LAM) process to engineering Nb-Si based alloy samples. A schematic drawing of LAM system is shown in Figure 1. In LAM process, CAD models of the components are constructed and sliced layer by layer for laser multilayer cladding, which directly forms the component shapes. LAM has the advantage of forming near-net shapes without the use of expensive cores and moulds for the reactive Nb-Si melt. Fine microstructure and even chemical composition distribution with reduced macro-segregation are obtained. With the use of power feeding system, new Nb-Si based alloys are LAMed with varying Ti, Si, Cr, Al, Hf, V concentrations. Microstructures and mechanical properties of the LAMed new alloys will be presented, the relationship between mechanical property, alloy chemistry and process variable will be analyzed and the challenges in powder feeding laser additive manufacturing of Nb-Si based composites will be reported.

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INFLUENCE OF INTERPHASE BOUNDARY ANISOTROPY ON EUTECTIC SOLIDIFICATION MICROSTRUCTURES

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Lamellar eutectic two-phase growth is in principle well understood for alloys in which the solid-liquid and solid-solid interfaces are isotropic. However, there are numerous experimental observations that cannot be explained by theories and numerical models with isotropic interfaces. Examples are the occurrence of lamellar growth directions that markedly differ from the direction of the temperature gradient, or the emergence of large regions of perfectly aligned lamellae in large samples. We have developed a phase-field model in which the anisotropy of each interface can be controlled separately, and we have investigated the case of anisotropic solid-solid (interphase) boundaries. Results will be presented (i) on the selection of lamellar growth directions in thin-sample directional solidification, (ii) on the ordering of lamellae in bulk samples, and (iii) on the dynamics of spacing homogenization in inhomogeneous lamellar arrays. Simulation data will be compared to available theories and experimental data.

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BREAKOUTS DURING CASTING (THE BIG CASTING MONSTER)

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To achieve the highest productivity and reach your targets, the plant stoppage should be decreased, the most and monster of any casting process is the breakout under the mold during casting as it causes plant stoppage from 1 hour to 9 hours (according to breakout severity, so analysis, controlling and review the crews' performance are considered to be some important things to control the breakout numbers, Many actions were taken, and many job instructions were issued to decrease the breakout numbers by half (from 42 to 24 breakout per year). In this paper, we will explain all the possible cause for breakout and actions taken to decrease the breakouts numbers.

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SOLIDIFICATION MODELLING IMPROVEMENT OF THE CONTINUOUS CASTING STEEL BILLET QUALITY

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DISTEMP solidification numerical model of the continuous casting steel has been a useful tool to explain billet surface and internal quality at Sidenor steel company. Work has been carried out along the years to adjust the appropriate heat transfer coefficients in the mould and secondary cooling to get a reliable description of the CC billet solidification. The numerical model has assisted to explain the influence of casting parameters on the formation of different defects in the CC process as the billet surface cracks for microalloyed steel grades; intercolumnar cracking for high temperature interval steel grades or the formation of central pipe/segregation for high carbon bearing steel grades. The solidification model has helped to find the optimum casting parameters to improve as cast semis quality

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GRAIN REFINEMENTS OF MAGNESIUM ALLOYS INOCULATED BY ADDITIONS OF EXTERNAL SiC PARTICLES

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A homogeneous microstructure of as-cast magnesium alloys is desired to improve the formability during their subsequent thermomechanical processing. Owing to its similar crystal structure to Mg, the part of Zr formed by peritectic reaction during solidification was considered to be the most effective nucleants for alpha-Mg. However, regarding the Al-containing magnesium alloys, up to now no suitable and effective external nucleants were found for them. Recently, it was demonstrated that the additions of SiC worked in refining both the Mg-Al and Mg-Zn alloys. The SiC particles acted as nucleants in magnesium alloys are attracting more attentions. The present work investigated and compared the effects of external SiC particle additions on the grain refinements of Mg-Al and Mg-Zn alloys. Their microstructures were characterized using XRD,

SEM and TEM. It was found that the additions of SiC particles could refine the grains of both Mg-Al and Mg-Zn alloys. The SiC particles cannot act as a direct heterogeneous nucleant for the nucleation of alpha-Mg in both Mg-Al and Mg-Zn alloys. The responsible mechanisms for their grain refinements are different. Regarding for Mg-Al alloys, the grain refinement caused by the addition of SiC particles is attributed to the formation of a ternary intermetallics Al2MgC2, which has a very similar crystal structure to that of Mg. As for Mg-Zn alloys, the grain refinement is attributed to the formation of a (Mn, Si)-enriched intermetallics by the interactions between SiC and impurity Mn in alloys.

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MULTISCALE MODELING OF DENDRITIC ALLOY MICROSTRUCTURES

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This talk will review recent progress to bridge the gap between phase-field modeling on the microstructure scale and grain structure modeling. While phase-field modeling has been used successfully to model quantitatively dendritic alloy microstructures, only volumes up to about a millimeter cube (or even smaller for concentrated alloys) can be simulated even on today's massively parallel computer architectures [1]. On a much larger scale, Cellular Automata coupled with Finite Elements (CAFE) models have yielded impressive predictions of grain structures of castings in both two and three dimensions [2]. However, those models do not resolve dynamical interactions between branches of hierarchical dendritic networks, which can strongly influence both intra-grain microstructure selection and the growth competition of different grains [3]. This talk will discuss efforts to overcome this limitation by using phase-field simulations to inform the choice of CAFE model parameters [4], thereby improving their predictions, or by developing coarse-grained models that can simulate dendritic microstructures on much larger length and time scales than phase-field models and that can be integrated into CAFE models. Among such approaches, the ones most explored and tested to date include the dendritic needle network (DNN) model that tracks the dynamical evolution of the hierarchical dendritic network on scale larger than the dendrite tip radius [5], and a mesoscopic model that approximates the complex dendritic morphology by its envelope [6]. Examples will be given that illustrate how those approaches have been used to model columnar and equiaxed microstructures, and transitions between them. Advantages and limitations of those approaches will be discussed to highlight ongoing challenges in scale-bridging and to provide an outlook for future developments.

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MESOSCOPIC MODELING OF POWDER BED BASED ADDITIVE MANUFACTURING

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Additive manufacturing (AM) is inducing some kind of next industrial revolution. Components develop layer by layer in a powder bed by selective beam melting according to 3D model data. This technique allows manufacturing of highly complex components and is especially interesting for high performance materials that are difficult to process in conventional technologies. Nevertheless, AM is challenged by material quality issues such as porosity, binding faults, surface roughness, selective evaporation, texture, etc. In this contribution, the variety of physical phenomena important during powder bed based AM of metallic alloys is discussed based on mesoscopic simulation also taking into account the effect of individual powder particles. We show the influence of the powder properties, such as bulk density or size distribution, on the consolidation process and stochastic appearing faults. Examples show the influence of the processing parameters and the consolidation strategy on phenomena such as selective evaporation or texture evolution. In summary we show, how mesoscopic simulation improves process understanding and represents the basis for further process development.

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MICROSTRUCTURAL ANALYSIS BASED ON COUPLING CFD AND CELLULAR AUTOMATA FOR CASTING PROCESS

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It is essential to predict the microstructure of the casting materials since it does not only influence on the mechanical properties, but also determine the process parameters during the casting process. The cellular automata (CA) is the one of the best efficient methods to analyse the microstructures by demonstrating the nucleation and grain growth during the solidification of materials. In this work, two-dimensional CFD-CA coupled analysis is performed to predict the microstructure in the casing based on the physical mechanism of the solidification. To validate the CFD-CA simulation results, experimental results are compared with the proposed analysis.

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RAPID SOLIDIFICATION MEDIATED LAMELLAR EUTECTICS FORMATION IN Nb-Si BASED ALLOY POWDERS AND THEIR SURFACE OXIDES

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Spherical pre-alloyed Nb-20Si-24Ti-2Cr-2Al (at.%) powders were prepared by plasma rotating electrode processing (PREP). The diameters of the pre-alloyed powders ranged from 45 μm to 380 μm. The microstructure and surface oxides of Nb-Si based alloy powders were investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray photoelectron spectra (XPS) and Auger electron spectroscopy (AES). The main phases of Nb-Si based alloy powders were Nb solid solution (Nbss), βNb5Si3 and Nb3Si. Fine lamellar eutectic structure was formed during solidification, taking the central parts of eutectic branches. Anomalous eutectics were

distributed at the edges of eutectic branches. The lamellar spacing (λ) of lamellar eutectics ranged from 0.12 μm to 0.38 μm, increasing with the increase of powder diameter. In addition to the fine lamellar eutectic colonies, large silicides (>15 μm) are occasionally observed in the sectional microstructures of some Nb-Si based alloy powders. The bulk oxygen content of the Nb-Si based alloy powders was as low as 0.06 wt.%. An oxygen-enriched layer with 5.14 nm in thickness, consisting of Nb2O5, SiO2, TiO2, Cr2O3 and Al2O3, was formed on the surface of pre-alloyed powders. The oxygen content was found to decrease exponentially with etch depth, and the amount in the oxygen-enriched layer accounts for 49.66 % of that in a whole single powder particle with a diameter of 120 μm. The outermost surface of Nb-Si based alloy powder was Nb-depleted and (Ti, Si)-enriched, resulting from the lower thermodynamic stability of Nb2O5 compared to the thermodynamic stability of TiO2 and SiO2.

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SINGLE-PIECE SIMULATION AND QUALITY CONTROL METHODS FOR THE COMPLEX SHAPE CASTING

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Numerical simulation technology has been widely used in the field of casting because of its visibility and forward-looking. However, for numerical simulation prediction of complex shape castings, the designer usually considers pouring under ideal conditions. The thermal property parameters used are uniform standardized parameters, and less consideration is given to the physical property parameters and boundary condition differences caused by process fluctuations in the casting process. Therefore, the numerical simulation prediction results are quite different from the actual production casting defects, which restricts the application and development of numerical simulation technology in casting process design and optimization. In this paper, a single-piece simulation and quality control method for complex shape casting is proposed considering the condition of process fluctuations. Firstly, the sensor, industrial data acquisition and casting single-piece full-cycle management technology is used to accurately obtain the key process parameters such as alloy casting temperature and time, initial temperature of casting and auxiliary materials during the forming process, and the volatility characteristics of the process parameters are derived. Secondly, the thermal property parameter reverse technique is used to carry out the pouring temperature measurement experiment of the standard test piece, and The orthogonal test and the anti-heat conduction method are applied to accurately obtain the thermal property parameters, and series of simulation of the whole process for casting process is performed. Thirdly, combined to the defect level analysis method, Fuzzy evaluation method and deep neural network method, the relationship model between key process parameters and differences is established, and then correct the model through differential reverse feedback to achieve accurate prediction of individual casting defects. Finally, based on the results of accurate prediction, multi-objective optimization algorithm is applied to find volatility characteristics of key parameters and sensitivity and influence mechanism of defects, and combining defect repair method of adaptive operation of casting to digitally control casting products quality in whole process. The research and implementation of the single-piece simulation and quality control method will provide scientific theory and technical support for high-quality and high-performance complex shape casting.

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ATOMISTIC SIMULATION OF CRACK PROPAGATION ALONG γ-TiAl LAMELLAR INTERFACE

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Due to start-up and shut-down operations of engine, TiAl structural components usually should undergo not only static but also cyclic mechanical loading. The crack propagation mechanisms of γ-TiAl under two types of loading are studied in this work to reveal the differences of the mechanisms under constant strain rate and cyclic loading. Since the crack prefers to nucleate at the interface, two types of loadings are applied to a γ-TiAl interface system with a pre-existing micro-crack at the interface by the means of classical molecular dynamics simulation, the loading direction is along [111] perpendicular to the interface. The evolution of crack tip and dislocation is observed in atomistic scale. The results show that, under both loading types, the crystal structure at the crack tip become disorder once the system yield, Shockley dislocations emit on the slip plane from the crack tip and slip along direction. The dislocations release the concentrated stress, and also blunt the extension of crack. During the cyclic loading, different with constant strain rate condition, the crack advances and dislocations slip with increasing loads and retreats during unloading. In addition, compared with the condition under static loading, more and shorter dislocations can be observed at the crack tip after several cycles.

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SIMULATION OF CASTING FILLING PROCESS USING THE LATTICE BOLTZMANN METHOD

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Numerical simulation of casting filling process with complex shape is time-consuming. Compared with the traditional SOLA method, the lattice Boltzmann method (LBM) calculates the pressure field by the particle distribution functions instead of the correction of velocity and pressure field, which greatly simplifies the calculation process. In addition, the LBM provides a flexiable approach which can be easily parallelized. In this study, the LBM is employed to simulate casting filling process. The calculation of filling process is performed on graphic processing unit (GPU) to accelerate the large-scale simulation. Volume of fluid (VOF) method is used to capture the free surface. A Smagorinsky LES model serves to increase fluid viscosity, which improves the stability of the LBM. As the LBM doesn't discretize the Navier-Stokes equations directly, the treatment of free surface boundary conditions is simple. An adaptive time stepping technique is adopted to ensure an efficient and stable simulation. The model is validated by the simulation results of Campbell box filling process. The filling process of complex casting is simulated, the result is compared with the filling process obtained by the SOLA method. The calculation accuracy of free surface profile and flow field is analyzed. The speed-up ratio of the GPU based parallel method is compared with the CPU based parallel method. The performance of the GPU based method under different conditions is investigated.

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USING MORPHOLOGY-EQUIVALENT METHOD TO SIMULATE THE EVOLUTION OF SHRINKAGE IN Ti6Al4V ALLOY CASTINGS DURING HIP

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Void is one of the main defects in titanium alloy castings, and hot isostatic pressing(HIP) is an effective method to eliminate this defect.In titanium alloy castings, the shape of real void is

complex, and there are structures such as sharp corners and small passages which would lead to a large number of meshes and easily divergent calculation. Therefore, the application of numerical simulation technology in HIP is limited. The real void is often simplified as a spherical void. However, this simplification ignores the characteristics of the true void and makes the simulation results unreliable. In this paper, the technique of morphology-equivalent ellipsoidal voidis applied to the numerical simulation of void evolution of titanium alloy castings during HIP.The volume evolution of morphology-equivalent ellipsoidal void is compared with that of real voids and spherical voids, the feasibility of the equivalent ellipsoidal void and the limitations of spherical void are verified.Firstly, the 3D shape of real void in Ti6Al4V alloy castings is obtained by computed micro-tomography. The radius of spherical void and the geometric size and orientation of ellipsoidal void are calculated by corresponding equivalent techniques.Secondly, the numerical simulation of HIP of the castings before and after the equivalent is carried out, and the volume of three kind ofvoids are recorded. The closure law of the true void, spherical void and morphology-equivalent ellipsoidal void are compared. The results show that the volume evolution of the morphology-equivalent ellipsoidal voidis closer to that of the real void. Finally, the distribution of equivalent strain and equivalent stress inside the casting are analyzed. It is found that the closure of the void is caused by stress concentration and equivalent strain at a certain value.

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THE INFLUENCE OF SHORT-RANGE ORDER IN THE LIQUID ON SOLIDIFICATION MORPHOLOGIES

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Frank in 1952 [1] already postulated that Icosahedral Short-Ranger Order (ISRO) in the liquid might explain the large undercoolings measured by Turnbull in fcc of hcp metals. ISRO was later confirmed by several observations such as the formation of quasicrystals or the atomic structure of their approximant intermetallic phases, neutron small angle scattering and atomistic simulations. In contrast to the explanation of Frank, Kurtuldu et al [2,3] have shown recently that ISRO can act as a precursor to what has been called "iQC-mediated nucleation" of fcc alloys. For two alloys based on Al and Au, it has been observed that minute additions of Cr and Ir, respectively, drastically change the final grain size and induce an abnormal fraction of twinned grain boundaries. The occurrence and geometrical configuration of multi-twinned nearest-neighbour grains can only be explained by heteroepitaxy relationships between 5-fold symmetry and fcc phases, where `[U+F0E1]`111`[U+F0F1]` and `[U+F0E1]`112`[U+F0F1]` directions of the fcc phase correspond to 3-fold and 2-fold symmetry axes of the icosahedron or interlocked icosahedron, respectively. The formation of these twins at the onset of solidification can explain the origin of twinned dendrites (or feathery grains), a morphology which has been observed in Al alloys since the mid-fourteens. But ISRO appears to also affect the dendrite growth directions via an attachment kinetics contribution, as first observed by Kurtuldu in Al-20wt%Zn with small additions of Cr [4] and very recently by Zollinger et al in Au-21.5wt%Cu-4.5wt%Ag with Ir traces [5]. This keynote will try to summarize these recent developments and outline future research directions that can confirm the influence of ISRO on nucleation and growth of metallic alloys.

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PREDICTION SOLIDIFICATION MICROSTRUCTURE IN HIGH PRESSURE DIE CASTING OF ALUMINIUM ALLOYS USING AN INTEGRATED COMPUTATIONAL MATERIAL ENGINEERING (ICME) APPROACH

Solidification microstructure of metal castings determines their as-cast mechanical properties. Accurate prediction of as-cast grain structure and key defects (such as porosity) is critical in the design and manufacturing of metal castings using an integrated computational materials engineering (ICME) approach. In this talk, a three-dimensional (3-D) model based on cellular automaton (CA) and process simulation will be presented for predicting grain growth coupled with hydrogen porosity evolution during solidification of aluminum alloys in high pressure die casting (HPDC). The 3-D CA model integrates the concurrent nucleation and growth of grains as well as those of hydrogen porosities. The diffusions of both solute and hydrogen are considered in the model. A test specimen casting, consisting of different wall thicknesses, was simulated using a finite element based software ProCAST®. The thermal history of the simulated casting was extracted

and used in subsequent mesoscale CA modeling to simulate the evolution of microstructure during HPDC. The grain morphology, grain density and grain size were obtained, and the porosity size and distribution were computed by CA modeling. The effects of cooling rates on final grain size and percentage of porosity were discussed. Electron backscatter diffraction (EBSD) analysis was performed on different wall thicknesses samples to validate the simulated results of grain size and distribution. X-ray micro computed tomography (microCT) technique was used to characterize the porosity morphology and distribution qualitatively and quantitatively. The 3-D simulated microstructure results, including grains and porosities, are in excellent agreement with the experimental results, which means the present model can be used in ICME design and development of aluminum castings.

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NUMERIC SIMULATION OF ADDITIVE MANUFACTURING

Additive Manufacturing enables manufacturing of parts by means of additive layer synthesis and thus getting complex topology parts. From the time AM technologies came into use significant progress has been achieved in understanding the processes, structure and properties of the parts being made. The objective of this work is to generate a set of mathematical models and user environment (APDL program set) based on ANSYS Finite Element Analysis System solver which would allow performing, with the required degree of accuracy, the technological operation of numeric prediction of manufacturing and residual stress fields formation and displacements in the process of Selective Laser Melting of gas turbine engine components blanks for further optimization of manufacturing process parameters.

The chosen simulation concept is based on the elements “birth and death” technique involving natural (unstrained) condition of the built-up part of material at the time it emerges. The tasks of unsteady heat transfer with moving boundaries and structural quasi-steady flow analysis are addressed successively. Mathematical substantiation of equations for recalculation of heat transfer parameters ensuring initial balance of heat energy is performed while switching to oversimplified spatiotemporal zoning unavoidable in numerical analysis. The next level of simulation involved averaging of thermomechanical and thermophysical properties of the supporting part of the structure.

The analysis of the obtained consistent patterns of temperature fields formation in the SLM process served the basis to develop an efficient analytical model of the next level which excludes powder and baseplate zones from consideration. Besides, heat transfer task solution is lacking, and the temperature in the structural task is set according to a special law ensuring minimum loss of accuracy. For complex topology parts the algorithm of laminated voxel mesh building was developed in APDL. For verification of the developed program suite, simulation of the physical process of the typical aircraft part additive manufacturing was performed. The results of mathematical simulation were matched with this part actual manufacturing process data sourced from UEC-Aviadvigatel. Simulation accuracy was verified by comparing design strain and results of measurement by the optical measurement system for 3D coordinate measurement.

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BRIDGING THE GAP BETWEEN ATOMISTIC AND MICROSTRU SCALE SIMULATIONS OF SOLIDIFICATION: FROM A PERSPECTIVE OF LARGE-SCALE MOLECULAR DYNAMICS SIMULATION

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Thanks to the recent advance in high-performance computing, the range of application of atomistic simulation is rapidly expanding. We have performed large-scale molecular dynamics (MD) simulations of solidification process including nucleation from undercooled melt and grain growth in the system [1], and discussed heterogeneity in homogeneous nucleation [1] and decrease of the grain boundary mobility during the grain growth [2]. The space scale of the large-scale MD simulation in our approach already reaches that of the phase-field method (PFM), which creates a new possibility for bridging the gap between MD and PFM [3]. For example, MD-generated microstructure is converted into interfacial profile of PFM to perform a direct comparison between

MD and PFM at the same spatiotemporal scale [4]. Moreover, the direct mapping of atomistic configuration into interfacial profiles of the phase-field model creates further new concept of the on-the-fly use of information combined with the data-driven technique. In the presentation, state-of-art collection of large-scale MD simulation of solidification will be introduced. Moreover, how MD simulation of solidification links to PFM will be discussed. [1] Y. Shibuta, et al., Nature Comm. 8 (2017) 10. [2] S. Okita, et al., Acta Mater. 153 (2018) 108. [3] Y. Shibuta, et al., Adv. Theor. Simul. 1 (2018) 1800065. [4] E. Miyoshi et al., Comp. Mater. Sci. 152 (2018) 118.

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ROLE OF SOLID-SOLID AND SOLID-LIQUID ANISOTROPIES IN EUTECTIC COLONY STRUCTURE FORMATION

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Eutectic alloys are self-organising composite materials with a wide variety of microstructural features. Size, shape, distribution, and orientation of these features can be modified by process parameters (temperature gradient, velocity of interface) as well as material parameters (volume fractions, anisotropy of interfacial energies, diffusivities, impurity nature and its percentage etc.). The objective of this work is to study the role of solid-solid and solid-liquid anisotropies in eutectic structure formation particularly the internal structure of colonies that arise due to a two-phase growth instability. We have chosen the Sn-Te eutectic system as the base binary system which has SnTe and Te phases, with Ag/Sb as impurity additions for triggering the colony formation. The binary and ternary (Ag/Sb addition) alloys are directionally solidified at different interfacial velocities to study the morphological evolution. In case of binary Sn-Te eutectic, broken labyrinth/ rod morphologies are observed (see left fig.). Upon addition of a third component, a diffusive instability (similar to a Mullins-Sekerka instability) leads to the formation of two-phase colonies that arise beyond a particular velocity. Critical velocities beyond which instabilities form are determined for each of the alloying additions. In our experiments we find colony structures having an internal sub-structure upon additions of both Ag/Sb. The internal structure due to Ag addition however, is different from Sb Addition (See figues). We explain the role of anisotropies in the free-energy of the interphase boundaries that lead to the formation of the different eutectic colony structures using results obtained from experimental characterization techniques (using SEM/TEM/EBSD).

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KEY DATA FOR SIMULATING THERMAL PROBLEMS - SWIFT MEASUREMENT OF THERMAL DIFFUSIVITY, THERMAL CONDUCTIVITY AND HEAT CAPACITY IN COMPLEX ALLOYS

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For the simulation of phase transformations and thermal problems in general, a set of input data is required that for the majority of alloys is unavailable with sufficient accuracy. ”Remedies” are to use data of the pure major alloying element, or use constant values that were measured at room temperature, neglecting their temperature dependence. The effort to gain temperature dependent data for thermal conductivity, thermal diffusivity and heat capacity is considerable, requires several measurement devices and a high degree of expertise. At present it is unlikely that this effort will be undertaken for numerous alloy systems and compositions. At FSU Jena a measurement method is being developed that allows to measure thermal conductivity, thermal diffusivity and heat capacity as a function of temperature in a single experimental run by evaluating transient and steady state temperature profiles. A state-of-the-art infrared camera is used to measure the temperature distribution of a rod-shaped sample in a temperature gradient with high resolution. Transient states are evaluated employing an inverse method to acquire thermal diffusivity, the

steady state is evaluated for thermal conductivity and the temperature dependent heat capacity is calculated from these two entities.
The accuracy of the measured data is comparable to those gained by conventional methods. This is demonstrated for Ni and 70:30 brass.

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COMBINING FLOW AND STRUCTURE MECHANICS MODELLING IN SOLIDIFYING REGIONS

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A casting process usually starts with a liquid alloy that solidifies on cooling. Forced and/or natural convection in the melt as well as stresses and deformations that occur from uneven cooling of the just solidified part can be described quite accurately. The challenging range is when the amount of solid increases so that melt flow becomes more and more difficult while solid starts to build up a coherent network that becomes more and more rigid. In such regions, the solid network starts to transmit stress while the flow is dammed to zero. A physically sound description of these regions are crucial for understanding the formation of shrinkage porosity, hot tearing and even (deformation-induced) macrosegregation. In the present contribution we are presenting an overview about up-to-date experimental and numerical findings that are relevant for the aforementioned topics and discuss related issues that are still unresolved and thus need more research.

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INFLUENCE OF SLAB SURFACE COOLING HISTORY ON CRACK SENSITIVITY OF MICRO-ALLOYED STEELS

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During continuous casting of steel, the strand is exposed to severe thermal and mechanical stresses. These may trigger formation and growth of cracks, which deteriorate the slab properties. Particularly, at temperatures in the region of the second ductility trough, deformation can become critical. A low ductility level is often observed in a temperature range of 600°C to 1200°C, where the bending of the strand is commonly performed. One of the concepts for prevention of this problem is known as “Surface Structure Control Cooling” (SSCC). SSCC aims to intensively chill the external section of the strand just below the mould. In the present study, the SSCC heat treatment is compared with the regular cooling conditions for the concast strand. Hot tensile tests, which have been found very useful in assessing a steels susceptibility to cracking, are performed on a thermo-mechanical simulator. Both thermal histories are applied to microalloyed steel with variations of the test temperature and the results are summarized in hot ductility curves. Furthermore, the microstructures are investigated by optical microscopy and the precipitation states are studied by transmission electron microscopy (TEM).