Three-dimensional mesoscopic modeling of equiaxed dendritic solidification in a thin sample: effect of convection flow

A. Olmedilla\textsuperscript{1,2}, M. Založnik\textsuperscript{1,2}, M. Cisternas Fernández\textsuperscript{1}, A. Viardin\textsuperscript{3}, H. Combeau\textsuperscript{1,2}

1 Institut Jean Lamour, Nancy, France
2 Labex Damas, Nancy/Metz, France
3 Access e.V., Aachen, Germany
Outline

- Introduction
- Motivation
- Model description
- Simulations and results
- Conclusions
- Perspectives
Introduction:
Our previous work in mesoscopic modeling
Mesoscopic modeling of XRMON-SOL experiment: growth by solute diffusion


Al-20%Cu

XRMON-SOL X-ray transmission

A. G. Murphy et al., J. Crystal Growth 440 (2016)

Numeric transmission of the mesoscopic Simulations (Beer-Lambert)
- Uniform T, constant cooling rate, 0.05k/s

- Small thickness of 200 µm aligned with gravity to minimize the effect of gravity

Observation window: 4124 x 2746 µm

Effect of the grain orientation on growth

Reference Grain

Mesoscopic modeling

XRMON-SOL
Effect of the grain orientation on growth

XRMON-SOL

0 deg  15 deg  30 deg  45 deg
Effect of the grain position on growth

XRMON-SOL

mid-plane

wall

A) B)

200μm

A B
Summary of RG's shape

a) $V_n [\mu m/s]$ $C_1 [wt\%]$ 

b) $V_n [\mu m/s]$ $C_1 [wt\%]$ 

c) $V_n [\mu m/s]$ $C_1 [wt\%]$ 

1e-07 

20 

21

1e-07 

20 

21

9e-06 

9e-06 

9e-06 

9e-06
Motivation:
What is the effect of the convection flow?
Simulation domain
Model description:
Mesoscopic envelope model with coupling of growth and melt convection
Tip kinetics

1. **Grain envelope**: virtual surface that wraps the dendrite arm tips

2. Define a **stagnant film of thickness** $\delta$

3. For each point of the grain envelope, compute:

   $v_n$: growth velocity along normal direction $n$

   Based on **Ivantsov’s tip growth kinetics**

   $$V_n = f(\Omega_\delta; \sigma; \delta)$$

   $\sigma$: tip selection parameter (material)

   $\Omega_\delta$: supersaturation at a distance $\delta$

   $\delta$: stagnant film thickness (the only adjustable parameter)

---


Volume-averaged solute transport equation

**Interior of the grain:** solid and liquid phases. Describe by the liquid fraction field $g_l$

**Exterior of the grain:** only liquid $g_l = 1$

Equation valid everywhere in the domain

$$
g_l \frac{\partial C_l}{\partial t} + g_l \langle \ddot{v}_l \rangle \cdot \nabla C_l = D_l \nabla \cdot (g_l \nabla C_l) + C_l(k_p - 1) \frac{\partial g_l}{\partial t}$$
Volume-averaged continuity and momentum equations

- **Solid**: immobile. No equations. Null velocity

- **Liquid**: volume-averaged momentum eq, using the Boussinesq approximation

\[
\nabla \cdot \left( g_l \langle \vec{v}_l \rangle^l \right) = 0
\]

\[
\frac{\partial}{\partial t} \left( g_l \langle \vec{v}_l \rangle^l \right) + \nabla \cdot \left( g_l \langle \vec{v}_l \rangle^l \langle \vec{v}_l \rangle^l \right) = -g_l \nabla \tilde{p} + \nabla \cdot \left( g_l \nu_l \nabla \langle \vec{v}_l \rangle^l \right) - \frac{\nu_l g_l^2}{K} \langle \vec{v}_l \rangle^l + g_l \tilde{\rho}_l \tilde{g}.
\]

*Buoyancy*

*Drag on liquid: grain is a porous medium*

\[
K = \frac{l_c^2 g_l^3}{180 (1 - g_l)^2}
\]

\[
\tilde{\rho}_l = (1 - \beta_C (C_l - C_0))
\]
Simulations and results
Simulation cases

For the 4 cases, sub-cases:

- No gravity
- Gravity
Grain projected area

Relative difference of projected area compared to the XRMON experiment

Low effect of convection when z is mid-thickness

Higher effect of convection when z is not mid-thickness
Primary arm length

Grain nucleus on the wall: higher effect of convection

Grain nucleus at mid-thickness: low effect of convection

Most similar cases to experimental case: C45+100 Grav, C100 Grav.
Gravity cases

When $z = 100\mu m$, $U_l(\text{tip}) \approx 30\mu m/s$

When $z$ mid-thickness, $U_l(\text{tip}) \approx 10\mu m/s$
Conclusions
Conclusions

- The **mesoscopic envelope** model is shown to be an useful tool to numerically simulate the equiaxed dendritic isothermal solidification including the **convection flow**.

- In case of isothermal solidification of a thin sample of Al-20 wt%Cu, we show that the **effect of** the thermo-solutal **convection flow** – consequence of the presence of gravity parallel to the sample thin thickness direction – **on the growth kinetics** of the reference grain depends on its initial **grain position** along the sample thickness.
Perspectives: Coupling between motion of grains, liquid convection, grain contact detection and grain growth
Coupling between motion of grains, liquid convection, grain contact detection and grain growth

Time = 0.0s
Coupling between motion of grains, liquid convection, grain contact detection and grain growth

Time = 0.5s
Coupling between motion of grains, liquid convection, grain contact detection and grain growth

Time = 1.0s
Coupling between motion of grains, liquid convection, grain contact detection and grain growth

Time = 1.5s
Coupling between motion of grains, liquid convection, grain contact detection and grain growth

Time = 2.0s
Coupling between motion of grains, liquid convection, grain contact detection and grain growth

Time = 2.5s
Coupling between motion of grains, liquid convection, grain contact detection and grain growth

Time = 3.0s
Coupling between motion of grains, liquid convection, grain contact detection and grain growth

Time = 3.5s
Coupling between motion of grains, liquid convection, grain contact detection and grain growth

Time = 4.0s
Coupling between motion of grains, liquid convection, grain contact detection and grain growth

Time = 4.5s
Coupling between motion of grains, liquid convection, grain contact detection and grain growth

Time = 5.0s
Thanks for your attention!

antonio.olmedilla.aero@gmail.com