Simulation of Nucleation and Grain Growth in Selective Laser Melting of Ti-6Al-4V Alloy

Dehao Liu, Yan Wang*

Georgia Institute of Technology

yan.wang@me.gatech.edu

http://msse.gatech.edu

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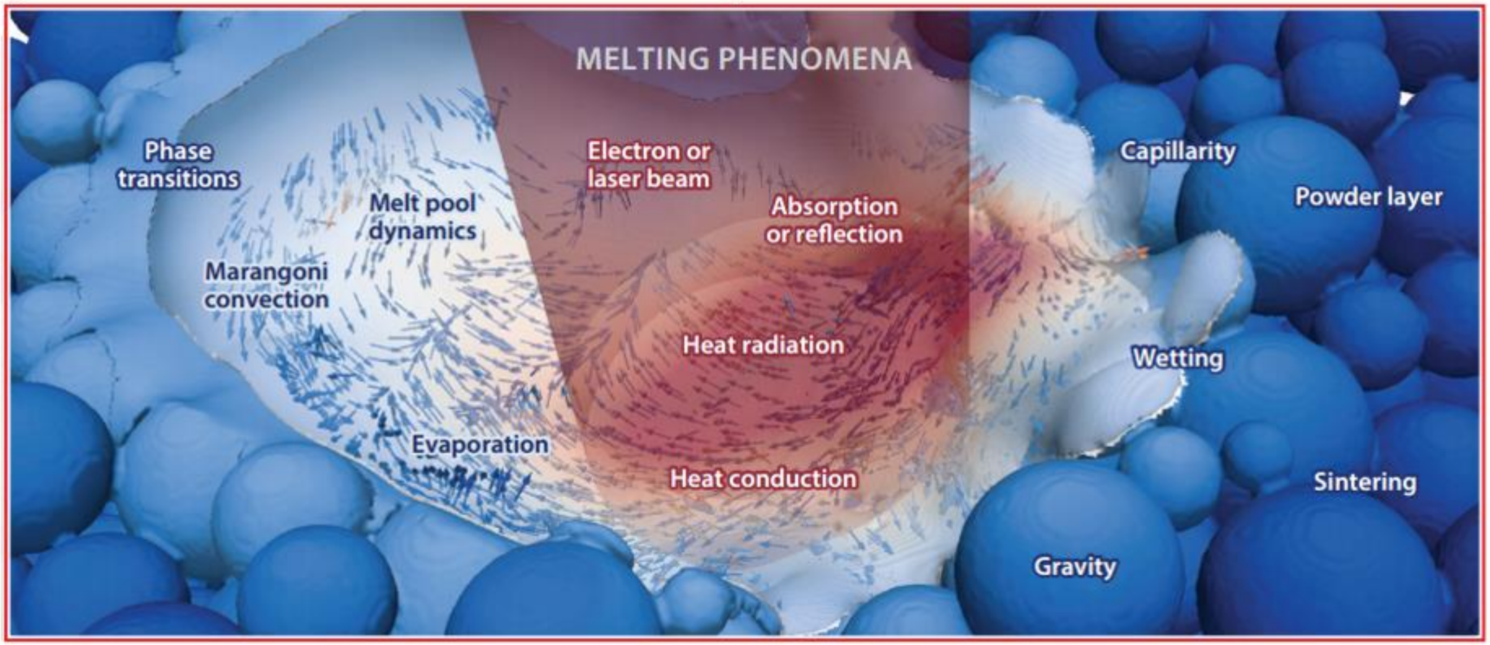
Outline

- **Background**
- **Methodology**
  - Phase Field Method
  - Thermal Lattice Boltzmann Method
  - Nucleation Model
- **Simulation Results**
  - Computational Setup
  - Dendritic Growth without Latent Heat
  - Dendritic Growth with Latent Heat
  - The Effect of Cooling Rate
  - Quantitative Analysis
- **Summary**

Background

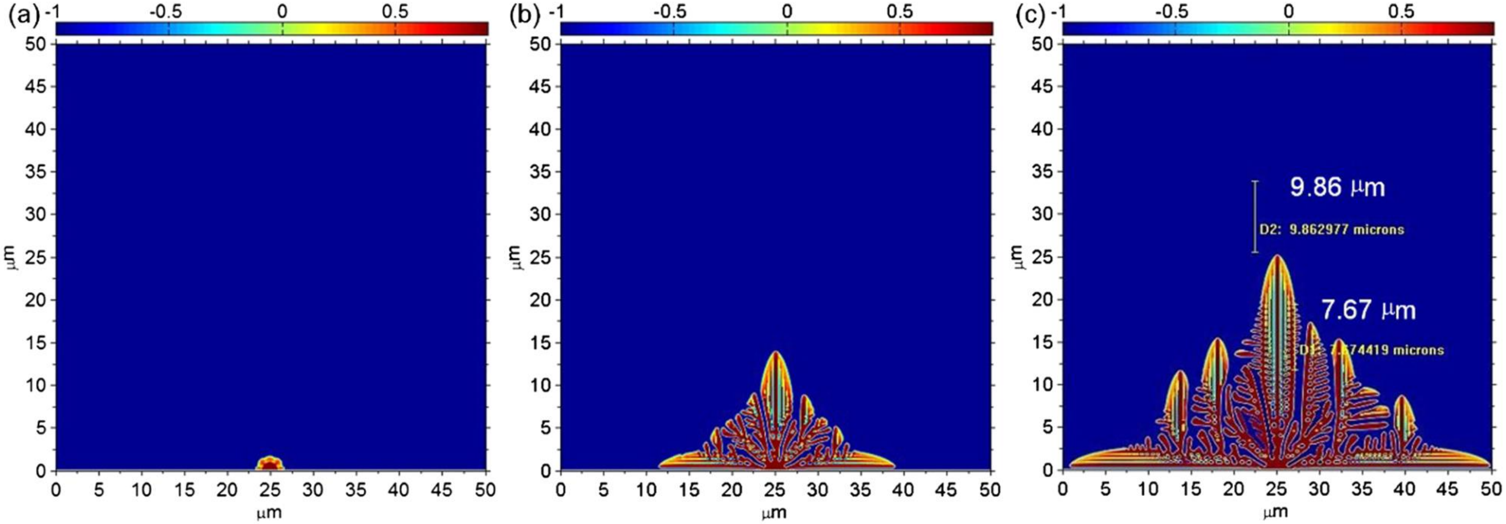
- Solidification in selective laser melting (SLM) process is very complicated, which involves multiple physical phenomena
- Challenge: Create a multi-physics based model to investigate the Process-Structure relationship



Markl, M., & Körner, C. (2016)

Phase Field Method for SLM

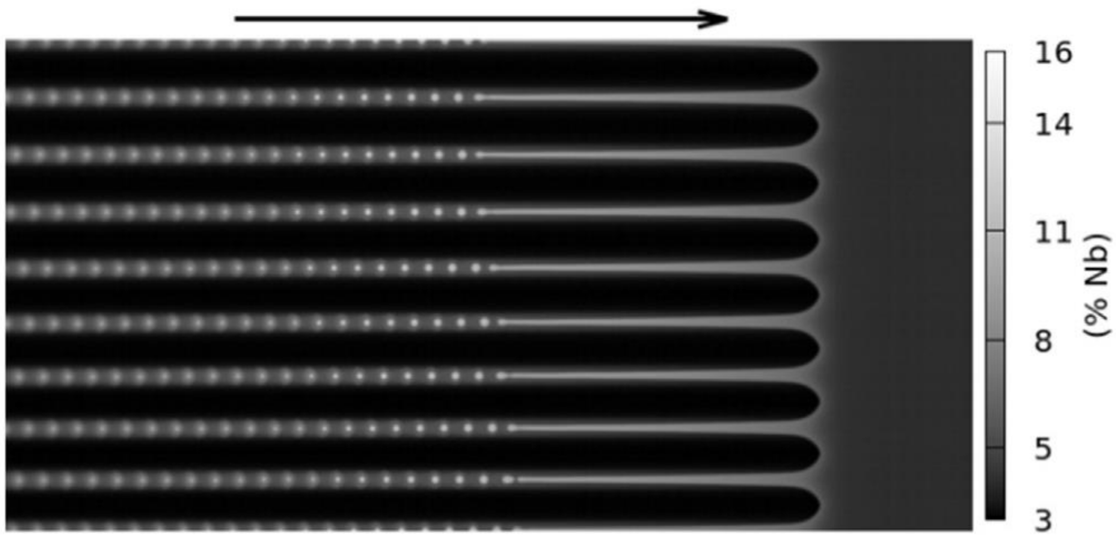
- Finite element thermal model and PFM were combined to investigate the effects of build height and scanning speed on the dendritic growth of IN718 alloy in SLM. (Wang and Chou, 2018)



  - Single grain growth
  - No latent heat
  - No nucleation

Phase Field Method for SLM

- Finite element analysis (FEA) was employed to obtain the geometric feature and the thermal history of the laser melt pool, which were used in the subsequent phase field method (PFM) simulation of dendritic growth of IN625 alloy. The predicted primary arm spacings agreed with the experimentally measured spacings (Keller et al., 2017)



  - No latent heat
  - No nucleation

Phase Field Method for SLM

- Computational fluid dynamics (CFD) analysis was utilized to predict melt pool shape and PFM was used to simulate dendritic growth of IN718 alloy in SLM. (Acharya et al., 2017)

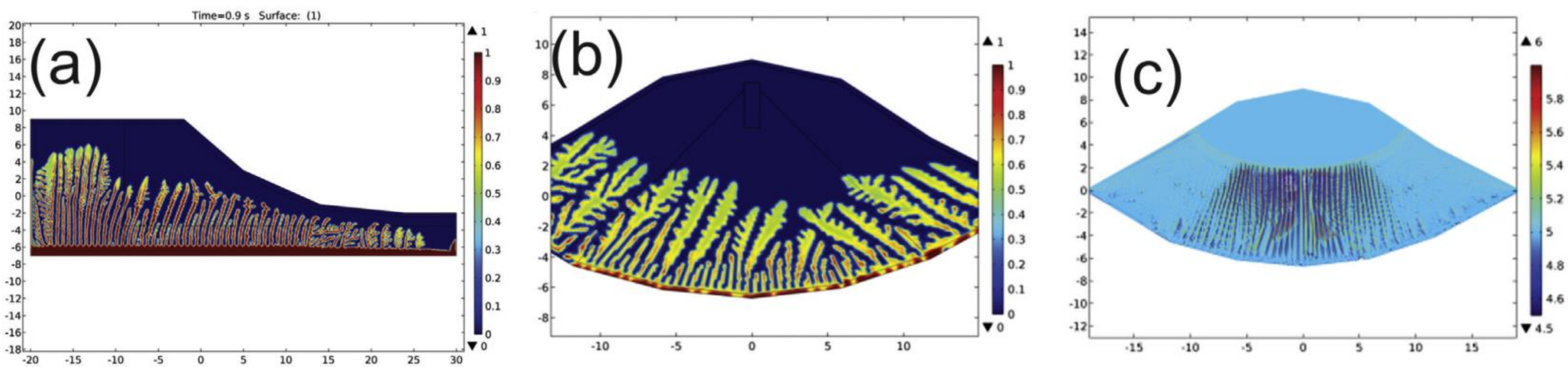
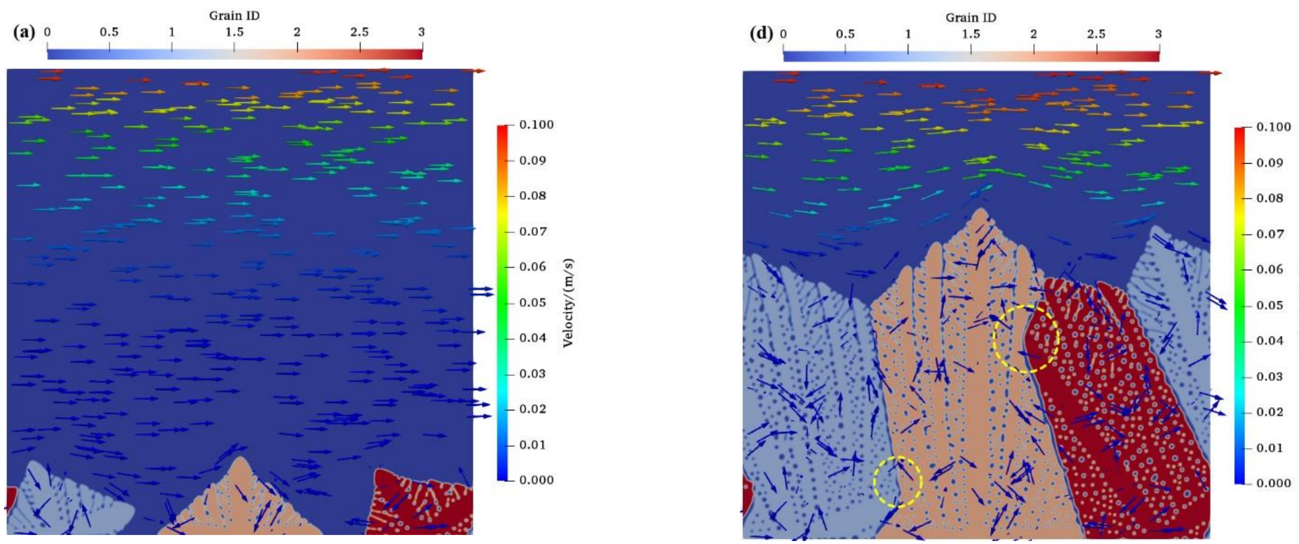


Fig. 7. a) Longitudinal cross section colored according to phase field (f = 0 indicates liquid, f = 1 indicates solid) showing dendritic structure, b) transverse cross section showing dendritic structure for higher undercooling, and c) dendritic structure observed from concentration contour.

  – No nucleation

Phase Field Method for SLM

- The phase-field and thermal lattice Boltzmann method (PF-TLBM) was used to investigate the effects of latent heat and forced melt flow on the dendritic morphology, concentration, and temperature field during SLM process. (Liu and Wang, 2018)



  - ➢ No nucleation

Nucleation Model in PFM

- A continuous Gaussian nucleation distribution was used to describe the grain density increase with the increase in undercooling (Shimono et al. , 2017)

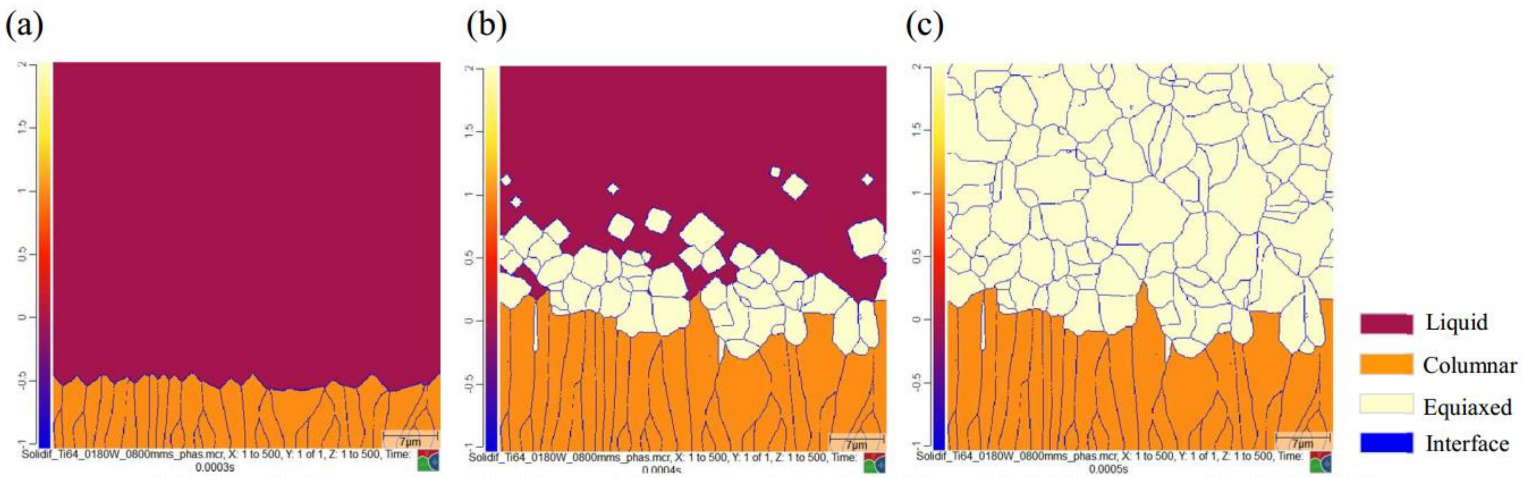
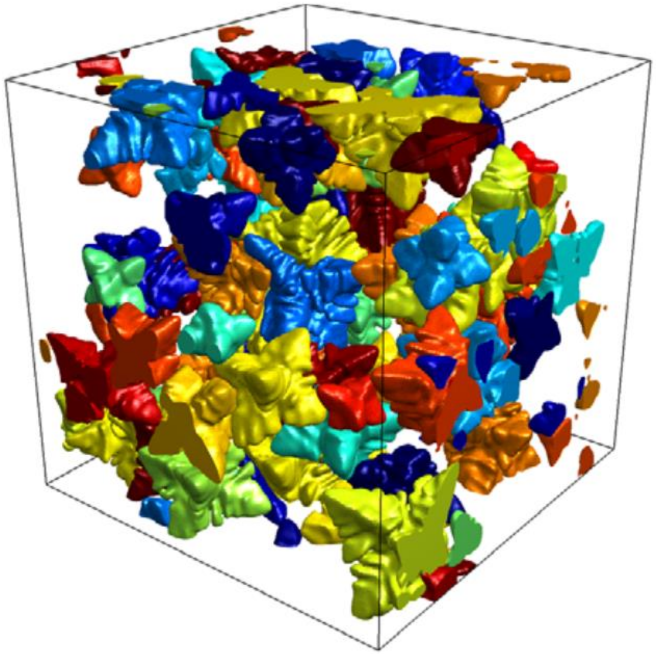


Figure 5. Phase distributions of Case 1 at (a) 0.0003 s, (b) 0.0004 s, and (c) 0.0005 s

  - 1D temperature field
  - No latent heat
  - Nucleation parameters are empirical

Nucleation Model in PFM

- Langevin noise terms could be introduced in PFM to simulate homogeneous and heterogeneous nucleation in polycrystalline (Pusztai et al. , 2008)



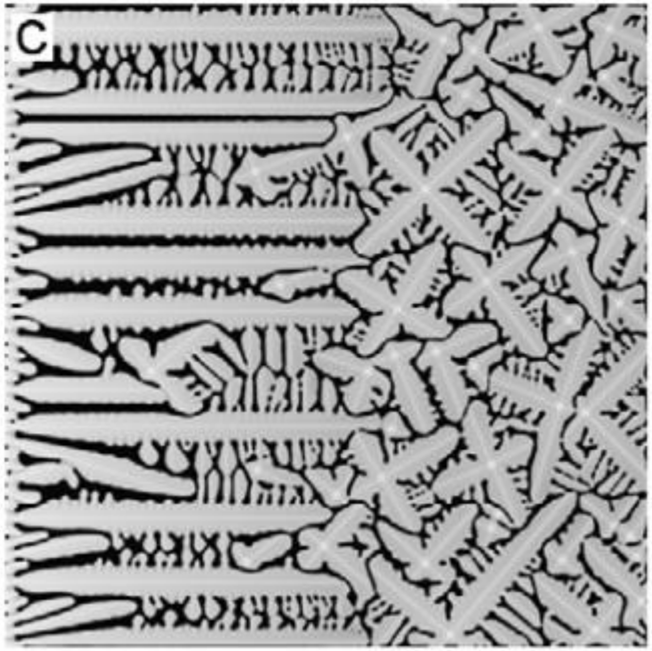
➢ Nucleation could occur at anywhere in the simulation domain rather than the solid-liquid interface

➢ The observation of nucleation would require an impractically large number of integration cycles

Nucleation Model in PFM

- Langevin noise terms in PFM could be replaced with a Poisson seeding algorithm, where viable nuclei were introduced at a time-dependent nucleation rate (Li et al., 2007)

- The nucleation kinetics of binary melts is calculated based on classical nucleation theory (CNT)



➢ The heterogenous nucleation occurred in the melt pool rather than the boundary of the melt pool, which cannot reflect the actual solidification process in SLM.

- **Methodology**
  - Phase Field Method
  - Thermal Lattice Boltzmann Method
  - Nucleation Model

Multi-Physics Model

- Phase Field + Thermal Lattice Boltzmann Method (**PF-TLBM**) integrates:
  - solute transport
  - heat transfer
  - phase transition

Phase Field

- Solute transport
- Phase transition

Thermal Lattice Boltzmann

- Heat transfer

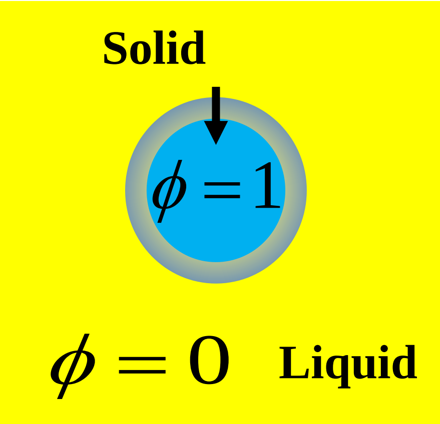
Phase Field Method

- Phase Field Method (PFM) is a versatile and accurate numerical tool to simulate solidification (Boettinger et al., 2002; Chen, 2002; Singer-Loginova and Singer, 2008; Moelans et al., 2008; Steinbach, 2009)
- *Phase field* or *order parameter* ϕ describes the distribution of phase
- Free energy functionals drive the evolution of microstructures

$$F = \int_{\Omega} (f^{GB} + f^{CH}) dV$$

$$f^{GB} = \frac{4\sigma(\mathbf{n})}{\eta} \left\{ |\nabla \phi|^2 + \frac{\pi^2}{\eta^2} \phi(1-\phi) \right\}$$

$$f^{CH} = h(\phi) f_s(C_s) + h(1-\phi) f_l(C_l) + \mu\left(C - (\phi_s C_s + \phi_l C_l)\right)$$



Our Implemented PFM

- Kinetic equation for the phase field

$$\frac{\partial \phi}{\partial t} = M_\phi \left\{ \sigma^*(\mathbf{n}) \left[\nabla^2 \phi + \frac{\pi^2}{\eta^2} \left(\phi - \frac{1}{2} \right) \right] + \frac{\pi}{\eta} \sqrt{\phi(1-\phi)} \Delta G_V \right\}$$

- Kinetic equation for the composition field

$$\frac{\partial C}{\partial t} = \nabla \cdot [D_l (1-\phi) \nabla C_l] + \nabla \cdot \mathbf{j}_{at}$$

  – Anti-trapping current

$$\mathbf{j}_{at} = \frac{\eta}{\pi} \sqrt{\phi(1-\phi)} (C_l - C_s) \frac{\partial \phi}{\partial t} \frac{\nabla \phi}{|\nabla \phi|}$$

Thermal Lattice Boltzmann Method

- Conservation equation of energy

$$\frac{\partial T}{\partial t} = \nabla \cdot (\alpha \nabla T) + \dot{q}$$

$$\dot{q} = \frac{L_H}{c_p}\frac{\partial \phi}{\partial t}$$

- Kinetic equations for the temperature particle distribution

$$g_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = \frac{1}{\tau_g}\left[g_i^{eq}(\mathbf{x}, t) - g_i(\mathbf{x}, t)\right] + Q_i(\mathbf{x}, t)$$

  – Heat source term

$$Q_i = \left(1 - \frac{1}{2\tau_g}\right)\omega_i \dot{q}$$

  – Temperature is calculated from g_i's

$$T = \sum_i g_i + \frac{\Delta t}{2}\dot{q}$$

Thermal Lattice Boltzmann Method

- Anti-bounceback scheme is used for the thermal boundary condition

$$g_{\bar{i}}(\mathbf{x}_b, t + \Delta t) = -g_i(\mathbf{x}, t) - \frac{1}{\tau_g}\left[g_i^{eq}(\mathbf{x}, t) - g_i(\mathbf{x}, t)\right] + 2\omega_i T_w$$

- The temperature of the wall

$$T_w = T_b - \frac{q_H \Delta x}{2\kappa}$$

Nucleation Model

- Nucleation can be treated as fully localized events and can be modeled as a Poisson process
- The nucleation probability

$$P_n = 1 - exp(-Iv\Delta t)$$

- The nucleation rate can be calculated based on classical nucleation theory (CNT)

$$I = I_0 exp\left[-\frac{\Delta G^*}{kT}\right]$$

$$I = I_0 exp\left[-\frac{16\pi\sigma^3 f(\bar{\theta})}{3kT(\Delta G_V)^2}\right]$$

$$f(\bar{\theta}) = (2 - 3cos\bar{\theta} + cos^3\bar{\theta})/4$$

Nucleation Model

1) During each time step, the nucleation probability P_n is calculated at each liquid cell at the boundary of the melt pool during the simulation.

2) A uniform random variable will be generated and compared with the nucleation probability P_n. If the random variable is less than the nucleation probability P_n, then the nucleus is planted.

Dendrite Growth in SLM Melt Pool

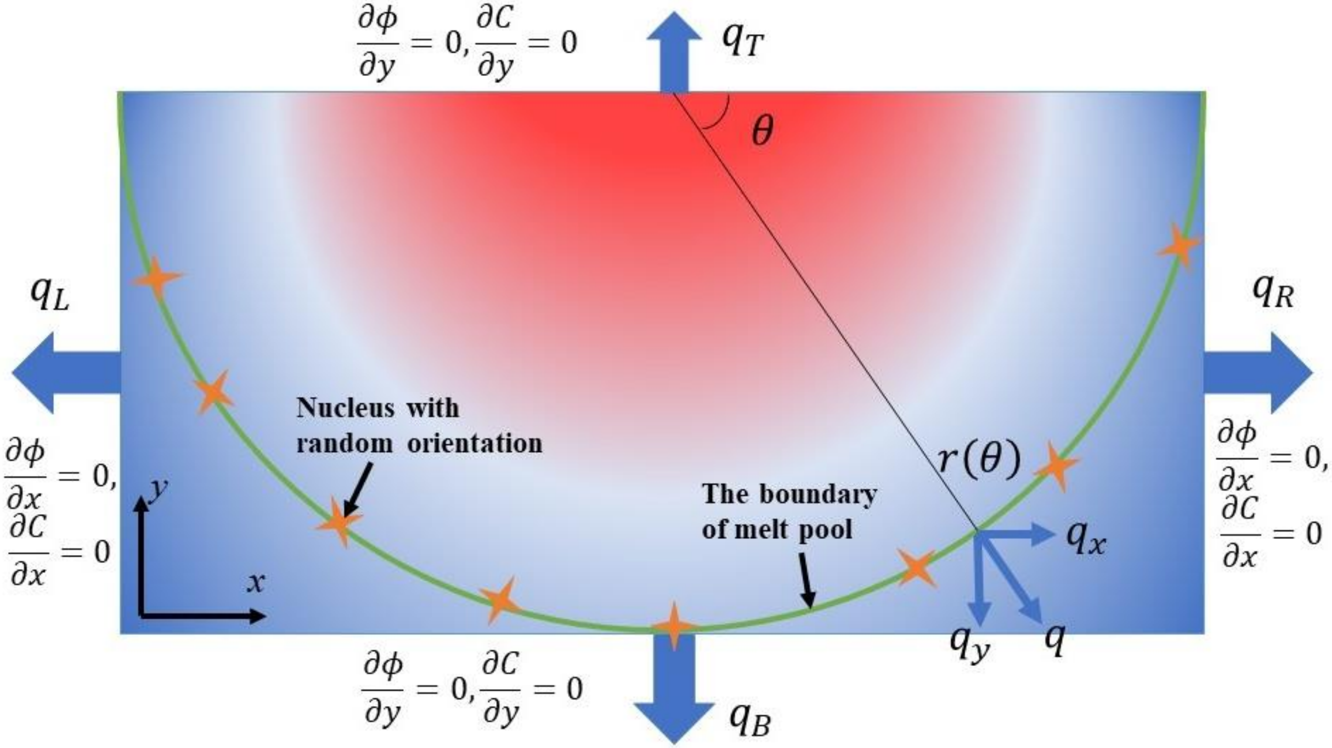
- Simulate **liquid-solid phase transition** in a **melt pool** for a **single pass** of laser beam in SLM

Assumptions

1) *Heterogeneous nucleation dominates with a lower activation energy than homogeneous nucleation*
2) *Nuclei with random orientations are influenced by the previous solidified layer along the curved boundary of the melt pool*

Computational Setup

- Cooling rate: $\dot{T} = 2 \times 10^4$ K/s
- Simulation domain: 100 μm × 50 μm
- Fine mesh $dx = 0.2$ μm for PFM and coarse mesh $\Delta x = 10$ μm for TLBM



Effect of Latent Heat

- Reveals the details of the formation of secondary arms
- Provides more realistic kinetics of dendrite growth

Without latent heat

With latent heat

Effect of Latent Heat

- Reduce overestimated microsegregation

Without latent heat

With latent heat

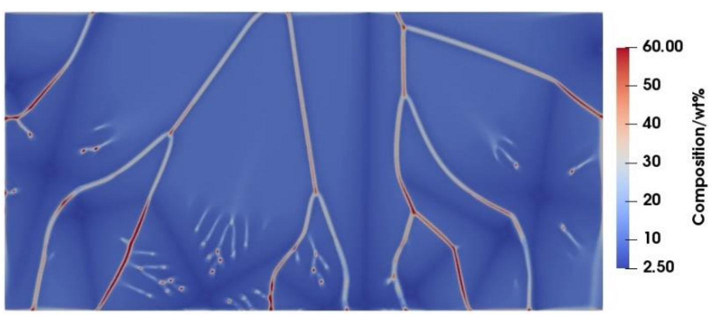
Without Latent Heat

(a) Phase field at 0.8 ms

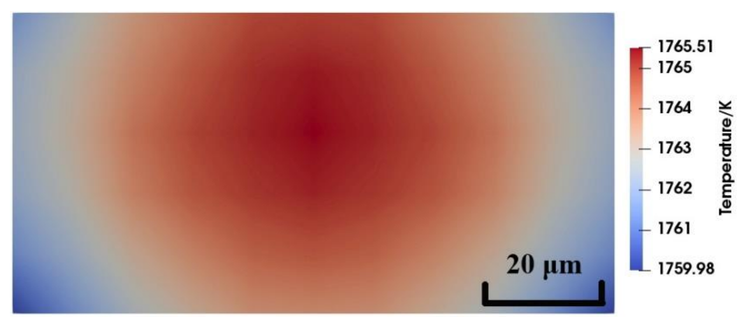
(b) Phase field at 1.6 ms

(c) Phase field at 2.4 ms

(d) Phase field at 3.2 ms



(e) Composition field at 3.2 ms

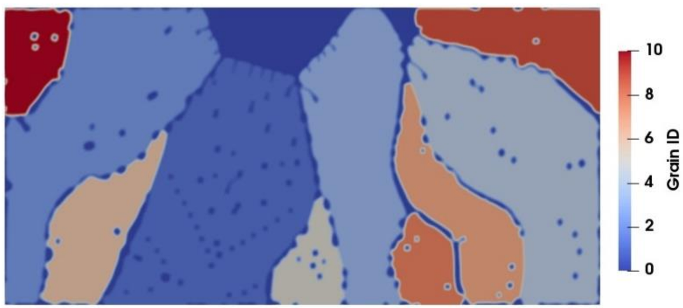


(f) Temperature field at 3.2 ms

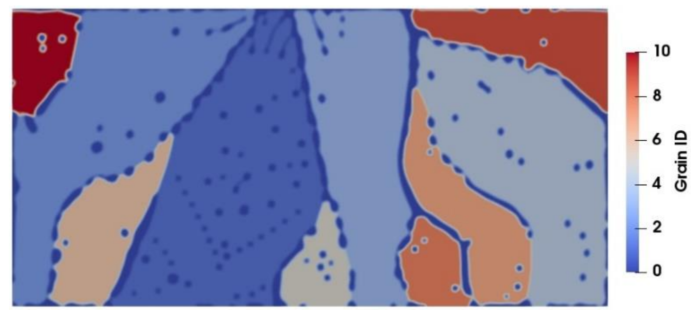
With Latent Heat

(a) Phase field at 0.8 ms

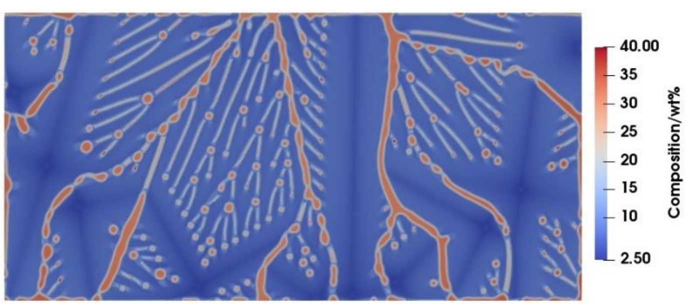
(b) Phase field at 1.6 ms



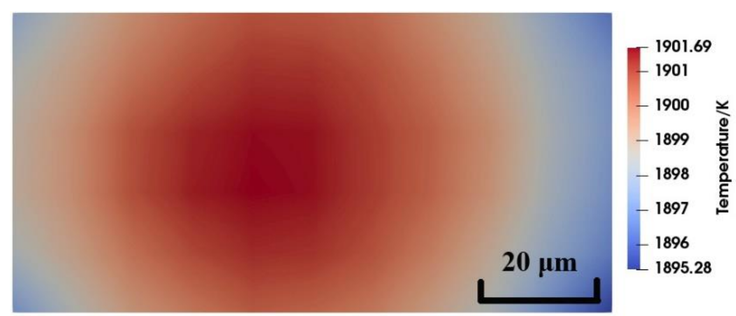
(c) Phase field at 2.4 ms



(d) Phase field at 3.2 ms



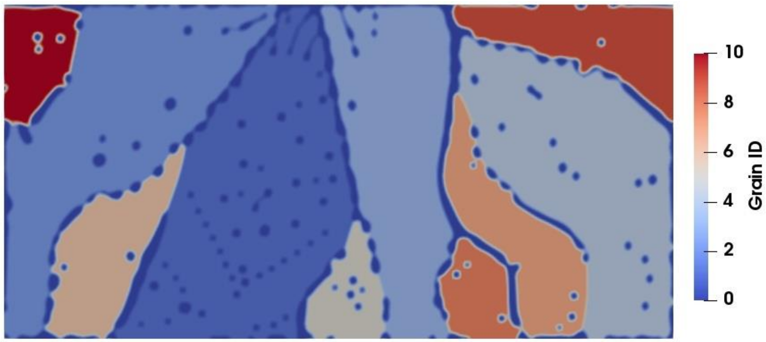
(e) Composition field at 3.2 ms



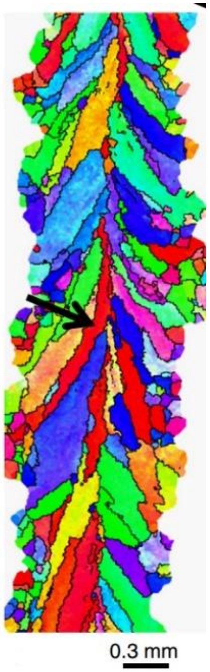
(f) Temperature field at 3.2 ms

Experimental Comparison

- Simulated secondary arm spacing $\lambda_2 = 2.8$ µm is close to the calculated value $\lambda_2 = 3.7$ µm, based on $\lambda_2 = 12\pi \left[\frac{4\sigma D_l^2}{C_0(1-k)^2 \rho L_H V_I^2}\right]^{\frac{1}{3}}$



Simultated Ti64 β grains



Ti64 sample from EBSM (Alphons Anandaraj, 2012)

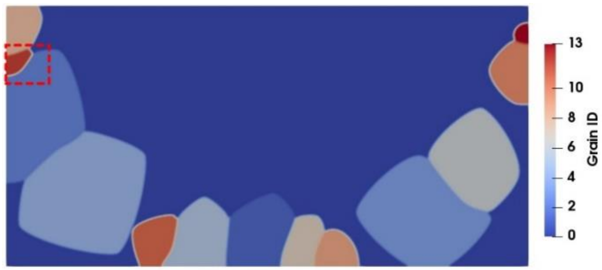
AlSi10Mg sample from SLM (LoreThijs et al., 2013)

Simulation

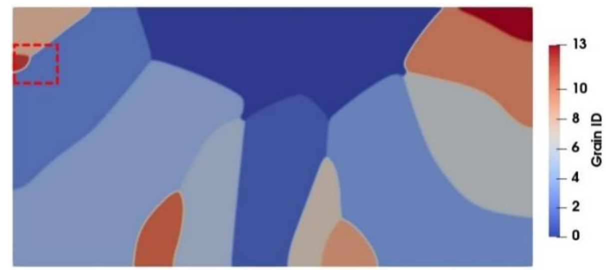
Experiment

The Effect of Cooling Rate

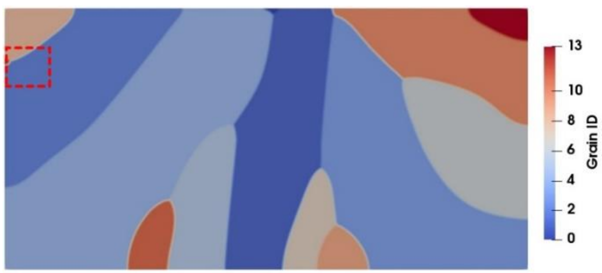
- A higher cooling rate leads to more nuclei and faster dendritic growth



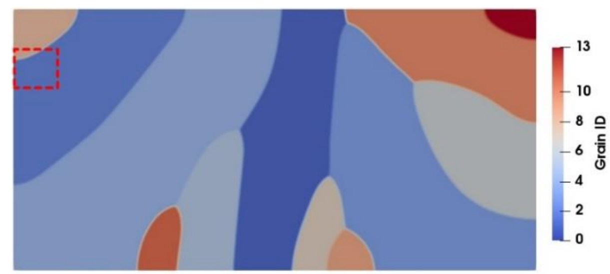
(a) Phase field at 0.8 ms



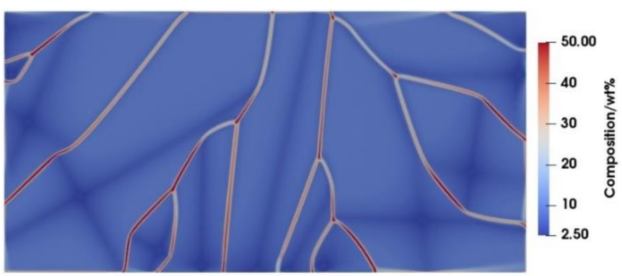
(b) Phase field at 1.6 ms



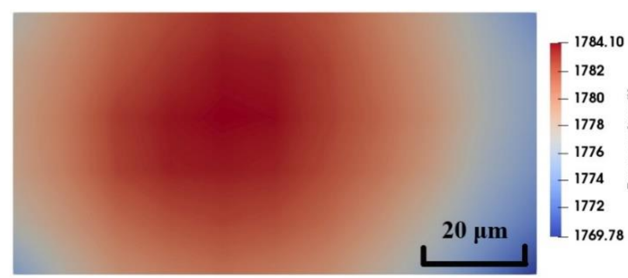
(c) Phase field at 2.4 ms



(d) Phase field at 3.2 ms



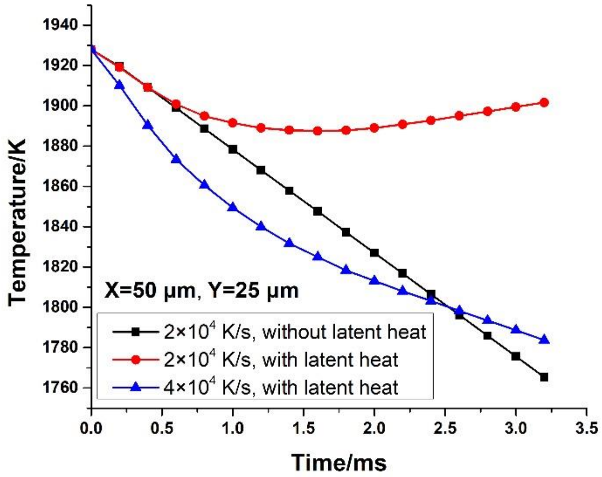
(e) Composition field at 3.2 ms



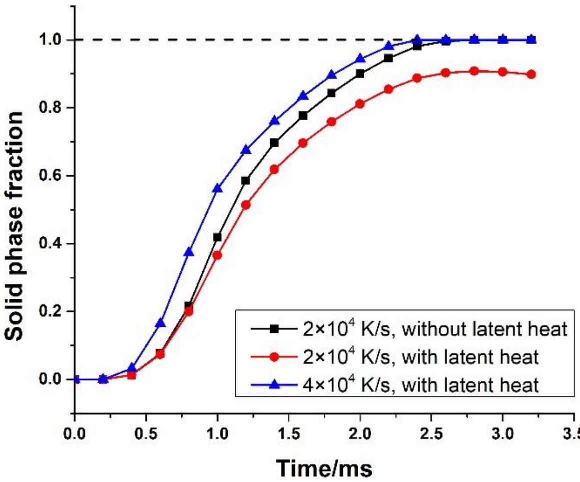
(f) Temperature field at 3.2 ms

Quantitative Analysis

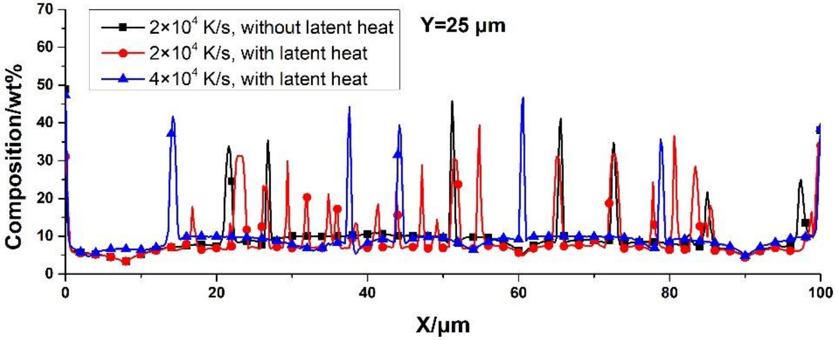
- The inclusion of latent heat results in the phenomenon called recalescence and reduces microsegregation at grain boundaries



Thermal histories



Time histories of solid phase fraction



Composition distributions

Future Work

- Inclusion of Marangoni flow, capillary, and motion of grains
- Calibration of simulation parameters
- Quantitative validation

Future Work

- Simulation of solid state phase transition
- Simulation of multiple laser passes
- Improve computational efficiency
  - parallelization
- Improve accuracy
  - Uncertainty quantification
    - Parameter uncertainty
    - Model form uncertainty
- Use simulation in process planning and optimization
  - Establishing Process-Structure-Property (P-S-P) relationship

Summary

- A mesoscale multi-physics model is developed to simulate the solidification process in SLM based on Phase Field and Thermal Lattice Boltzmann Methods

- The PF-TLBM model incorporates solute transport, heat transfer, fluid dynamics, kinetics of phase transformation, nucleation and grain growth

- It simulates systems at a reasonable time scale for manufacturing processes while providing fine-grained material phase and composition information.

Thanks!
Any questions?