

## Multiscale Modeling of μ-Structure Evolution during Rapid Solidification

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• Industrial Partner (Arconic)

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Yijia Gu	co-PI (moved to academia since November 201	18)
Alojz Kajinic	(replaced Yijia until March 2019)	
Shihuai Zhou	current PI (since last week)	

• National Laboratory

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## About Arconic



Arconic (NYSE: ARNC) creates breakthrough products that shape industries. Working in close partnership with our customers, we solve complex engineering challenges to transform the way we fly, drive, build and power.

Through the ingenuity of our people and cutting-edge advanced manufacturing techniques, we deliver these products at a quality and efficiency that ensure customer success and shareholder value. For more information: <a href="http://www.arconic.com">www.arconic.com</a> .



- The need to improve the quality and minimize fragility of the final product during AM process, requires a deeper understanding of the kinetics of rapid solidification of alloys.
- Information and data that leads to a kinetic phase-diagram for alloy rapid solidification is very useful to AM industry in order to understand better at what condition should they operate in order to have a homogeneous equiaxed final product.



- Metal additive manufacturing (AM) enables the fabrication of near-net-shape metallic objects with reduced manufacturing time and minimal finishing.
- The ability to design the AM processing conditions that yield desired microstructures would accelerate and streamline the entire fabrication process by reducing the manufacturing cost and enhancing the energy efficiency.
  - A vast majority of alloys can not be AM-ed because melting and solidification in the process lead to anisotropic microstructure (columnar grains and periodic cracks)
  - Achieving homogeneous μ-structures i.e. crack-free, equiaxed (grains equal in space) is very sought after in this industry.
- A bottom-up multiscale computational approach (from atomistic -> continuum) enabled by HPC will be very valuable to inform the industry of the range of conditions they need to tune their experiments.

#### Multiscale Modelling of Microstructure Evolution During Rapid Solidification for Additive Manufacturing (continued)

Var: concentra 0.5800 - 0.5255 - 0.4710 5 - 0.4165

r-Axis

-4.0-3.0-2.0-1.00.0 1.0 2.0 3.0 X-Axis



- At the atomistic level, extracting information for the partition coefficient as a function of thermodynamic driving force.
  - ► Kinetic phase-diagrams
  - Identify the transition from partition -> partitionless solidification
  - ▶ This informs for the columnar to equiaxed transition
  - More reliable kinetic models that can be used in phasefield
- At the mesoscale level phase-field informed from MD will provide more realistic microstructure





Example of MD for Ni-Cu system for partition coefficient as a function of interface velocity. Yang et al. PRL 107, 025505 (2011)

#### Continuum phasefield simulation with AMPE

## Secondary Dendrite Arm Spacing (Al-4.5wt%Cu, 3.5 $\mu$ m) MR

- Can we simulate microstructures and study with between cooling rate?
- Relation between cooling rate and grain size
- Aluminum alloys (of interest to industrial Partner) studied
  - Mixtures of 10, 20 and 30% Cu or Fe with Al will be exposed to different degrees of undercooling(30, 50, 100, 120, ..., 200 K) to map a transition from partition to partitionless solidification.
  - Similar conditions for the study of microstructure evolution in phase-field meso-scale simulations.



## Meso-scopic Phase-Field for Rapid Solidification:



MD informed PDE to account for rapid phase-transformation

$$\tau_{\phi} \frac{\partial^2 \phi}{\partial t^2} + \frac{\partial \phi}{\partial t} = M_{\phi} \left( \varepsilon_{\phi}^2 \nabla^2 \phi - \frac{\partial f}{\partial \phi} \right)$$

 $\vec{j}_{AT} = -a\delta(1-k_e)c_l e^{u(c,\phi)}\frac{\partial\phi}{\partial t}\frac{\vec{\nabla\phi}}{|\vec{\nabla\phi}|}$ 

$$\left|\tau_{D}\frac{\partial^{2}c}{\partial t^{2}}\right| + \frac{\partial c}{\partial t} = \vec{\nabla} \cdot \left[M_{c}\left(\frac{\partial^{2}f}{\partial c^{2}}\vec{\nabla c} + \frac{\partial^{2}f}{\partial c\partial \phi}\vec{\nabla \phi}\right)\right] - \vec{\nabla} \cdot \vec{j}_{AT}$$



 $M_c$  - mobility of the atoms  $M_{\Phi}$  - mobility of the phase-field

#### Rapid solidification

 $\tau_{\Phi}$  - timescale for relaxation of rate of change of  $\,\phi$ 

 $\tau_{\text{D}}$  - relaxation time for the diffusion flux



## Effect of partition coefficient on $\mu$ -Structure



T = 915 K. Low undercooling by ~ 17 K. Initially the solid grain has a 0.3% Cu and is surrounded by the melt with 2% Cu concentration.

At this dilute limit and low driving force, the microstructure produced by AMPE with its current development provide reliable results

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## Effect of partition coefficient on $\mu$ -Structure



T = 700 K. High undercooling by ~ 150 K. Initially the solid grain has a 1.5% Cu and is surrounded by the melt with 15% Cu concentration.

At these conditions close to eutectics and at very high driving force, the microstructure produced by AMPE will not be the correct one. As we improve the kinetic models that go in AMPE by MD studies we will be able to assess the effects in the microstructures.





## Cross comparing equilibrium phase diagrams



Liquidus from MD



Liquid-Solid-Liquid interfaces .Snapshot taken after equilibration of joined system for a <110> oriented 90% Al-10% Cu system at 800 K.

Kinetic Part with Molecular dynamics using LAMMPS A solid fcc nuclei with 2% Cu has been equilibrated with a surrounding Al with 8% Cu and then undercooled to rapidly solidify







#### Kinetic Part with Molecular dynamics using LAMMPS (10% molar Cu)



Solid seed and liquid has the same composition picked at he liquidus line.

Color scheme is based on the calculation of the order parameter, blue corresponding to the highest value.

## Order parameter computed from MD



<110> orientation

$\Delta T = 50 K::$	v <sub>I</sub> ~ 3.93 m/s
$\Delta T = 100 K$ :	v <sub>I</sub> ~ 10.02 m/s
$\Delta T = 150 K$ :	v <sub>I</sub> ~ 16.85 m/s

solid/liquid interface from an order parameter calculated from local entropy oriented. Base curve taken for 0 ns, all others taken at 2.25 ns.



## Kinetic Part with Molecular dynamics using LAMMPS HECK Simulations for pure Al for different Cooling rates

- We also explored different cooling rates to track the nucleation events and the kinetics of the solid-liquid interface
- For pure Al a extreme high cooling rate 10<sup>13</sup> K/s leads to vitrification.
- We are exploring this at the eutectics



# Opportunities for leveraging project to support/foster future activities



- Exascale computing effort among LLNL and other labs
- The extreme conditions that are explored here fall in the category of materials under extreme conditions, which is very active in the lab. Phase transition (melting/solidification) of materials under shock compression.
- Experimental work in the lab, NIF, dDAC, dTemp etc.
- Other additive manufacturing modelling efforts in LLNL.





- We have initiated we a multi-scale study of Rapid Solidification of Al alloys invoking Atomistic and Mesoscopic phase-field.
- Atomistic simulation of rapid solidification of AlCu alloys has been performed. We have done this by
  using a solid seed inside a liquid AlCu alloy as an initial condition in a pencil-like geometry. In the work
  presented we chose to have the same Cu composition in solid and liquid phase at the liquidus T.
- Partition to partitionless transition is being identified. Information and data that lead to a kinetic phase-diagram for alloy RS is very useful to AM industry in order to understand better at what condition they should operate in order to have a homogeneous alloy.
- Larger size systems are needed to determine a solute-based solidification for improving the accuracy of the mesoscopic models. We will explore different compositions as well as different cooling rates.
- We also are exploring the cooling rate range for the possibility of the vitrification of Al alloys at eutectics