Multiscale modeling of μ–structure Evolution During Rapid Solidification for Additive Manufacturing

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INTRODUCTION

This project aims at developing the advanced understanding and data necessary to establish the processing-microstructure relationship for metal additive manufacturing (AM). Using high-performance computing and multiscale modeling capabilities, we are studying the highly non-equilibrium kinetic behaviors of solute chemistry at an overdriven liquid/solid interface and their impact on rapidly solidified microstructures during AM. In particular, we (i) employ large-scale classical molecular dynamics (MD) simulations to investigate the kinetic behavior of interfacial atoms at or near a rapidly migrating liquid/solid interface; and (ii) apply the MD-derived non-equilibrium interfacial parameters to a mesoscopic phase-field model to analyze the effects of the non-equilibrium interfacial chemistry on the solidification microstructure during AM. Our research is expected to provide the essential kinetic information for tailoring mechanical performances of AM alloys by controlling their solidification microstructures.

NEED

- 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 processes by reducing the manufacturing cost and enhancing the energy efficiency.
    i. 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)
    ii. 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.
- The need to improve the quality and minimize fragility of the final product during the AM process, requires a deeper understanding of the kinetics of rapid solidification of alloys .
- Information and data that lead to a kinetic phase-diagram for alloy rapid solidification is very useful to AM industry in order to understand better at what condition they should operate in order to have a homogeneous equiaxed final product.
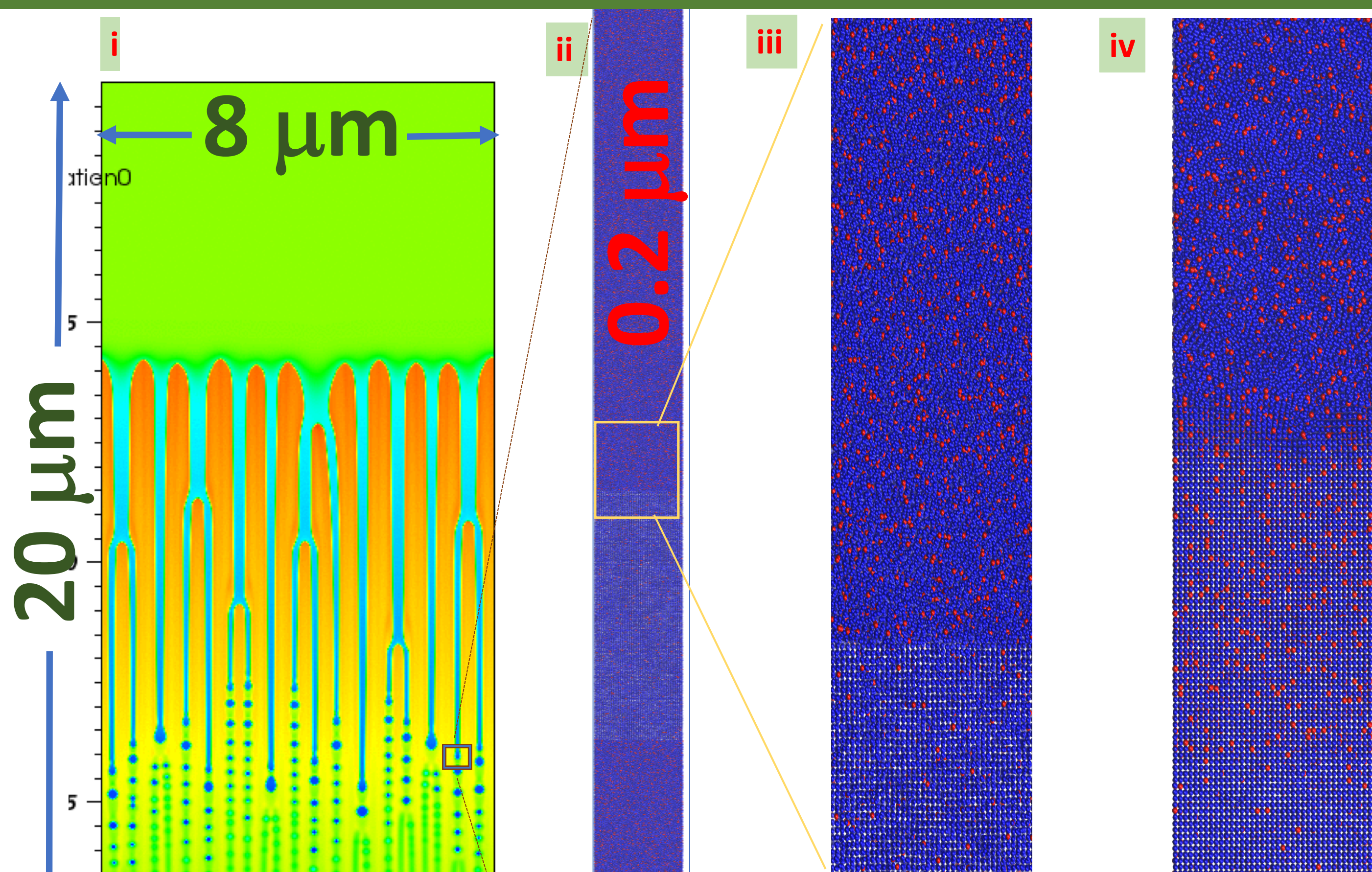
APPROACH

Atomistic kinetic behaviors of interface evolution during rapid solidification: For the atomistic level aspect of this work, we are using large scale molecular dynamics (MD) to study the growth velocity and interface kinetics during rapid solidification. We extract 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 phase-field
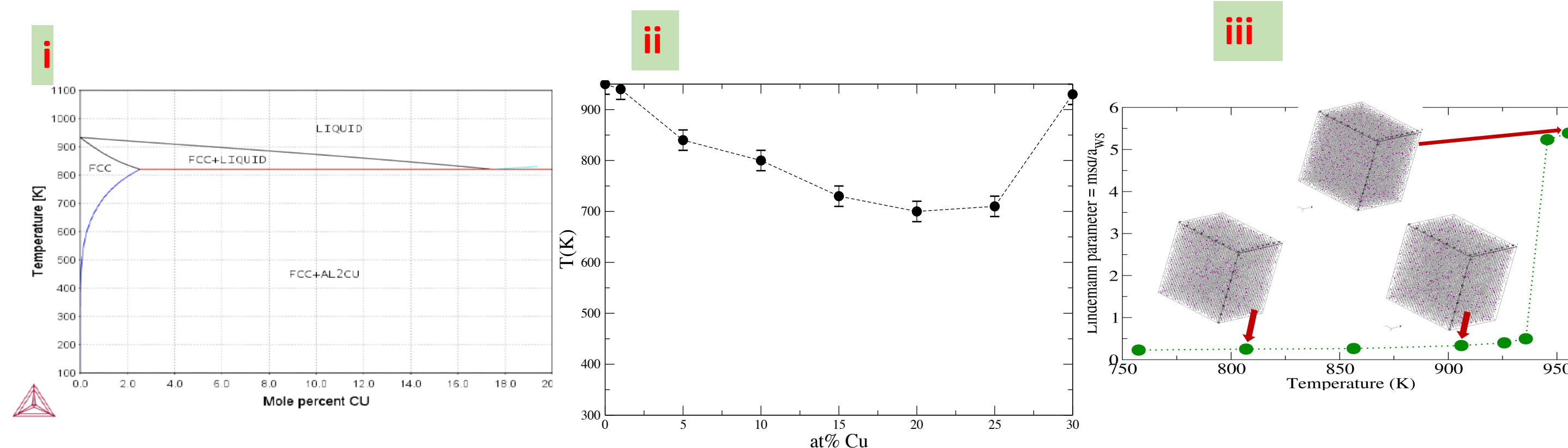
i phase-diagram of AlCu from Calphad calculations
ii Liquidus part of the AlCu phase-diagram computed from MD, corresponding to T values of zero velocity of solid-liquid interface
iii computing the solidus through Lindemann criterion as one example

Mesoscopic impact of the non-equilibrium interfacial chemistry on the solidification microstructure: Conventional solidification phase-field models are essentially based on local transport which encompasses two assumptions: 1) local equilibrium at the liquid/solid interface; and 2) linear kinetics of interface motion. However, these assumptions are considered invalid for rapid solidification, which is a process far from equilibrium inherent to AM. We will initially modify phase-field models to capture the non-local transport and highly non-equilibrium nature of rapid solidification. We will apply the extracted interfacial information from MD simulations to the mesoscopic phase-field model to relax the assumptions, and assess the impact of the non-equilibrium interfacial processes on the rapidly evolving solidification microstructures.

RESULTS

8 μm
20 μm
0.2 μm

i Preliminary results with phase-field simulation with AMPE using phenomenological kinetic models close to equilibrium. The color represents Cu composition profile.

ii MD equilibrated system for AlCu alloy at 875 K. The solid nuclei in the middle has a composition of 2% Cu and 98% Al, whereas the surrounding liquid is composed of 8% Cu and 92% Al. The sample is equilibrated at ambient pressure with a solid-liquid interface along <100> crystallographic orientation. The blue spheres correspond to Al atoms; the red to Cu.
iii Zoomed in view of the equilibrated upper solid-liquid interface.
iv Solute trapping at the partitionless solidification limit, after exposing the equilibrated sample for 48 ps to an 100K undercooling.

BENEFITS AND FUTURE WORK

The proposed multiscale approach follows the bottom-up paradigm which requires an extensive use of leadership-class HPC resources with practically more reliable quantitative outcome. In this regard, this work will open a new venue for LLNL toward the study of rapid solidification of alloys. In particular, the successful implementation of the proposed approach in LLNL's AM modeling framework will enhance its predictive capability, which will be beneficial for LLNL's entire integrated effort on the metal AM research. The proposed work is very synergetic with LLNL's general interest in developing multiscale models of different far-from-equilibrium physical phenomena, which are associated with materials under extreme conditions. Thus it will contribute in enhancing U.S. competitiveness by utilizing DOE-developed intellectual property and capabilities.

References
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