Application of Phase Field and CALPHAD Methods to Additive Manufacturing in IN625

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AM Inconel 625 As-Built Microstructure



S. Cheruvathur (NIST)

Partitioning is expected.



AM Inconel 625 Stress-Relieved Microstructure



Y. Idell and F. Zhang (NIST)

Precipitates are unwelcome.



Modeling Microsegregation in AM Inconel 625

T. Keller, G. Lindwall, S. Ghosh, L. Ma, et al., "Application of Finite Element, Phase-field, and CALPHAD-based Methods to Additive Manufacturing of Ni-based Superalloys." Acta Materialia (2017), DOI: 10.1016/j.actamat.2017.05.003. Laser Direction 1328 1587 1440 1294 1294 147 1000 50 µm 0.30 0.30 0.25 ≥ 0.20 16 Cr > 0.20 Nass fraction in 0. 14 0.10 11 (qN % 149 Mo Distance from secondary dendrite core (nm) 0.10 Nb 0.05 Fe 0 50 100 150 Distance from secondary dendrite core (nm)

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Modeling Microsegregation in AM Inconel 625

T. Keller, G. Lindwall, S. Ghosh, L. Ma, *et al.*, "Application of Finite Element, Phase-field, and CALPHAD-based Methods to Additive Manufacturing of Ni-based Superalloys." *Acta Materialia* (2017), DOI: 10.1016/j.actamat.2017.05.003.

Thermodynamic driving force for nucleation of secondary phases from γ for the enriched (interdendritic) composition, Ni–0.13 % C–13.6 % Cr–0.35 % Fe–13.9 % Mo–23.5 % Nb, at the stress relief treatment temperature.

Interdendritic composition favors precipitation. Carbides are inevitable, but intermetallics?

J				
$1143\mathrm{K}$				
Phase	$-\Delta G^{ m nuc}$			
\underline{MC}	$20.5\mathrm{kJ/mol}$			
M_2C	$15.6\mathrm{kJ/mol}$			
μ	$8.0\mathrm{kJ/mol}$			
\overline{M}_6C	$7.9\mathrm{kJ/mol}$			
BČC	$6.3\mathrm{kJ/mol}$			
$\underline{\sigma}$	$5.2\mathrm{kJ/mol}$			
Laves	$4.1\mathrm{kJ/mol}$			
$\underline{\delta}$	$3.5\mathrm{kJ/mol}$			
γ''	$3.5\mathrm{kJ/mol}$			
$M_{23}C_6$	$3.4\mathrm{kJ/mol}$			

Phase-field Model: Unary Solidification

Model free energy:

$$\begin{aligned} \mathcal{F} &= \int_{V} \left[f_{\text{bulk}} + f_{\text{bias}} + f_{\text{grad}} \right] \mathrm{d}V \\ f_{\text{bulk}} &= W \phi^2 (1 - \phi)^2 \\ f_{\text{bias}} &= L \frac{T_M - T}{T_M} p(\phi) \\ f_{\text{grad}} &= \frac{1}{2} \epsilon^2 |\nabla \phi|^2 \end{aligned}$$

Non-conserved dynamics (Allen-Cahn):

$$\begin{split} \frac{\delta \mathcal{F}}{\delta \phi} &= \frac{\partial f_{\text{bulk}}}{\partial \phi} - \epsilon^2 \nabla^2 \phi = 0\\ \frac{\partial \phi}{\partial t} &= -M \frac{\delta \mathcal{F}}{\delta \phi} \end{split}$$

Boettinger, Ann. Rev. Mater. Res. **32** (2002) 163 T. Keller & J. Guyer (NIST MSED) AM Modeling



Multicomponent Multiphase Model

Represent Inconel 625 as Cr–Nb–Ni with γ , δ , and Laves phases:

$$\begin{split} f_{\text{bulk}} &= \sum W_i \phi_i^2 (1 - |\phi_i|)^2 + \alpha \sum \phi_i^2 \phi_j^2 \\ f_{\text{bias}} &= n_\gamma f_\gamma (x_{\text{Cr}}^\gamma, x_{\text{Nb}}^\gamma) + n_\delta f_\delta (x_{\text{Cr}}^\delta, x_{\text{Nb}}^\delta) \quad f_{\text{bulk}} \\ &+ n_{\text{L}} f_{\text{L}} (x_{\text{Cr}}^\gamma, x_{\text{Nb}}^{\text{L}}) \\ f_{\text{grad}} &= \sum \kappa_i (\nabla \phi_i)^2 \\ i \in \delta, \text{Laves} \\ \frac{\partial x_j}{\partial t} &= V_m^2 M_j \nabla^2 \left[\frac{\partial f_\gamma (x_{\text{Cr}}^\gamma, x_{\text{Nb}}^\gamma)}{\partial x_j^\gamma} \right] \\ j \in \text{Cr}, \text{Nb} \\ \frac{\partial \phi_i}{\partial t} &= -M_i \left(\frac{\partial f_{\text{bulk}}}{\partial \phi_i} - 2\kappa \nabla^2 \phi_i \right) \quad \text{htt} \end{split}$$

 $f_{\text{bulk}}(\phi_1, \phi_2, 1 - \phi_1 - \phi_2)$



https://github.com/tkphd/ multiphase-interfaceplanarization

After Zhou et al., Acta Mater. 65 (2014) 270.

Ternary Analogue to Inconel 625: Cr–Nb–Ni



CALPHAD Free Energy Domain Restrictions



 γ landscape δ landscape Laves landscape

Physically reasonable, but numerically unforgiving.

Cr–Nb–Ni Phase Diagrams



Sublattices: Physically reasonable

Paraboloids: Numerically forgiving

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Simulation Software

MMSP

This repository	Search	Pull requests	Issues Marketplace	Explore	♠ +• _M •
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github.com/mesoscale/mmsp

parallel grid (MPI)

- C++, templated by type & dimension
- user supplies kernel code
- 20+ examples: phase-field & Monte Carlo, finite difference

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Early: flux from γ toward particles

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Middle: flux from γ and δ toward Laves

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Late: flux from δ toward Laves

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Cr-Nb-Ni at 1143K

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2D Evolution Trajectories

Small sample of ternary coexistence field, small domains

Hardware and Software Changes

Goals

Explore

- Compare
- Share

CPU

- Serial
- OpenMP
- ∎ TBB
- GPU
 - CUDA
 - OpenACC
- OpenCL
 KNL
 Hybrid

HiPerC

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API Reference

- CPU Specifics
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High Performance Computing Strategies for Boundary Value Problems

Ever wonder if a GPU or Xeon Phi accelerator card would make your code faster? Fast enough to justify the expense to your manager, adviser, or funding agency? This project can help answer your questions!

The example codes in this repository implement the same basic algorithm using whichever of the mainstream accelerator programming methods apply. Running the code on different parallel hardware configurations — CPU threading, GPU offloading, and CPU coprocessing — provides a benchmark of these tools using common computational materials science workloads.

hiperc.readthedocs.io

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HiPerC Diffusion: Carburizing Process

Preliminary HiPerC Diffusion Results

Preliminary HiPerC Diffusion Results

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More Interesting Benchmarks

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CHiMaD Phase Field

Integrating the phase field community

In January 2015 a group of phase field theorists and code developers met at Northwestern University to discuss ways for the community to improve code collaboration efforts. Everyone agreed that the community needs to become more open and work in a more collaborative manner.

A key factor to improving community code collaboration is to develop resources to compare and contrast phase field codes and libraries. This site aims to provide some of these resources and become a useful web service for phase field practitioners.

pages.nist.gov/chimad-phase-field

Benchmarks:

- Spinodal decomposition
- Ostwald ripening
- Dendritic growth
- Precipitation & elasticity
- Stokes flow
- Cahn-Hilliard with electrostatics

Conclusions & Future Work:

- Phase-field modeling shows competition between δ and Laves particles in a ternary analogue to Inconel 625
- Further analysis needed to distinguish ripening from reversion (interfacial vs. bulk thermodynamics), finite size effects
- Extension to larger systems with more accurate free energy requires changes to
 - \blacksquare Model formulation: Kim-Kim-Suzuki \rightarrow grand potential
 - \blacksquare Computer architecture: CPU \rightarrow GPU
 - Sublattice description or ternary system

Refactoring code for new architectures is worthwhile. It can also be easy. Contact me if you're curious: trevor.keller@nist.gov

