

Phase-Field Modeling of Non-Isothermal Microstructure Evolution in Titanium

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Motivation and Introduction

Titanium alloys, including commercially pure Ti (cp-Ti), are important for low-weight, high-strength, and corrosion resistant applications. Thermal history dictates Ti-alloy microstructures, which are determined by the transition from high-temp bcc β phase to low-temp hcp α phase and other non-equilibrium phases.

Phase-field modeling is extensively used to predict microstructure evolution, but few models fully account for non-isothermal conditions. The current work seeks to develop quantitative non-isothermal modeling of microstructure evolution for pure Ti.

Model Details

Each possible crystallographic variant is represented by a non-conserved order parameter, where the $\alpha \leftrightarrow \beta$ transformation is represented by:

$$\frac{\partial \eta_i}{\partial t} = -L \frac{\delta F}{\delta \eta_i} = -L \left(\frac{\partial f}{\partial \eta_i} - \kappa \nabla^2 \eta_i \right) \quad i=1,2,\dots,12$$

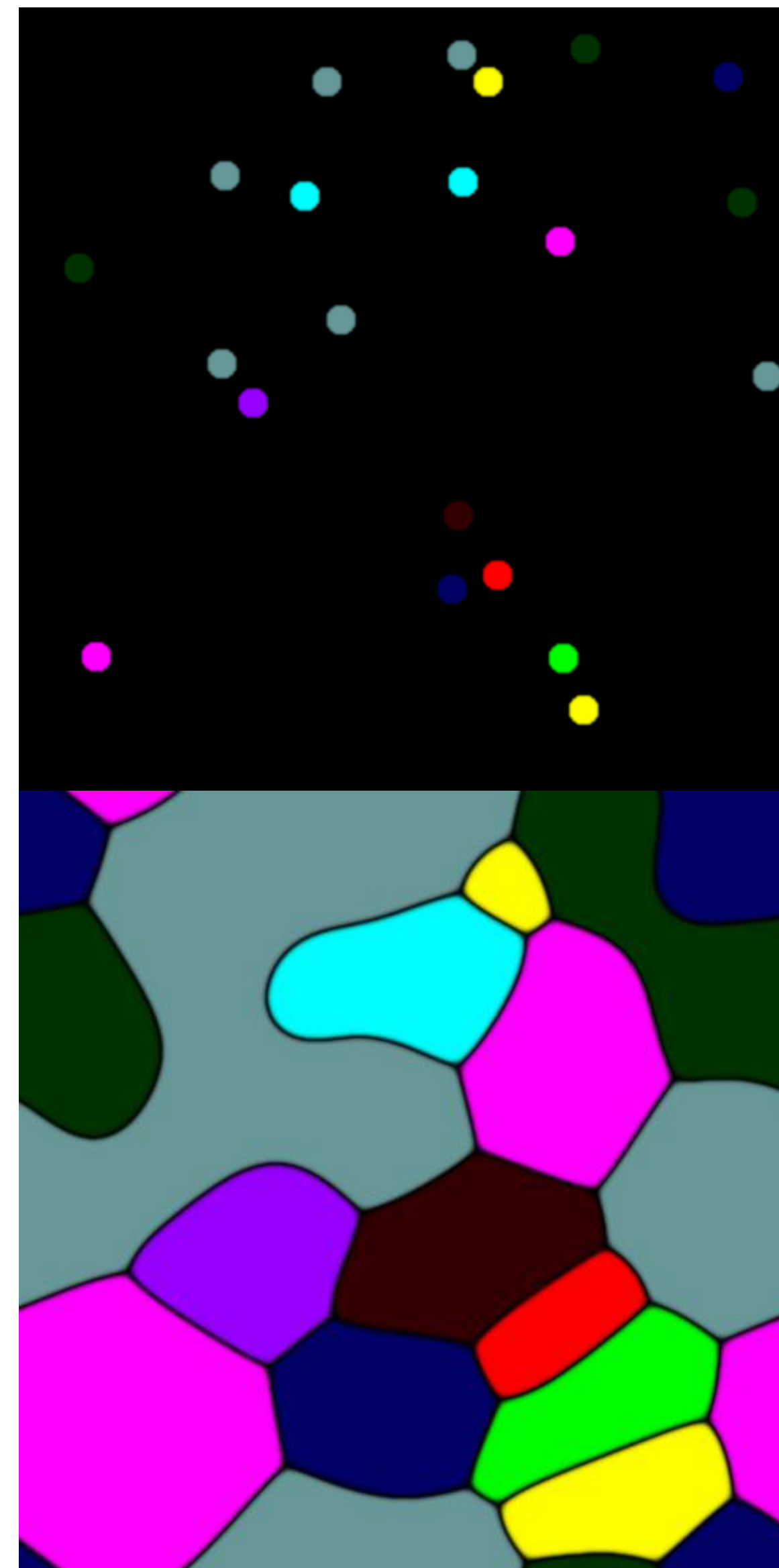
$$\frac{\partial \phi_j}{\partial t} = -L \frac{\delta F}{\delta \phi_j} = -L \left(\frac{\partial f}{\partial \phi_j} - \kappa \nabla^2 \phi_j \right) \quad j=1,2,\dots,6$$

where $\eta=1.0$ and $\phi=1.0$ indicate alpha phase and beta phase, respectively. The energy functional f incorporates a double-well function and the temperature-dependent Gibb's free energy of the phase transformation, with the equation fitted from NIST thermodynamic data. The gradient energy coefficient is κ . [1]

Non-isothermal kinetics are also accounted for by converting scaling each non-reduced time-step to a temperature-dependent value of $L(T)$:

$$\Delta t = \frac{\Delta t^*}{L(T)E}$$

where Δt is real time, Δt^* is the reduced time-step, and E is a characteristic energy.



Initial, site-saturated conditions (top), and final configuration: 100% transformation, 180,000 time-steps (bottom)

Non-isothermal Kinetics

For validation, the model results are compared to theoretical transformation kinetics. Isothermal transformations can be described by (JMAK) equations. Non-isothermal transformed fraction X can be described similarly. For site-saturated nucleation conditions (i.e. all nuclei exist at start of transformation) with random particle impingement, the theoretical equation simplifies to: [2.]

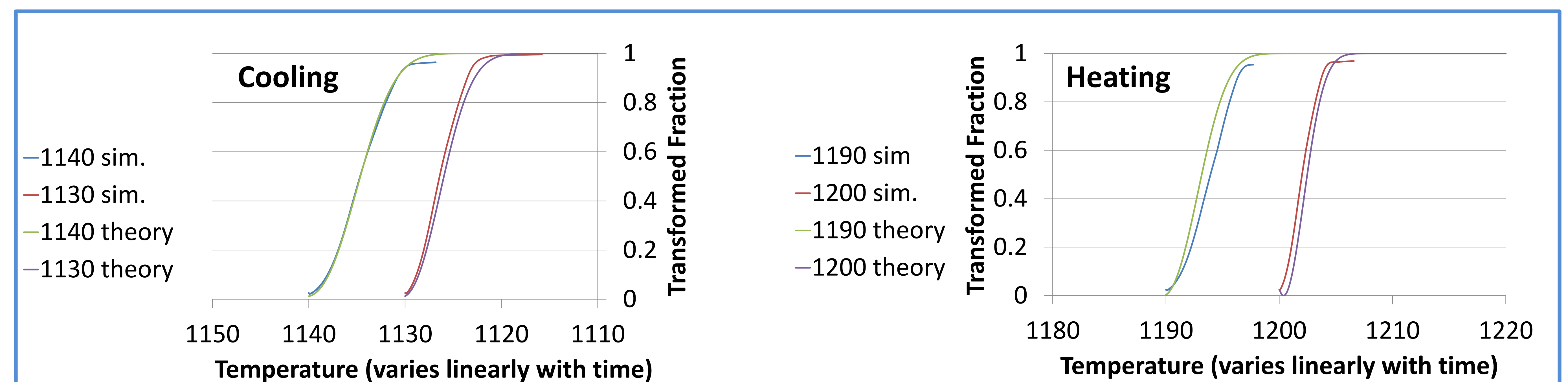
$$X = 1 - \exp \left[N g \left(\int_{\tau}^t v dt' \right)^n \right]$$

where N is number of nuclei present, g describes the geometry of the particles, n is the Avrami exponent related to geometry and growth mode, and v is interface velocity. The velocity v is temperature dependent, and relates to $L(T)$ as:

$$L(T) = \frac{\sigma}{\kappa_0} v_0 \exp \left(\frac{-G_a}{RT(t)} \right) \left(1 - \exp \left(\frac{\Delta G}{RT(t)} \right) \right) / -\Delta G$$

where σ is surface energy, κ_0 is a gradient energy coefficient, v_0 is a interface velocity pre-factor, G_a is activation energy, ΔG is the driving force (free energy), and $T(t)$ is temperature as function of time.

Simulations of isochronal (constant temperature change) cooling and heating agree well with the theoretical equations (below), and models indicate the effect of thermal history on microstructure (left). Continued efforts will verify non-isothermal nucleation behavior and important effects of elastic terms.



References:

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- [2] F. Liu, F. Sommer, C. Bos, and E. J. Mittemeijer, "Analysis of solid state phase transformation kinetics: models and recipes," *International Materials Reviews*, vol. 52, no. 4, pp. 193–212, Jul. 2007.
- [3] T. W. Heo, "Phase-field Modeling of Microstructure Evolution in Elastically Inhomogeneous Polycrystalline Materials," Pennsylvania State University, 2012.

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