Hybrid Model for the Simulation of Radiation Induced Segregation and Phase Transformation

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Introduction

Ion irradiation has been shown to cause different types of microstructural changes in materials, e.g. phase transformations [1]. In order to understand how radiation damage affects microstructural evolution, we developed a deterministic–statistical hybrid model. This model incorporates different types of radiation–generated defects to study the effects these have on the microstructure. The hybrid model uses a digitized voxelated microstructure, where each voxel's state is defined by a set of discrete order parameters and overlayed with continuum field parameters. This type of hybrid model is able to efficiently model microstructural changes by taking advantage of each method's strengths [2].

Our model was influenced by the model developed by Wiedersich et al. [3], where a set of equations is defined to describe the evolution of the defects and the atomic elements. Our model couples an equivalent set of equations with a Potts Monte Carlo model to simulate the microstructural evolution of an irradiated binary (AB) system. The deterministic equations evolve the continuum fields, which then lead to changes in the system's thermodynamics. Due to these changes, phase nucleation and transformation takes place, which is simulated by the Potts Monte Carlo model. We simulate the microstructural changes due to surface irradiation in a generalized binary material.

Microstructure Representation

- Divided into distinct order parameters
  - Discrete: grain id (orientation) and phases
    - Features with a sharp interfaces
  - Continuum: composition and defect concentration

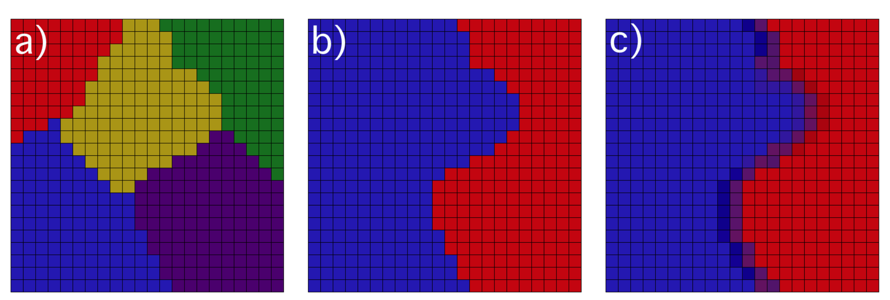

Figure 1 : Schematic showing the different types of order parameters and their inter–relationship. The order parameters used to model the microstructural evolution include: (a) grain id, (b) phase, and (c) concentration.

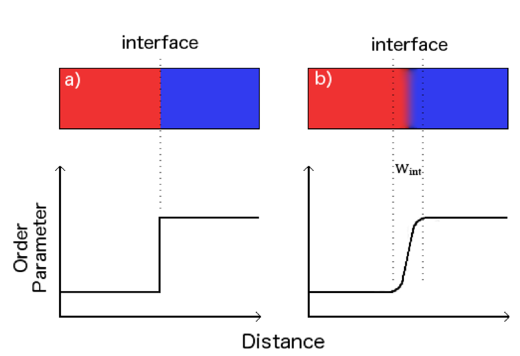

Figure 2 : Microstructural evolution has been model with both diffuse and sharp interfaces. Our hybrid model incorporates both types into an efficient description of microstructural evolution.

Radiation Damage

- Use SRIM's TRIM application to determine distributions

$$\Upsilon(z) = \Upsilon_0 \cdot \exp\left(-\left[\frac{z-\bar{z}}{\sigma}\right]^2\right) \quad (1)$$

- Energy deposited used to calculate number of net defects
  - Stochastically chosen to capture spatial variation in damage
- The number of *surviving* defects is given by *Hobler* et al. [4]

$$\underbrace{\eta_s}_{\text{Surviving}} = \underbrace{\eta_{TRIM}}_{\text{\# Defects}} \cdot \underbrace{f_{rec}}_{\text{Recombination Collision Cascade}} \cdot \underbrace{(1-2p_{rec})}_{\text{... Pre–existing Defects}} \quad (2)$$

Thermodynamics, Phase Transformation & Diffusion

- The equation of state (EoS) is defined as

$$F_{EoS} = \int_{\mathcal{V}} \left(G + \gamma|\nabla C_b|^2\right) dV \quad (3)$$

where the interfacial energy is given by the concentration gradient

- The molar free energy, G, is by the molar bulk free chemical energy (G_q), Figure 3, plus the energy of mixing (regular solution equation)

Thermodynamics, Phase Transformation & Diffusion (cont.)

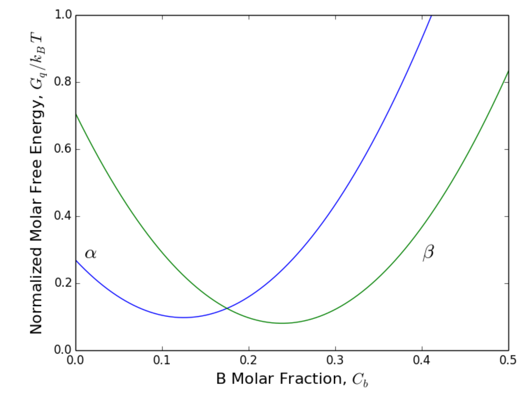

Figure 3 : Isothermal chemical free energy curves for the *AB* system being modeled. The equilibrium concentrations for this example are $C_\alpha = 0.12$ and $C_\beta = 0.23$.

Phase Transformation Events:

- Compare the bulk free energy before and after a phase change attempt event
  - Interfacial energy from EoS is replaced by a sharp interfacial energy term, i.e. Potts Monte Carlo

$$F_d = \sum_{i=1}^{N} F_{d,i} = \sum_{i=1}^{N}\left(G_i + \underbrace{J\sum_{j=1}^{n}\left[1-\delta_{s(i)s(j)}\right]}_{\text{Interfacial energy, i.e. PMC}}\right) \quad (4)$$

where δ is the Kronecker delta and $s(i)$ is the grain id of site i

- The probability of accepting the microstructural change event follows Boltzmann statistics

$$P_i = \begin{cases} 1, & \Delta F_d \leq 0 \\ \exp\left(-\frac{\Delta F_d}{k_B T}\right), & \Delta F_d > 0 \end{cases} \quad (5)$$

where $\Delta F_d = F_{d,final} - F_{d,initial}$

- Ensuring that the system evolves by energy minimization

Diffusion Equations:

- The phenomenological behavior of the compositional evolution is captured by the a set of PDE's

$$\frac{\partial C_i}{\partial \tilde{t}} = \frac{\eta_s(\vec{x})}{\Delta \tilde{t}} + \tilde{\Theta}_b \tilde{\nabla}\cdot\left(\frac{D_i}{D_b}\tilde{\nabla} C_i + C_i \tilde{\nabla} C_b\right) - \tilde{k}_{iv} C_i C_v - \tilde{S}_{fs} - \tilde{S}_{\alpha\beta} \quad (6a)$$

$$\frac{\partial C_v}{\partial \tilde{t}} = \frac{\eta_s(\vec{x})}{\Delta \tilde{t}} + \tilde{\Theta}_b \tilde{\nabla}\cdot\left(\frac{D_v}{D_b}\tilde{\nabla} C_v - C_v \tilde{\nabla} C_b\right) - \tilde{k}_{iv} C_i C_v - \tilde{S}_{fs} - \tilde{S}_{\alpha\beta} \quad (6b)$$

$$\frac{\partial C_b}{\partial \tilde{t}} = \tilde{\nabla}\cdot\left(\tilde{\nabla}\left[\frac{\partial \tilde{G}}{\partial C_b} - \tilde{\nabla}^2 C_b\right] + \tilde{\Theta}_b C_b\left[\frac{D_i}{D_b}\tilde{\nabla} C_i - \frac{D_v}{D_b}\tilde{\nabla} C_v\right]\right) \quad (6c)$$

where the "tilde" denotes that the parameter is non–dimensional

- We also include a *free surface* as a fixed sink for the radiation defects
- Then, the boundary condition at the surface is

$$\mathbf{J}\cdot\mathbf{n} = 0 \quad \text{on } \partial\mathcal{V} \quad (7)$$

Concentration Distribution

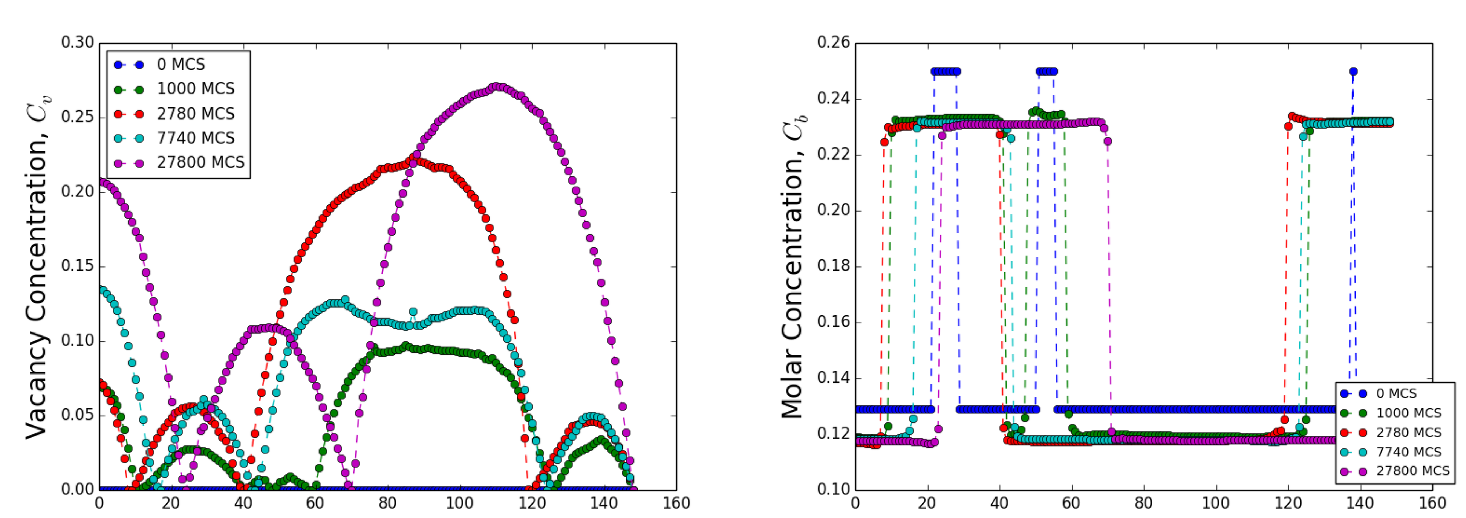

Figure 4 : We show the vacancy defect (C_v) and chemical (C_b) concentration as a function of depth. As also evident from Figure 5, there seems to be "relaxation" effect on the defect concentration as it reaches a critical density. Furthermore, it can be seen that the chemical concentration accurately matches the respective equilibrium concentration for each phase. The concentration profiles were taken across the same path (black dashed line) shown in Figure 5. We are performing parameterization studies to obtain physically sensible results to compare them to experimental results.

Microstructural and Defect Evolution

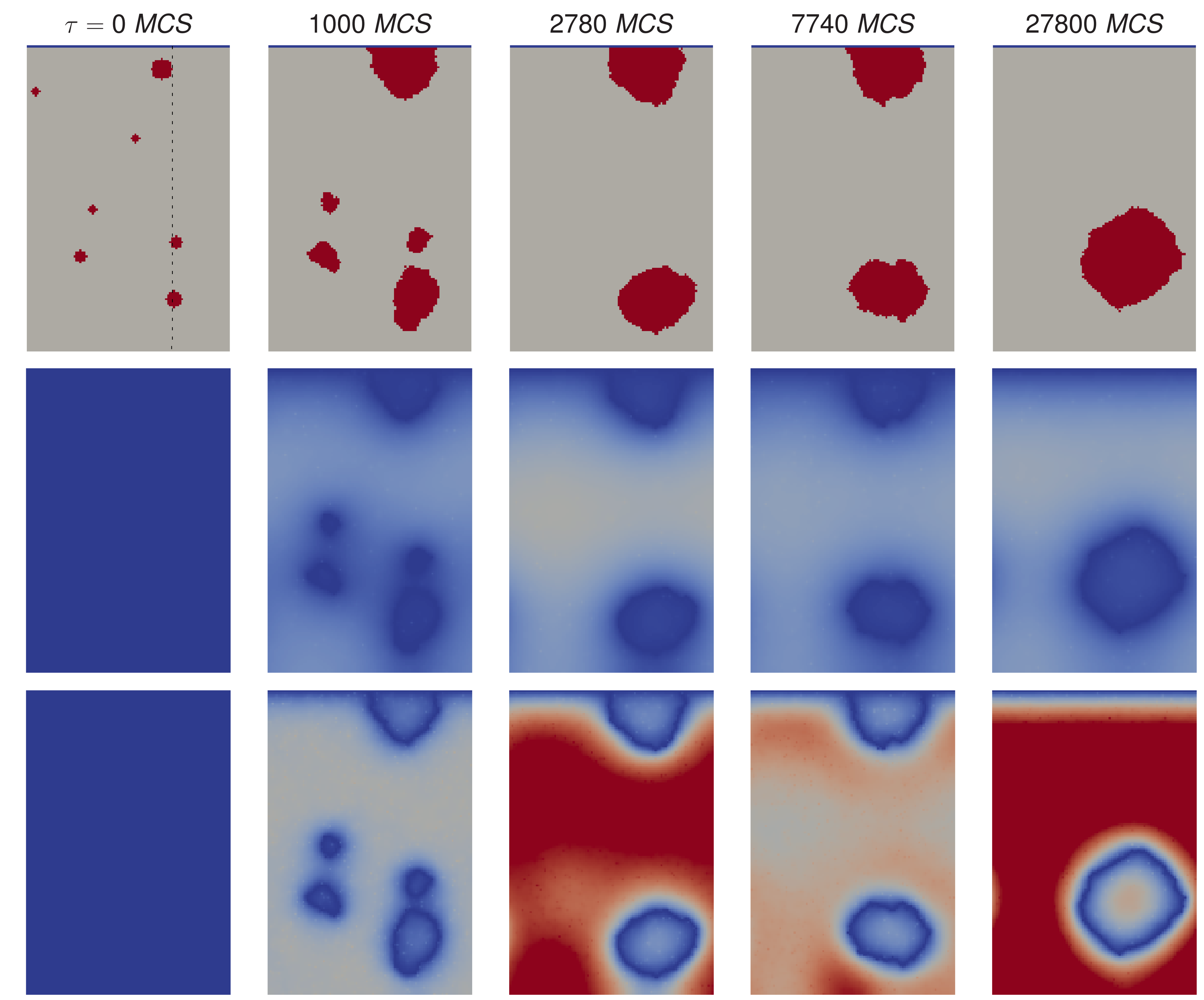

Figure 5 : Simulation results showing the evolution of the different order parameters used to evolve the microstructure. From top–to–bottom: phase (q), interstitial (C_i) and vacancy (C_v) concentrations. It can be clearly seen that the creation of these defects influences the microstructural evolution. During the initial accumulation of defects stage, the diffusion of interstitials to the sinks leads to the growth of the precipitates. Eventually, coarsening becomes the dominant behavior, as evident from the final microstructure.

Conclusion

A model that can simulate radiation–induced segregation, which then leads to phase transformation, has been demonstrated. It is a hybrid that combines deterministic and statistical approaches to simulate defect creation, diffusion, component segregation and phase transformation in a binary, two–phase system. Initially the precipitates grow by continued component segregation and later coarsening of the precipitates dominates. Initially defects densities increase with irradiation until it reaches a steady–state between defect creation, phase transformation and defect recombination.

We successfully applied a hybrid model to a radiation induced segregation and phase transformation problem:

- The hybrid model consists of a deterministic–statistical approach to simulating microstructural evolution
- We can see how radiation defect creation and evolution has an effect on the microstructural changes
- Small precipitates initially grown until coarsening dominates
- Defects are accumulated until a critical density is reached, where recombination becomes a dominant factor

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