

# Coarsening of Cu-rich Precipitates Located on Grain Boundaries in $\alpha$ -Fe Matrix

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## Introduction

Copper is being used in  $\alpha$ -Fe P/M parts as an alloying element for improving their mechanical properties by solid solution strengthening and particle strengthening. At higher operating temperature, as the Cu-rich precipitates undergo coarsening with time that cause poor tensile strength. Computational modeling of the precipitate coarsening behavior requires an understanding of its physical processes and effect of heterogeneity in the matrix. To clarify the behavior precipitate coarsening on heterogeneous regions, specific quantitative studies would be helpful. Our current simulation is obtained from a multiphase field model which uses the thermodynamics database.

## Multi-phase field model formulation

Microstructural evolution is governed by phenomenological minimization of grand potential functional;

$$\Omega(\mu, \vec{\phi}, T) = \int_V \left( \Psi(\mu, \vec{\phi}, T) + \left( \epsilon a(\vec{\phi}, \nabla \vec{\phi}) + \frac{1}{\epsilon} w(\vec{\phi}) \right) \right) dV,$$

The grand potential density  $\Psi$ , as an interpolation of individual grand potential densities of  $\Psi_\alpha$ ,

$$\Psi(\vec{\phi}, \mu, T) = \sum_{\alpha=1}^N \Psi_\alpha(\mu, T) h_\alpha(\vec{\phi}),$$

where  $\Psi_\alpha$  are functions of the chemical potential  $\mu$  and of the temperature  $T$  in the system:

$$\Psi_\alpha(\mu, T) = f_\alpha(\vec{c}^\alpha(\mu), T) - \sum_{i=1}^{K-1} \mu_i c_i^\alpha(\mu, T)$$

$c_i^\alpha(\mu, T)$  are the inverse functions of the chemical potentials  $\mu_i(\vec{c}^\alpha, T)$ .

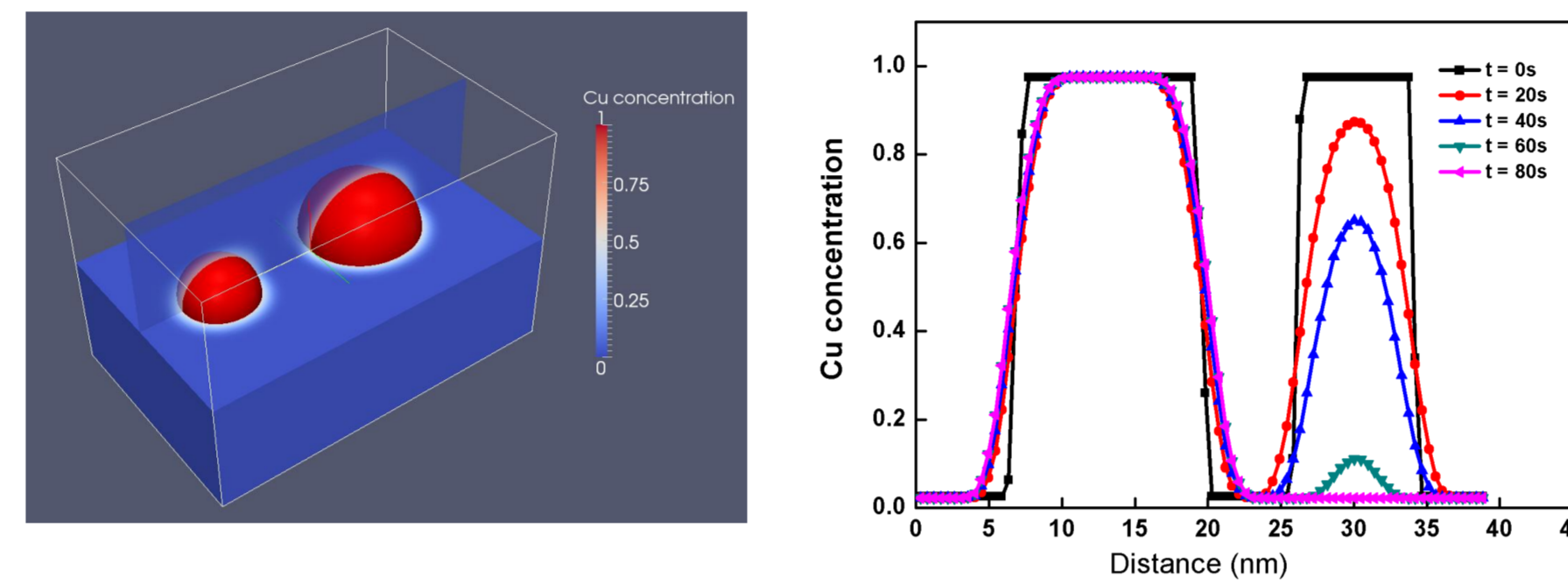
Evolution equations for the concentration fields;

$$\frac{\partial c_i}{\partial t} = \nabla \cdot \left( \sum_{j=1}^{K-1} M_{ij}(\vec{\phi}) \nabla \mu_j \right),$$

The evolution equation for the N-phase field variables,

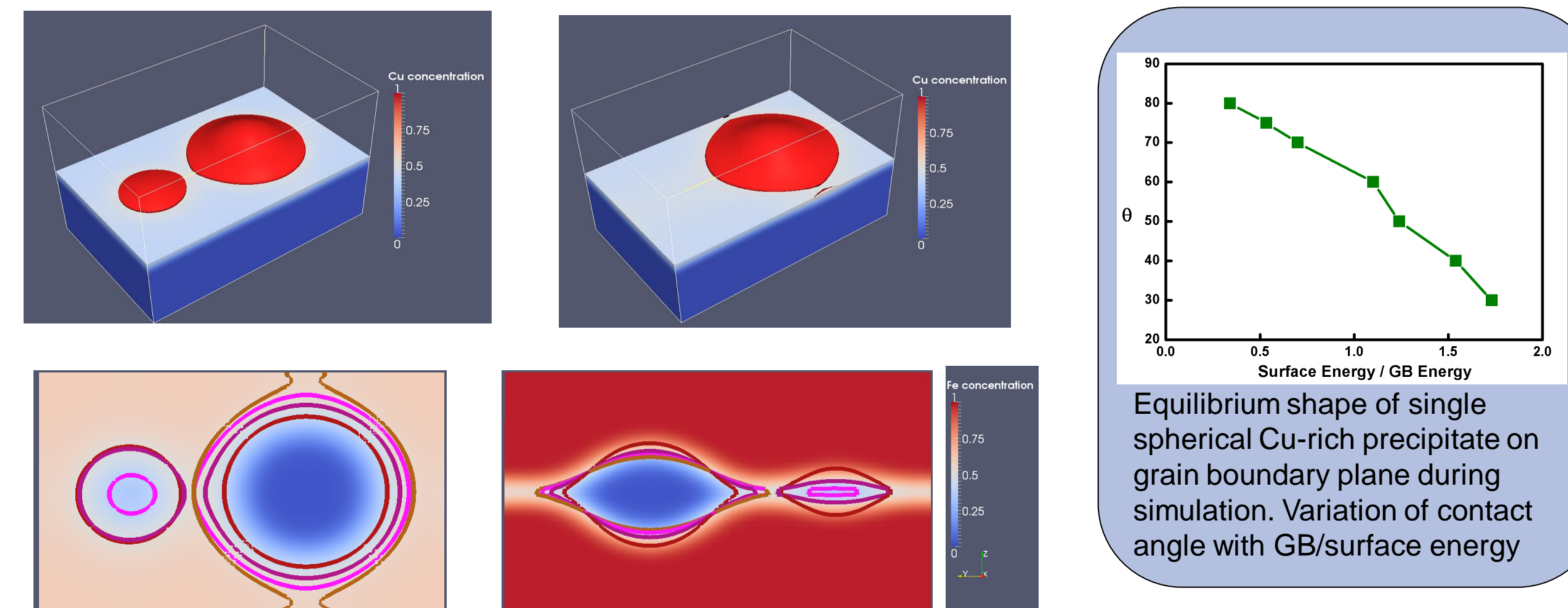
$$\tau_\epsilon \frac{\partial \phi_\alpha}{\partial t} = \epsilon \left( \nabla \cdot \frac{\partial a(\vec{\phi}, \nabla \vec{\phi})}{\partial \nabla \phi_\alpha} - \frac{\partial a(\vec{\phi}, \nabla \vec{\phi})}{\partial \phi_\alpha} \right) - \frac{1}{\epsilon} \frac{\partial w(\vec{\phi})}{\partial \phi_\alpha} - \frac{\partial \Psi(T, \mu, \vec{\phi})}{\partial \phi_\alpha} - \lambda,$$

## Cu-rich precipitates on Fe Matrix



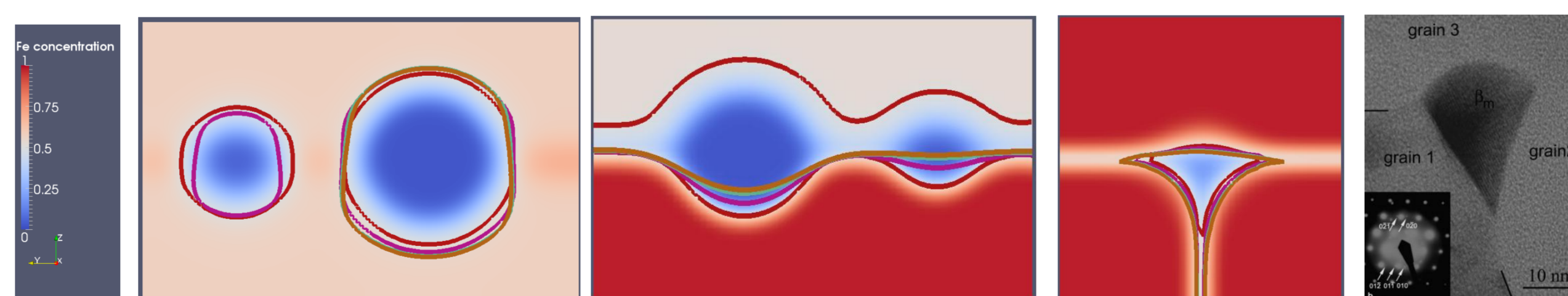
Due to the Gibbs-Thomson effect, smaller Cu-rich precipitates shrink by diffusion of Cu through the matrix grain. System grid size is 40x64x40 lattice cells. One grid size is 0.289nm.

## GB precipitates during coarsening



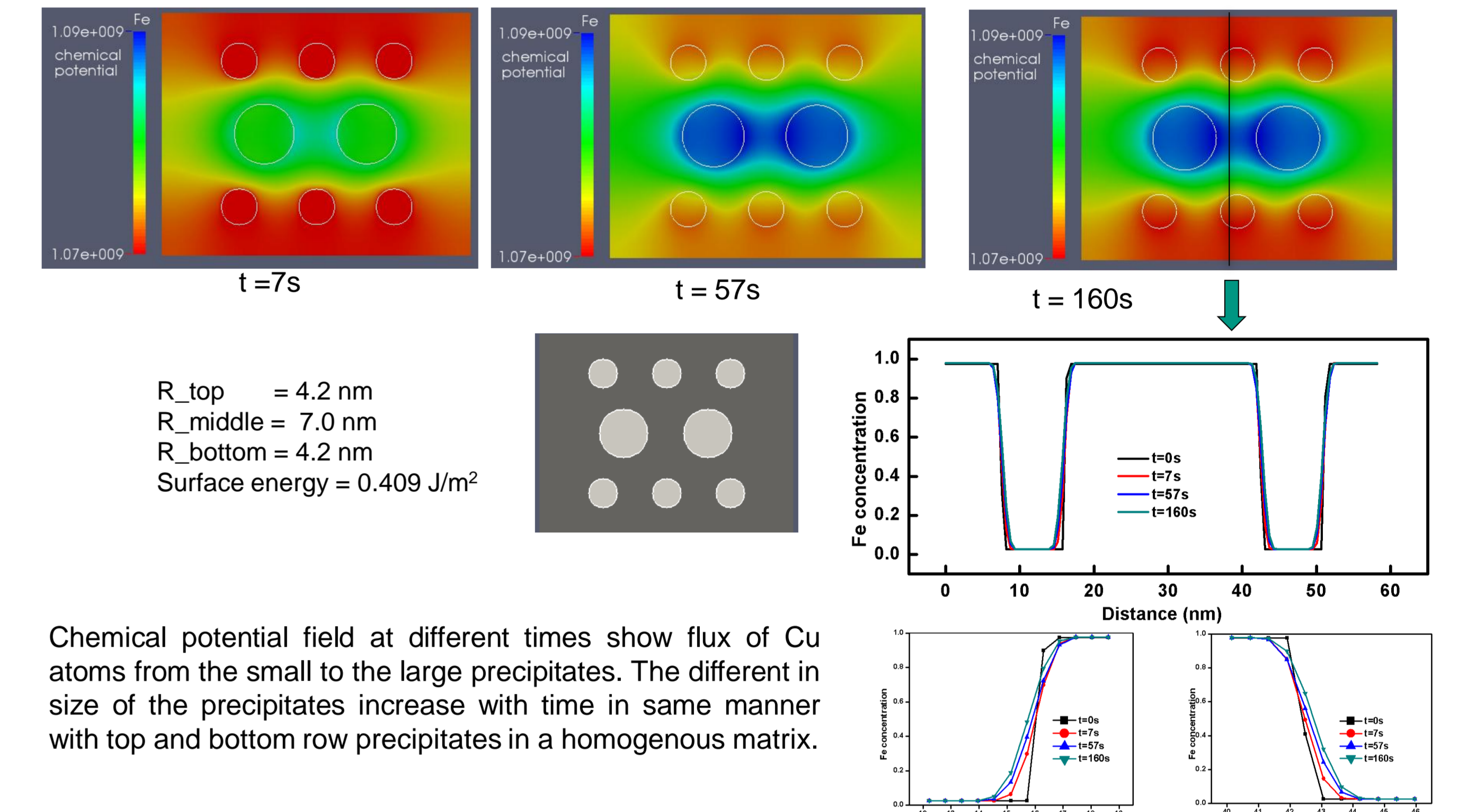
Simulation images of diffusion along grain boundary plane. System size is 40x64x40 lattice cells. The possible path of Cu transfer to the growing precipitate other than volume diffusion is diffusion along the grain boundary, visible on cross sectional view.

## Triple junction precipitates during coarsening



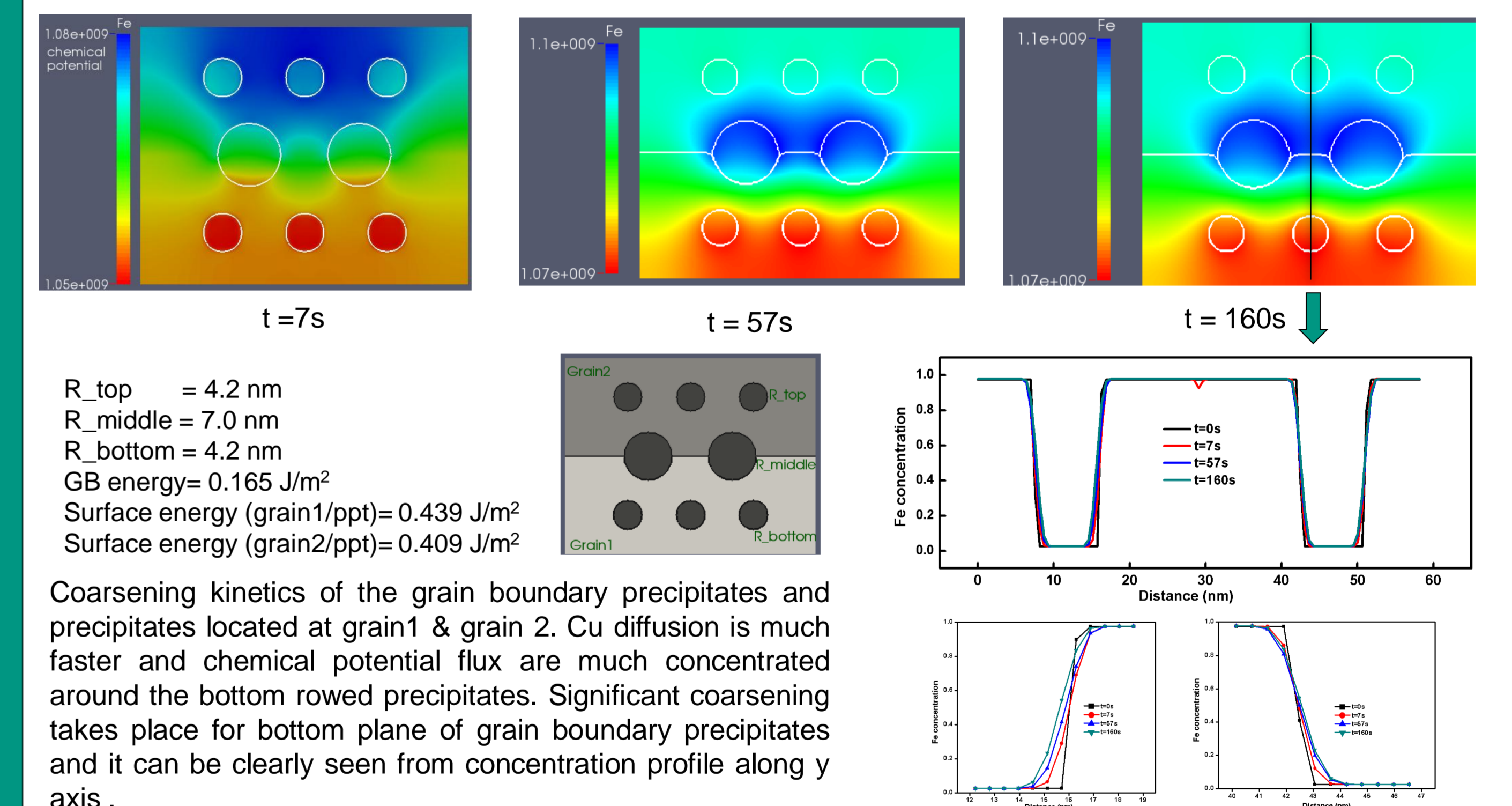
3D system has three grains with the system size of 40x64x40 lattice cells. System tends to minimize their interfacial energy and triple lines also offer kinetic advantages of the growth of precipitates. It provides larger feed area than single grain boundary plane. Concentration diffusion potential between the precipitates increases with the grain-grain interaction planes.

## Kinetics of precipitates on Single crystalline structure



Chemical potential field at different times show flux of Cu atoms from the small to the large precipitates. The different in size of the precipitates increase with time in same manner with top and bottom row precipitates in a homogenous matrix.

## Kinetics of Precipitates on Bicrystalline structure



Coarsening kinetics of the grain boundary precipitates and precipitates located at grain1 & grain 2. Cu diffusion is much faster and chemical potential flux are much concentrated around the bottom rowed precipitates. Significant coarsening takes place for bottom plane of grain boundary precipitates and it can be clearly seen from concentration profile along y axis.

## Summary

Coarsening simulations conducted with the objective of testing the theories and control of the real parameters involved. We have shown how the short-circuit diffusion paths such as surfaces and grain boundaries have a major influence on the kinetics of the processes. This study specifically relevant to the growth stage of precipitates without considering nucleation stage. However we attempt to refine the current theory which can be applied to predict the coarsening behavior of the real systems.

## References

- [1] Choudhury A, Nestler B, Phys Rev B 2007:76
- [2] David M, et al., Acta Materialia, 2012, 60, 6961-6971
- [3] Straumal B, Kogtenkova O, et al., Materials Science & Engg. A 2008, 495, 126-131