Three-Dimensional Grain Growth Model Using the Phase Field Approach

James Fletcher
Alabama A & M University

Research Alliance in Math and Science
Computer Science and Mathematics Division
Mentors: Dr. G. Sarma and Dr. B. Radhakrishnan

http://www.csm.ornl.gov/Internships/rams_05/abstracts/j_fletcher.pdf

Abstract

Metallic materials exhibit grain growth when exposed to high temperatures encountered in industrial processing. While a fine grain size is required for obtaining good ductility and toughness, large grain size is required for high temperature applications for resisting creep deformation. Therefore, a fundamental understanding of the grain growth process is required in order to optimize grain size. This research project involves computational modeling of grain growth in three-dimensions using a Phase Field approach. The input for the phase field code is an initial grain structure that is obtained using a 3-D Monte Carlo Code. The grain structure is further evolved using Monte Carlo and the Phase Field Codes separately. The resulting grain structure and growth characteristics are compared.

Introduction

Grain growth occurs due to thermally activated atomic jumps across grain boundaries. The driving force for grain growth is the reduction in the grain boundary area. This poster presents three-dimensional (3-D) grain growth computations using Phase Field and Monte Carlo techniques. The Phase Field simulations show the occurrence of a grain coalescence process which is an artifact and needs to be eliminated. One possible solution is to use a coarse grain structure obtained by a Monte Carlo technique as input to the Phase Field simulations.

Phase Field Model

In a phase field model, a polycrystalline microstructure is described by many orientation field variables, called order parameters, which describe the orientation of grains, as shown in Fig. 1. The computational algorithm for evolving grain structures is shown in Fig. 2.

$$\eta_i = 1 \qquad \sum_{j=1, j\neq i}^{n} \eta_j = 0$$

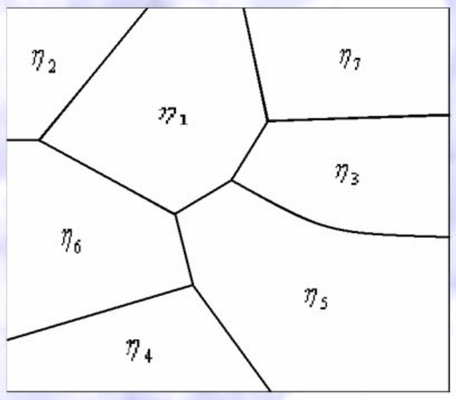

Fig. 1. Grain structure with assigned order parameters

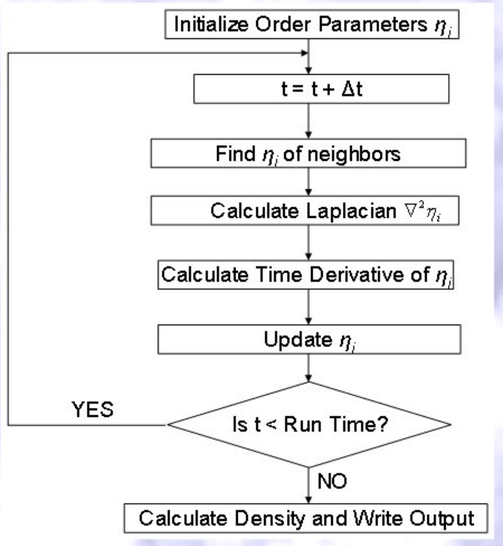

Fig. 2. Flowchart of phase field model

- An equation describes the free energy of the system of grains

$$F = \sum_{i-1}^{p}\left(-\frac{\alpha}{2}\eta_i^2 + \frac{\beta}{4}\eta_i^4\right) + \gamma\sum_{i=1}^{p}\sum_{j\neq i}^{p}\eta_i^2\eta_j^2$$

- F satisfies multiple troughs in energy corresponding to grain interior
- Order parameters are evolved using Ginzburg-Landau equation

$$\frac{\partial\eta_i(r,t)}{\partial t} = -L_i\frac{\delta F}{\delta\eta_i(r,t)},$$

- The final equation that is solved is

$$\frac{\partial\eta_i}{\partial t} = -L_i\left(-\alpha\eta_i + \beta_i^3 + 2\gamma\eta_i\sum_{j\neq i}^{p}\eta_j^2 - \kappa_i\nabla^2\eta_i\right)$$

Monte Carlo Model

In a Monte Carlo model, a polycrystalline microstructure is described by Monte Carlo numbers assigned to each site. Sites with the same MC number represent a single orientation, as shown in Fig. 3. The computational algorithm for evolving grain structures is shown in Fig. 4.

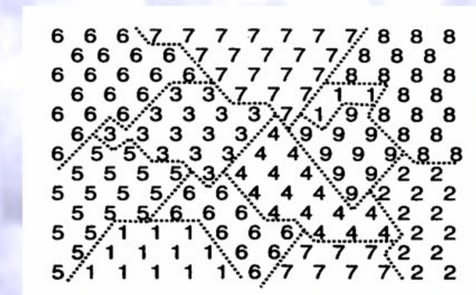

Fig. 3. Grain structure with assigned MC numbers

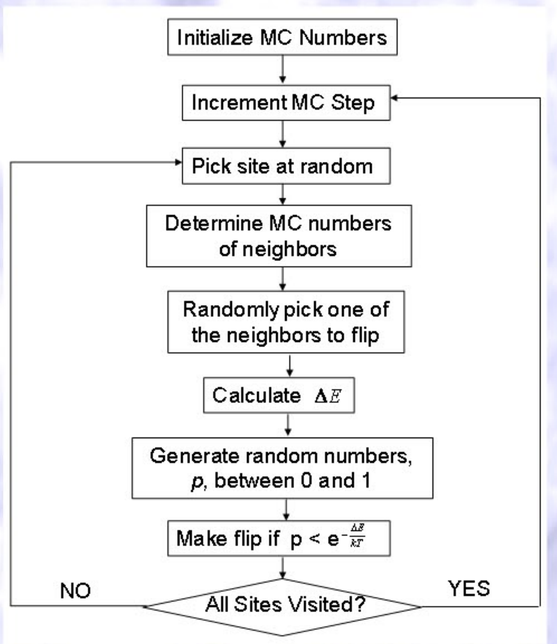

Fig. 4. Flowchart of Monte Carlo model

Summary of Results

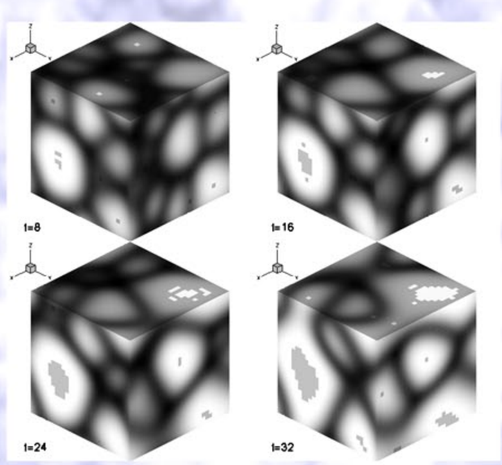

Fig. 5. Phase field simulation showing grain coalescence

Fig. 5 shows grain coalescence due to limited number of order parameters. Using a coarse grain structure as input, with as many order parameters as grain orientations eliminates grain coalescence, as shown in Fig. 6. Monte Carlo simulation with the same initial grain structure as in Fig. 6 also shows no coalescence (Fig. 7).

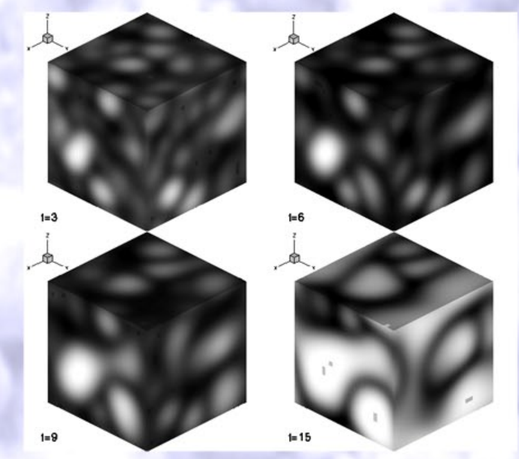

Fig. 6. Phase field simulation showing absence of grain coalescence

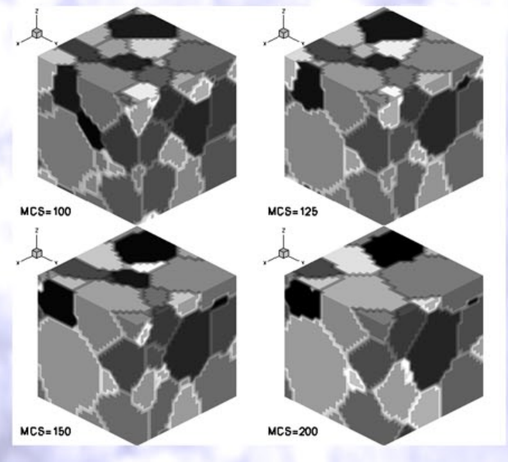

Fig. 7. Monte Carlo simulation showing absence of grain coalescence

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