Investigating the effects of grain boundary energy anisotropy and second-phase particles on the grain growth of an HCP metal

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Introduction

In recent years, a drastic effort has been put forth by material scientists to model the complexities associated with the grain boundaries of common alloys and pure metals. Grain boundaries are highly influential in determining a grain's microstructural anatomy, an anatomy that evolves through various material processing. Predicting and controlling the microstructural evolution during material processing is vital to material development and structural design, as the grain microstructure determines mechanical and material properties such as Young's modulus, ductility, and hardness.

Grain Growth

The heating process of metals leads to a phenomenon known as grain growth by which a number of grains expand in size while others shrink. With heating, grain growth results from excess free energies at the grain boundaries, resulting in a thermodynamically unstable system. To reach a state of equilibrium, grain growth occurs to reduce the total grain boundary area, thus the total grain boundary energy.

Previous models have done much to further the knowledge of grain growth, but many of these models did not consider the effects made by the presence of second-phase particles or grain boundary energy anisotropy on the microstructural evolution of hexagonal-close packed (HCP) metals.

Phase-Field Model

The phase-field model was used because it eliminates the need to track interfaces during microstructural evolution. This removes the need to make previous assumptions on the shape or mutual distribution of the grains. The time dependent variables of the phase-field method are a set of partial differential equations which are solved numerically. The phase-field method is derived with general thermodynamic and kinetic principals in mind. Material specific properties must be introduced into the model through phenomenological parameters which are derived by experimental and theoretical results.

Using the phase-field model, a polycrystalline microstructure can be described by numerous orientation field variables or non-conserved order parameters.

$$\eta_i(\mathbf{r},t) \qquad i = 1, 2, \dots n$$

where n is the number of different orientations. The total grain boundary energy is a function of these field variables. The free energy of the system including the inert particles can be determined by

$$F = \int_V \left[f(\eta_1, \eta_2, \dots, \eta_n) + \sum_{i=1}^{n} \frac{\kappa_i}{2} (\nabla \eta_i)^2 \right] dV$$

where κ is the gradient energy coefficient.

The local free energy density, f, takes the form

$$f(\eta_1, \eta_2, \dots, \eta_n) = \sum_{i=1}^{n} \left[-\frac{\alpha}{2} (\eta_i)^2 + \frac{\beta}{4} (\eta_i)^4 \right] + \gamma \sum_{i=1}^{n} \sum_{j \neq 1}^{n} \eta_i^2 \eta_j^2 + \varepsilon\, \Phi^2 \sum_{i=1}^{n} \eta_i^2$$

where α, β, γ, and ε are phenomenological parameters based on the material's properties. When Φ is inside a particle the value is one and when outside a particle the value is zero.

In order to account for misorientation angles between adjacent grains, θ_{ij}, which is the basis for anisotropic grain boundary energy, the relationship between the gradient energy coefficient and the grain boundary energy is shown to be

$$\kappa_i = \bar{\kappa}_i\, E^2(\theta_{ij})$$

where $\bar{\kappa}$ is a constant.

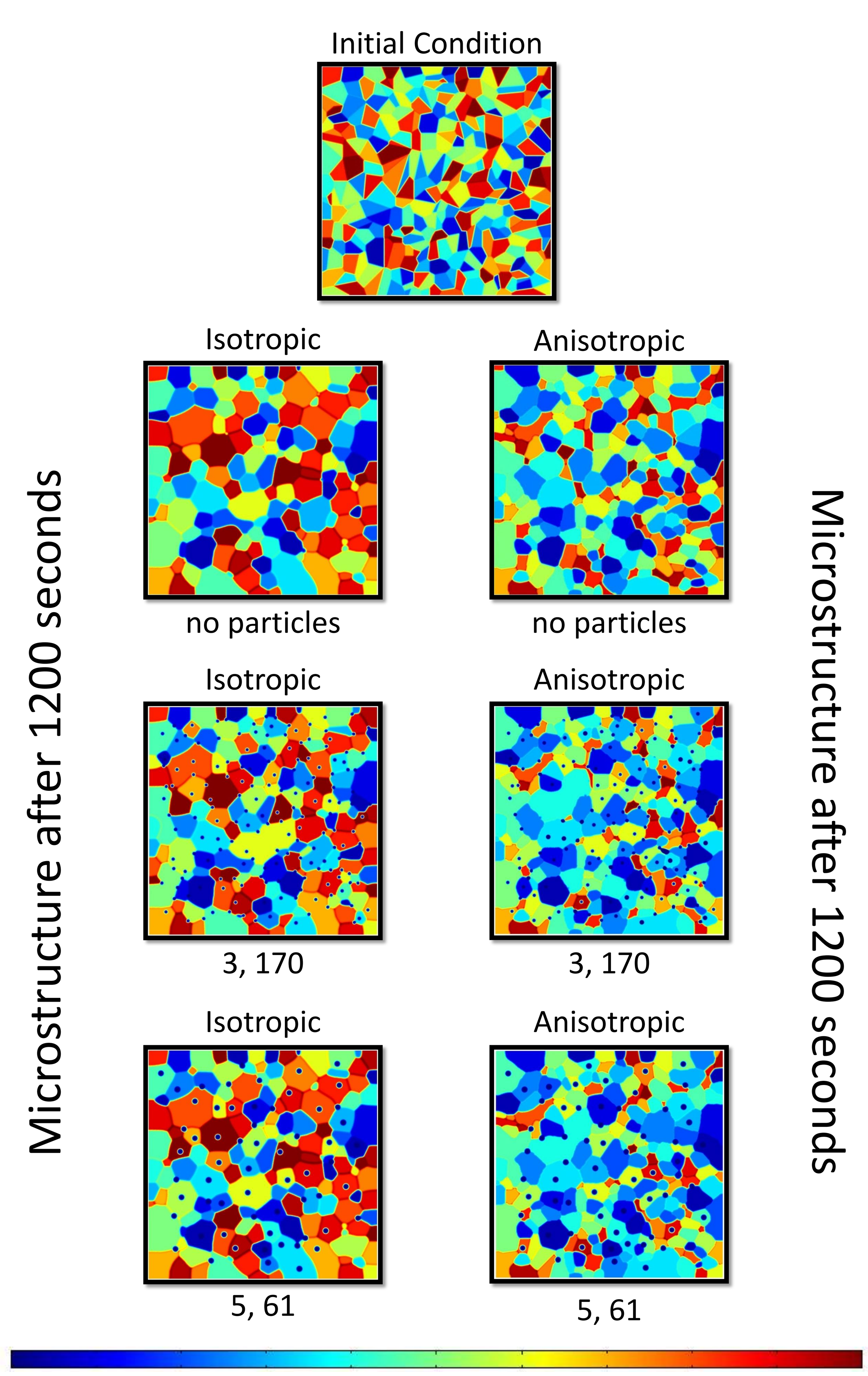
When considering large misorientation angles, the grain boundary energy was expressed as

$$E(\theta_{ij}) = E_0 \sin(3\theta_{ij}) \left[1 - r \ln\left|\sin(2.5\theta_{ij})\right|\right]$$

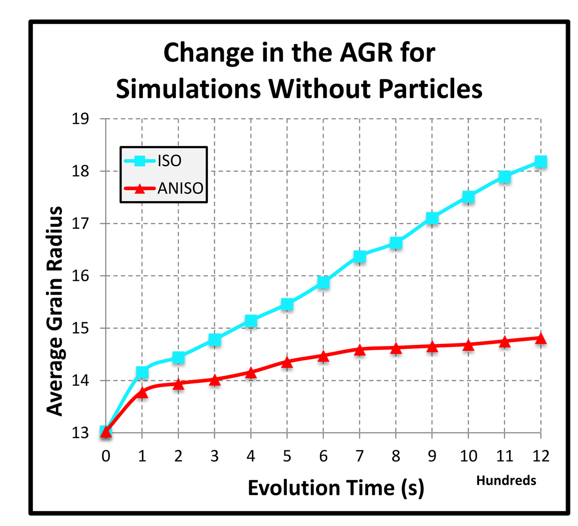
where E_0 is a material constant and r is a constant value.

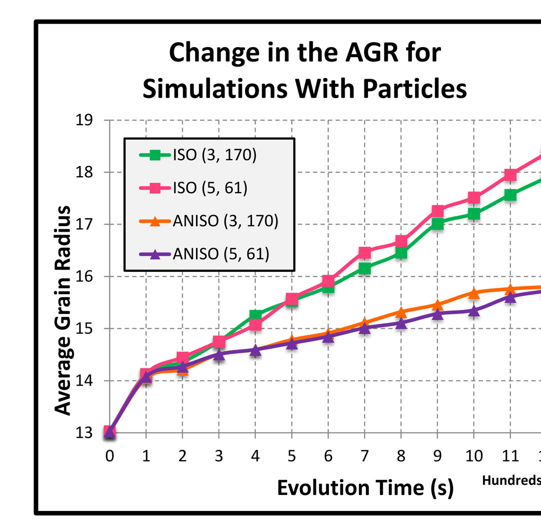
Results

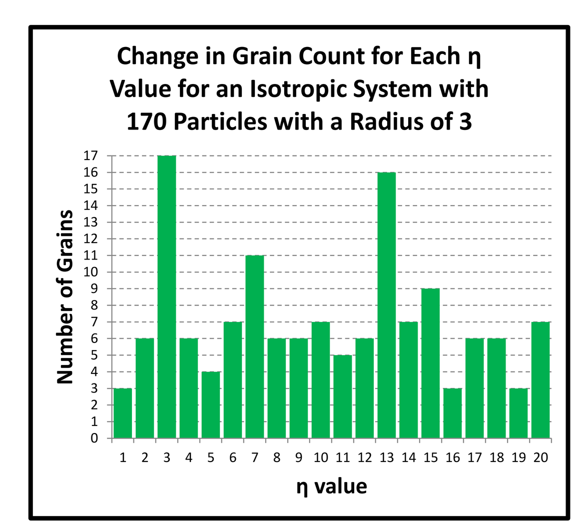
Both the isotropic and anisotropic models were simulated using COMSOL Multiphysics, which is a finite element analysis, solver, and simulator. The first figure shows the initial grain microstructure followed by the end of time (1200 s) microstructure change. For the simulations with second-phase particles, the particles had a radius of 3 and 5, with a particle count of 170 and 61 respectively.

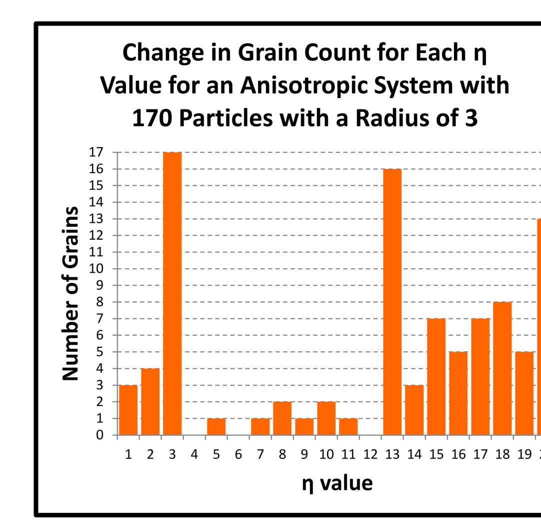


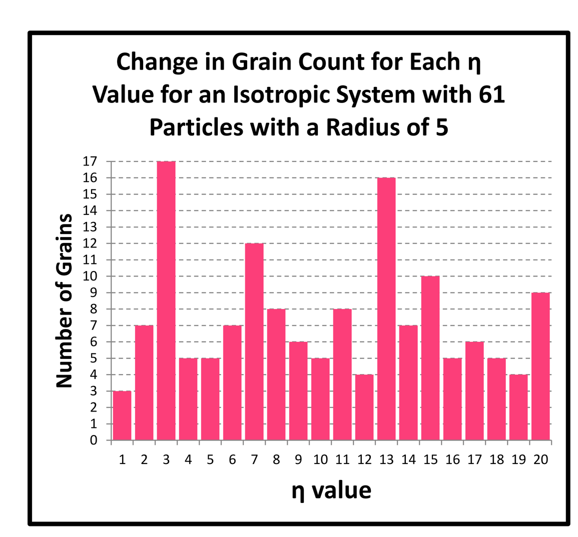
The Plots below show the change in the average grain radius (AGR) for the entire system and the change in number of grains for each η value over the evolution time.

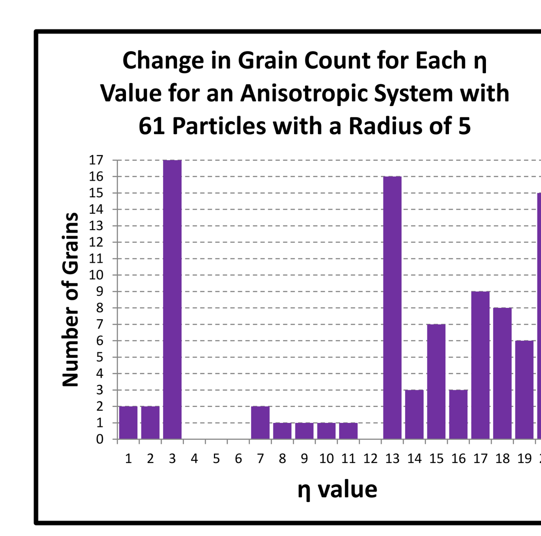












Conclusion

Many differences can be noticed when comparing grain growth of and HCP metal while considering grain boundary energy anisotropy versus isotropic conditions. Some examples are:

- The isotropic model over predicts the rate of grain growth.
- Grains with η values of 3 and 13 disappear completely for both the isotropic and anisotropic models.
- For the anisotropic simulations, η values 4 through 12 experience the least amount of grain count reduction.
- The second-phase particles' volume fraction affects the rate of grain growth independently from the particles' radius.

References

1. M. A. Zaeem, H. E. Kadiri, P. T. Wang, and M. F. Horstemeyer, "Investigating the effects of grain boundary energy anisotropy and second-phase particles on grain growth using a phase-field model," *Computational Materials Science*, vol. 50, no. 8, pp. 2488-2492, 2011.
2. D. Fan and L. Q. Chen, "Computer simulation of grain growth using a continuum field model," *Acta Materialia*, vol. 45, no. 2, pp. 611–622, 1997.
3. N. Moelans, B. Blanpain, and P. Wollants, "An introduction to phase-field modeling of microstructure evolution," *Calphad*, vol. 32, no. 2, pp. 268-294, Jun. 2008.