

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

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EXTENDED ABSTRACT

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. 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 of materials during manufacturing processes 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. Specifically, high temperature processes lead 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 takes place to reduce the total grain boundary area, thus the total grain boundary energy.

Since researchers began investigating the use of computer simulations to characterize grain growth, many advances have been made to understand and predict the grain growth phenomenon of face-centered cubic (FCC) metals. Numerical methods have been utilized such as the sharp interface, Monte Carlo, continuum field, and phase-field methods to characterize grain growth. 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. There are several HCP metals such as magnesium and zirconium which are of great interest to industries. Magnesium appeals to the automotive and aerospace industry because it provides a lightweight, high-strength alternative to commonly used metals steel and aluminum. Replacing steel and aluminum with magnesium eases the ability to create more fuel efficient vehicles. Zirconium alloys are the primary materials for nuclear energy power plants where safety is a main concern when choosing materials.

This work was created to study the effects made by inert second-phase particles and grain boundary energy anisotropy on the microstructure evolution of an HCP crystal system using the phase-field method. The phase-field model was used because it eliminates the need to track interfaces during microstructural evolution, as well as making it possible to include grain boundary energy anisotropy and second-phase particles without enforcing extra complexity to the governing equations of grain growth. The simulations show that not only do second-phase particles reduce or inhibit grain growth, but the effect of grain boundary energy anisotropy also reduces the kinetics of grain growth. The simulations were also compared to previous models where isotropic conditions were explored.