11th. World Congress on Computational Mechanics (WCCM XI)
5th. European Conference on Computational Mechanics (ECCM V)
6th. European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

A PHASE FIELD MODEL FOR THE STABILIZATION OF NANOCRYSTALLINE MICROSTRUCTURES WITH SOLUTE SEGREGATION

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Keywords: *Phase Field Model, Microstructural Evolution, Nanocrystalline Materials, Mesoscale Model*

Creating nanocrystalline microstructures are one route to creating materials with superior strength and hardness, or tunable electrical properties. The Hall-Petch relationship indicates that the achieving nano-crystalline grain sizes should enhance these properties in a material.[1-2] However, decreasing the average grain size increases the amount of grain boundary area, and thus leads to a system with a very large driving force for grain growth, and unstable microstructures, which may even demonstrate grain growth at room temperatures.[3] To achieve stable nanocrystalline microstructures in some systems, stabilization with a solute that preferentially segregates to grain boundaries is proposed. A solute past its solubility limit will collect at grain boundaries, and the driving force for grain growth would be offset by the energy of adding solute past the solubility limit into the grain crystal. A theoretical model, termed the Regular Nanocrystalline Solution

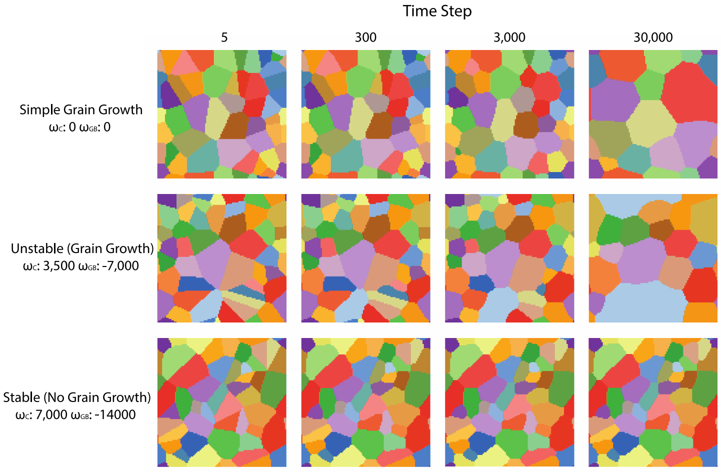

Figure 1: Microstructural evolution over time as a function of order parameters of the crystalline and grain boundary regimes.

(RNS) model, proposed by Schuh *et al*. gives a theoretical basis for this with macroscopic arguments.[4]

Here, we report the use of a phase field model to simulate this behavior at the grain structure scale in two dimensions. A phase field model has been developed which includes diffusion of solute and to include the RNS model. This model demonstrates, based on thermodynamic inputs and concentration of solute, a stabilization or lack thereof of the grain structures, and indicates whether or not the system is stable against phase separation. In general, stabilization occurs as a function of both the order parameter at grain boundaries and in the crystal, a the combination of the two creates the driving force for stabilization. The order parameter in the crystalline region is primarily responsible for phase separation, as expected. In cases with driving forces insufficient for stabilization, slowing of grain growth is observed.

Future work includes expanding this work into three dimensions, and parameterizing the system to model actual physical systems, and allow for predictive power in determining the stability of grain boundaries.

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