Three-Dimensional Grain Growth Model Using the Phase Field Approach

Grain boundaries are defects in a polycrystalline material that cause the free energy of the material to increase. A low overall energy can be established in the material if the amount of grain boundary area is reduced by grain growth. Grain growth involves the movement of grain boundaries, which allows larger grains to grow and smaller grains to shrink and eventually disappear. The growth of the grains is related to the minimal amount of energy needed for an atom to jump across the boundary. The driving force for grain growth to occur is the reduction in the grain boundary area. Therefore, the tendency of polycrystalline materials, when heated is to transform into materials that have a larger average grain size. This research project involves development of a three-dimensional parallel code for simulating the micro structural grain growth of a material using the phase field approach. The new code will be generated by modifying an existing grain growth code which uses a Monte Carlo approach. This technique will be used to simulate grain structures in large 3-D domains using the phase field model which will be compared to the grain structures produced using the Monte Carlo approach.

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