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A NEW LEVEL SET-FINITE ELEMENT FORMULATION FOR ANISOTROPIC GRAIN GROWTH

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Grain growth in metallic materials is often detrimental to the desired properties of finished components. As such, predicting the evolution of a microstructure undergoing grain growth under specific conditions of temperature and stress is crucial to controlling the microstructure, and therefore the properties, of formed metal parts.

Even so, a grain boundary Γ is a complex 5 dimensional object [1] that evolves in order to minimize thermodynamic potentials [2] and whose movement is thermally activated. The intrinsic properties of these boundaries vary based on crystallographic variables, the misorientation M, as well as topological ones, the normal to the grain boundary n, which vary in space. This means that quantities commonly associated to grain boundaries such as grain boundary energy, γ, or mobility, m, are not constants for a given material at a given temperature, but functions of the grain boundary character $B = (M, n)$. Models for driving forces do exist for normal dependent grain boundary energies $\gamma(n)$ [2]. However, the dependence of the grain boundary energy to crystallographic variables $\gamma(M)$, and more notably the gradients of this component of the energy, is not clearly formulated in the classical models for grain growth.

This work aims to formulate, develop and implement a grain growth simulation framework that can take into account aspects of the gradient of anisotropy of grain boundary energy using a level-set (LS) description of the microstructure and a finite element (FE) resolution of the physical problem. This framework is tested for high ratios of anisotropies, with the max-min ratio of energy values of the order of ten (the order of a twin boundary with respect to a general grain boundary). The behavior of anisotropic systems in this new formulation is different and closer to analytical values as compared with anisotropic systems in the classical formulation of the problem. The new formulation is able to predict the equilibrium angles of triple junctions associated with the energies of the boundaries that meet at the triple point. In polycrystal simulations, the results in terms of microstructural evolutions and their kinetics follow new tendencies as compared with results from classical formulations.

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