A Statistical and Multiscale Perspective on Solute Induced Embrittlement for Intergranular Fracture

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Abstract

Intergranular fracture is a common form of fracture in polycrystals and can be influenced by the presence of solutes (for alloying) and impurities at grain boundaries (GBs). One approach to assess the influence of solute segregation to a GB on intergranular fracture is via the calculation of an embrittling potency. Historically, studies have reported embrittling potency as a single, scalar value, assuming a single segregation site of importance at a GB and a particular cleavage plane. However, the topography of intergranular fracture surfaces is rarely known a priori. Thus, the objective of this work is to take a statistical ensemble approach to solute embrittling potency, where distributions of embrittling potencies are computed via atomistic simulations and such calculations motivate the use of local fracture property distributions in phase-field fracture simulations. Specifically, atomistic calculations are used to compute embrittling potency distributions for Cr segregation to GB sites at two Ni $< 111 >$ symmetric tilt grain boundaries. The average embrittling potency for a particular GB site, considering the ensemble of fracture permutations, is not equal to the embrittling potency computed using the lowest energy fracture path. Then, phase-field fracture simulations are performed where the local fracture toughness of a GB within a two-dimensional polycrystal is sampled from a distribution that depends on local solute composition and GB type. Assigning local properties to GBs stochastically influences the global stress-strain response of the polycrystal, the stress necessary for fracture initiation, and the fracture path, relative to the case where each GB has uniform fracture properties. The effect of different distribution widths for solute induced embrittlement is also explored.

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