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Computational simulations of intergranular fracture of polycrystalline materials and size effect

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Abstract

Grain boundaries are important elements associated with micro-structural heterogeneity in polycrystalline materials. The influence of the grain boundary character distribution on intergranular fracture of polycrystals is investigated in this paper. Considering the random heterogeneity of materials, a two-dimensional stochastic finite element method (SFEM) is used to simulate the intergranular damage and failure process of polycrystals. The impact of the fraction and distribution of random grain boundaries on the fracture behavior is discussed, and the effect of model size on results is also evaluated.
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1. Introduction

Grain boundaries and interphase boundaries strongly affect the mechanical properties in polycrystalline materials. The Hall–Petch effect is a well-known example. Intergranular brittleness is another detrimental effect of grain boundaries on mechanical properties. Grain boundaries can be preferential sites for crack nucleation and propagation.

Based on the coincident-site lattice model (CSL), grain boundaries can be geometrically described by a parameter, Σ, a measure of the reciprocal density of coincident lattice sites. It has been found that the propensity for intergranular fracture is closely related to the type and structure of grain boundaries. Low angle boundaries and certain special boundaries with $\Sigma < 29$ are found to confer high resistance to intergranular fracture [1]. Therefore, $\Sigma < 29$ boundaries can be referred as special boundaries and $\Sigma > 29$ as random

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boundaries. The optimization of the grain boundary character distribution (GBCD) and the grain boundary connectivity are a key to produce desirable bulk mechanical properties in both structural and functional polycrystalline materials [2].

In this paper, a micro-mechanical stochastic finite element method is used to model the intergranular micro-crack initiation and evolution in polycrystalline micro-structures. The heterogeneity and grain boundary character distribution are considered. Cohesive interface elements are embedded along grain boundaries to simulate initiation and evolution of micro-cracks.

2. Computational model

We shall focus on the fraction and distribution of random grain boundaries and their effect on the intergranular fracture. The material data for aluminum polycrystal are taken as an example in the model, though it is not a typical material for grain boundary engineering because of its relatively lower faction of special grain boundaries. The stiffness data of aluminum single crystal are taken from Ref. [3] that

$$C_{11} = 108.2\ \text{GPa}, \quad C_{12} = 61.3\ \text{GPa}, \quad C_{44} = 28.5\ \text{GPa}, \quad 2C_{44}/(C_{11} - C_{12}) = 1.22$$

where the last parameter, $2C_{44}/(C_{11} - C_{12})$, describes its elastic anisotropy. Single crystal of aluminum shows little elastic anisotropy.

The crystal-plasticity-based computational micro-mechanic models can offer better prediction of the local deformation and texture evolution in polycrystals than continuum elastic–plastic theory [4]. As our interest is the intergranular fracture, the following continuum elastic–plastic stress–strain relationship of individual grain is adopted [5],

$$\sigma = \begin{cases} E\varepsilon & (\varepsilon \leqslant \varepsilon_0^e) \\ \sigma_0^e + E'(\varepsilon - \varepsilon_0^e) & (\varepsilon_0^e < \varepsilon \leqslant \varepsilon_{01}^e) \\ \sigma_{01}^e + k(\varepsilon - \varepsilon_{01}^e)^{1/2} & (\varepsilon_{01}^e < \varepsilon) \end{cases} \tag{1}$$

where ε_0 and σ_0 are the equivalent yielding strain and stress, respectively, E' is the hardening coefficient in stage I, ε_{01} and σ_{01} are the equivalent strain and stress, respectively, when stage I is finished, and k is a material parameter.

A multi-body contact-interface algorithm describing the kinematics at the grain boundaries is used to simulate crack initiation and propagation. A cohesive zone model through a so-called "spot welds" in the ABAQUS code [6] is employed to simulate the intergranular cracking. It is assumed that a spot weld carries a force normal to the surface onto which the node is welded, F^{n}, and a shear force tangent to the surface, F^{s}. Once failure is detected, the weld constraint is relaxed linearly over a time period T_{f}. Hence the failure initiation and post-failure behavior of a spot weld is described by,

$$\left(\frac{\max(F^{\text{n}}, 0)}{F_{\text{f}}^{\text{n}}}\right)^2 + \left(\frac{F^{\text{s}}}{F_{\text{f}}^{\text{s}}}\right)^2 = \left(1.0 - \frac{t}{T_{\text{f}}}\right)^2 \tag{2}$$

where F_{f}^{n} is the force required to cause failure in tension, F_{f}^{s} the force required to cause failure in pure shear, and t the time since the initial failure of the weld is detected. If the normal force is compressive, it is replaced by zero in Eq. (2).

Eq. (2) can be converted into stress and strain description as:

$$\left(\frac{\max(\sigma^{\text{n}}, 0)}{\sigma_{\text{cr}}^{\text{n}}}\right)^2 + \left(\frac{\sigma^{\text{s}}}{\sigma_{\text{cr}}^{\text{s}}}\right)^2 \leqslant \left(1.0 - \frac{\Delta\varepsilon}{c}\right)^2 \tag{3}$$

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