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Homogenization scheme for brittle intergranular decohesion in polycrystalline aggregates

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ABSTRACT

The overall fracture behaviour of polycrystalline aggregates is strongly conditioned by intergranular failure, as is the case in copper alloys subjected to dynamic embrittlement. The self-consistent scheme is extended to account for grain boundary decohesion using a nonlinear cohesive law. The effective tensile response up to failure is computed for a Cu–Ni–Si alloy based on the homogenization method. In particular, the proposed approach allows for identification of the grain boundary critical energy release rate from the macroscopic tensile curve.

1. Introduction

Precipitation-strengthened copper alloys are good candidates for electrical applications, such as lead-frames, connectors or rotors in large electrical machines. These alloys offer a relative high strength without deteriorating significantly electrical conductivity. However, some copper alloys such as Cu–Cr (Misra et al., 1996; Nathani and Misra, 2004), and Cu–Ni–Si (Sun et al., 2008) have been found to suffer from dynamic embrittlement in the temperature range 400–700 K, which results in brittle intergranular cracking (Fig. 1). This phenomenon involves stress-induced segregation of an embrittling element into grain boundaries, causing the reduction of their cohesive strength and eventually their failure. The effect of dynamic embrittlement is amplified by environmental and loading conditions, such as temperature increase and/or strain rate decrease as shown by Sun et al. (2008). According to Priester (2011), sufficient quantities of the embrittling element at grain boundaries can change the fracture mode of the copper alloys from ductile to brittle intergranular mode. For example, addition of a small quantity of bismuth can provoke brittle fracture of copper along grain boundaries (Schweinfest et al., 2004). Thus, it is of great importance in technological applications of metals to consider the effects of dynamic embrittlement, especially on the material effective behaviour.

In our study, an approximate analytical model is proposed to find easily the polycrystal homogenized behaviour, while taking account of the grain boundaries decohesion. Through this model, degradation of the mechanical properties of grain boundaries due to dynamic embrittlement can be considered in a more simplified and less time-consuming manner than simulations based on finite element computation. The model relies on the concept of imperfect interface as originally incorporated into the solution of the inclusion problem by Qu (1993a). In this latter approach, the inclusion-matrix interface is considered as a layer of vanishing thickness, where traction remains continuous while displacement is discontinuous. In this case, the nonlinear behaviour of the material is the result of both crystal plasticity inside grains and interface debonding at grain boundaries (Fig. 2). A viscoplastic crystal plasticity law is used to model the mechanical behaviour of each grain as function of its crystallographic orientation. As for the representation of grain boundary weakening, a nonlinear cohesive law with an exponential declining shape is introduced in the homogenization scheme. The paper is structured as follows. First, the constitutive equations for single crystal plasticity and the homogenization model of Hill (1965) for the polycrystalline aggregate are recalled. Then, intergranular failure resulting from grain boundary decohesion is incorporated in the homogenization scheme using a nonlinear cohesive law. A new transition rule, that does not presuppose continuity of displacement at grain boundaries, is then derived from the self-consistent scheme of Hill. Finally, the analytical model is used to predict the overall brittle failure behaviour of a Cu–Ni–Si alloy resulting from intergranular

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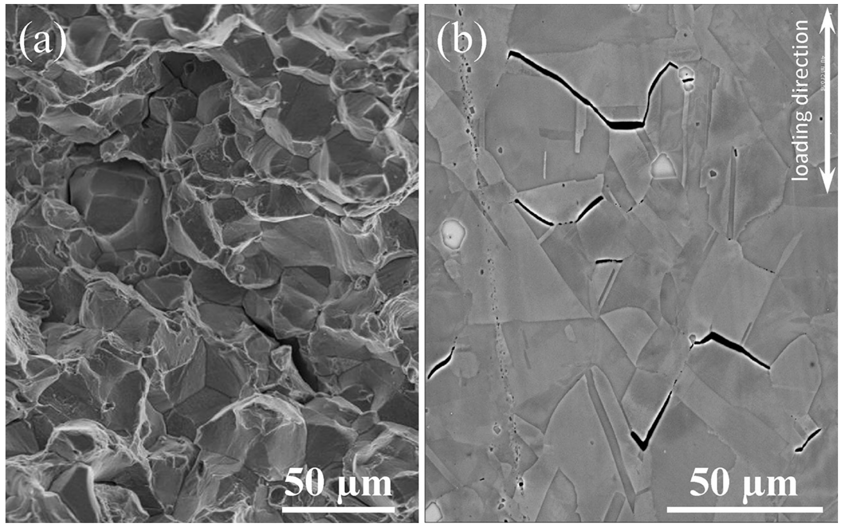

Fig. 1. MEB observations showing (a) intergranular fracture surface, and (b) presence of microcraks at grain boundaries on a longitudinal section (after tensile test performed at temperature 200 °C with strain rate $\dot{\varepsilon} = 5 \times 10^{-6}\ \mathrm{s}^{-1}$).

cracking. Grain boundary features are identified from tensile tests performed under different strain rates and temperatures.

2. The original mean field theory for nonlinear polycrystals

2.1. Single crystal plasticity

Single crystal plasticity is defined at the grain scale where slip occurs by dislocation motion along a crystallographic direction. For FCC polycrystalline, 12 octahedral slip systems are considered, based on slip planes {1 1 1} and slip directions ⟨1 1 0⟩. According to the Schmid's law, the resolved shear stress for system s in the grain g can then be obtained by:

$$\tau^s = \underline{\sigma}^g : \underline{\underline{m}}^s \quad \text{with} \quad \underline{\underline{m}}^s = \frac{1}{2}(l^s \otimes n^s + n^s \otimes l^s) \tag{1}$$

where n^s and l^s are respectively the normal to the slip system s and the slip direction in this plane. A viscoplastic framework, as proposed by Méric and Cailletaud (1991), is used by introducing isotropic κ^s and kinematic χ^s hardening variables, respectively, associated with the state variables ρ^s and α^s. In this model, the resolved shear is used as a critical variable to evaluate the viscoplastic slip rate:

$$\dot{\gamma}^s = \left\langle \frac{|\tau^s - \chi^s| - \kappa^s}{k} \right\rangle^n \mathrm{sign}(\tau^s - \chi^s) \tag{2}$$

where k and n are material coefficients characterizing the viscosity (Norton's law). The hardening variables, as well as the evolution of the state variables, are given by:

$$\kappa^s = \kappa_0 + bQ\sum_r h_{sr}\rho^r \quad \text{with}\ \dot{\rho}^s = (1 - b\rho^s)\dot{\upsilon}^s \tag{3}$$

$$\chi^s = c\alpha^s \quad \text{with}\ \dot{\alpha}^s = \dot{\gamma}^s - d\alpha^s\dot{\upsilon}^s \tag{4}$$

where κ_0 represents the initial critical shear stress, $\dot{\upsilon}^s = |\dot{\gamma}^s|$, the parameters c and d characterize the kinematic hardening, while b, Q and the matrix h_{sr} define the isotropic hardening. Eventually, the plastic strain rate in grain g, which results from the contribution of all slip systems, is calculated as $\underline{\dot{\varepsilon}}^{pg} = \sum_s \dot{\gamma}^s \underline{\underline{m}}^s$.

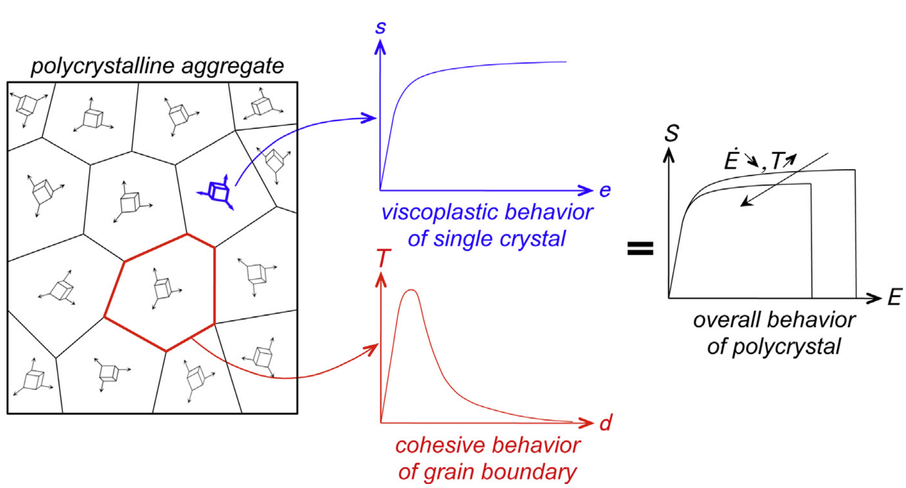

Fig. 2. Schematic representation of the various nonlinearities in the polycrystal and their effect on the overall response.