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Grain boundary interfacial plasticity with incorporation of internal structure and energy

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ABSTRACT

Modelling the behaviour of grain boundaries in polycrystalline metals using macroscopic continuum frameworks demands a multi-scale description of the underlying details of the structure and energy of grain boundaries. The objective in this work is the incorporation of a multi-scale atomistic-to-continuum approach of the initial grain boundary structure and energy into a grain boundary extended crystal plasticity framework in order to investigate the role of the grain boundary energetics on the macroscopic response. To this end, the methodology includes: (i) the generalisation of the atomistic-to-continuum results of the initial grain boundary structure and energy, (ii) an analytical analysis of the resulting grain boundary energetics in the continuum framework, (iii) the numerical implementation of the developed framework in the case of a periodic bicrystal subjected to simple shear deformation considering a symmetric tilt boundary system in the full misorientation range. This work provides a step forward towards the physically based continuum modelling of grain boundary interfacial plasticity.

1. Introduction

In polycrystalline materials, differences in the orientation of the crystals that constitute the material play a significant role in the macroscopic behaviour. In spite of numerous investigations in the past, the physical understanding of the underlying deformation mechanisms defining this macroscopic behaviour and its incorporation into continuum level modelling are still the subject of ongoing studies. A well-known example is the increased strength and hardening due to grain size refinement, i.e. the Hall–Petch effect, which has led to advanced material models capturing these size effects. However, when the average grain size reduces, also the behaviour of the grain boundaries (GB) and their interaction with crystal defects become of key importance. Various types of interactions between dislocations and grain boundaries have been reported experimentally (Gemperlová et al., 2002; Lee et al., 1990; Shen et al., 1988; Smith, 1982; Valiev et al., 1986) and in atomistic simulations (Bachurin et al., 2010; de Koning et al., 2003; Pestman et al., 1991; Sangid et al., 2012; Zhang and Wang, 1996). Dislocations can be accumulated, transmitted, absorbed or nucleated at the interfaces.

From a continuum modelling point of view, conventional continuum plasticity models, even those enhanced to include strain gradients and interface behaviour (Dahlberg et al., 2013; Fredriksson and Gudmundson, 2007; Massart and Pardoen, 2010; Polizzotto, 2009; Voyiadjis et al., 2014), do not explicitly account for crystallographic misorientation across a grain boundary, which is an important quantity defining micro-scale interactions between dislocations and grain boundaries. Classical crystal plasticity models overcome this deficiency, but they generally do not account for grain boundary phenomena, i.e. grain boundaries are only incorporated as planes where the crystallographic orientation changes. Gradient

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enhanced crystal plasticity alleviates this limitation. While these approaches mostly incorporate the limiting situations of either impenetrable or completely transparent grain boundaries through higher-order boundary conditions (Bayley et al., 2006; Evers et al., 2004a; Gurtin, 2002; Kuroda and Tvergaard, 2008; Mayeur et al., 2011), several attempts have been made to elaborate these frameworks to include grain boundary interface mechanics (Ekh et al., 2011; Gurtin, 2008; Kim and Oh, 2012; Liu et al., 2011b; Özdemir and Yalçinkaya, 2014; Wulfinghoff et al., 2013). Among the different constitutive choices that have to be made, the grain boundary energy often follows a simple ad hoc expression. However, atomistic simulations indicate that the grain boundary energy is dependent on the grain boundary structure (Hasson et al., 1972; Rittner and Seidman, 1996; Tschopp and McDowell, 2007; Wang et al., 1984; Wolf, 1990). Furthermore, the dislocation interaction behaviour depends on the grain boundary structure. It should be emphasised that the macroscopic gradient crystal plasticity models discussed above do not directly account for the detailed grain boundary processes, but incorporate idealised grain boundary conditions. Currently, a limited number of the continuum modelling approaches (can) address the underlying initial and evolving grain boundary structure (Fressengeas et al., 2014; Taupin et al., 2013).

In recent work, van Beers et al. (2015) developed a multi-scale approach leading to a continuum representation of the initial grain boundary structure and energy based on the output of atomistic simulations. The proposed approach introduces an intrinsic net defect density, representing the grain boundary structure, which is related to the atomistically calculated grain boundary energies through a logarithmic expression. It was shown that this multi-scale method can accurately describe the grain boundary energies in the complete misorientation range of symmetric tilt grain boundary systems in aluminium and copper. In the present paper, this atomistic-to-continuum approach is incorporated into the grain boundary extended crystal plasticity model, developed earlier by van Beers et al. (2013). The resulting model is implemented numerically in order to examine the particular role and influence of the grain boundary energetic contributions on the macroscopic response. The modelling approach is illustrated on a periodic copper bicrystal subject to simple shear deformation, considering symmetric tilt boundaries with the [0 0 1] rotation axis in the full misorientation range, including both low- and high-angle grain boundaries.

The outline of this paper is as follows. In Section 2, a summary of the grain boundary extended crystal plasticity framework is provided. Section 3 briefly describes the multi-scale atomistic-to-continuum approach of the initial grain boundary structure and energy, and covers the incorporation of the atomistic-to-continuum approach into the grain boundary interface model within the strain gradient crystal plasticity framework. In Section 4, the resulting initial grain boundary energetics is analysed analytically. The numerical implementation and the results of the effect of the energetic contributions of the grain boundaries on the macroscopic response of copper bicrystals are described in Section 5. This is followed by a discussion in Section 6. Finally, conclusions are made in Section 7.

Cartesian tensors and tensor products are used throughout the paper: $\mathbf{a}$, $\mathbf{A}$ and ${}^{n}\mathbf{A}$ denote respectively a vector, a second-order tensor and an nth-order tensor, unless stated otherwise. The following notation for vector and tensor operations is employed: transpose $A^{\mathrm{T}}_{ij} = A_{ji}$, the dyadic product $\mathbf{ab} = a_i b_j \mathbf{e}_i \mathbf{e}_j$, the dot product $\mathbf{A}\cdot\mathbf{B} = A_{ij}B_{jk}\mathbf{e}_i\mathbf{e}_k$ and the double dot product $\mathbf{A}:\mathbf{B} = A_{ij}B_{ji}$ with $\mathbf{e}_i$ $(i = 1,\ 2,\ 3)$ the unit vectors of a Cartesian basis.

2. Bulk and interface frameworks

The microstructurally motivated strain gradient crystal plasticity framework including a grain boundary interface model as developed in van Beers et al. (2013) is summarised next.

2.1. Bulk crystal formulation

The bulk crystal formulation originates from the one proposed by Evers et al. (2004a,b) and Bayley et al. (2006), restricted to small deformations. The total distortion is given by the sum of elastic (e) and plastic (p) components

$$\nabla\mathbf{u} = \mathbf{H}^{\mathrm{e}} + \mathbf{H}^{\mathrm{p}}. \tag{1}$$

The plastic distortion is given by

$$\mathbf{H}^{\mathrm{p}} = \sum_{\alpha}\gamma^{\alpha}\mathbf{s}^{\alpha}\mathbf{m}^{\alpha}. \tag{2}$$

Here, γ^{α} represents slip on slip system α having slip plane normal $\mathbf{m}^{\alpha}$ and slip direction $\mathbf{s}^{\alpha}$. In the crystal plasticity approach adopted, dislocation densities on individual slip systems act as key variables. Geometrically necessary dislocation (GND) densities of edge and screw character, denoted $\rho_{\mathrm{G}}^{\alpha(e)}$ and $\rho_{\mathrm{G}}^{\alpha(s)}$, respectively, arise from gradients in slip as follows

$$\rho_{\mathrm{G}}^{\alpha(e)} = \rho_{\mathrm{G0}}^{\alpha(e)} - \frac{1}{b}\nabla\gamma^{\alpha}\cdot\mathbf{s}^{\alpha}, \quad \rho_{\mathrm{G}}^{\alpha(s)} = \rho_{\mathrm{G0}}^{\alpha(s)} + \frac{1}{b}\nabla\gamma^{\alpha}\cdot\mathbf{p}^{\alpha}, \tag{3}$$

with unit vector $\mathbf{p}^{\alpha} = \mathbf{s}^{\alpha}\times\mathbf{m}^{\alpha}$. The quantities $\rho_{\mathrm{G0}}^{\alpha(e)}$ and $\rho_{\mathrm{G0}}^{\alpha(s)}$ represent the initial GND densities and b is the Burgers vector magnitude. For a given slip system α the resolved shear stress or Schmid stress τ^{α} is given by

$$\tau^{\alpha} = \boldsymbol{\sigma} : \mathbf{s}^{\alpha}\mathbf{m}^{\alpha}, \tag{4}$$

where the Cauchy stress tensor $\boldsymbol{\sigma}$ is determined through the conventional elastic relationship

$$\boldsymbol{\sigma} = {}^{4}\mathbf{C} : \mathbf{E}^{\mathrm{e}} \text{ with } \mathbf{E}^{\mathrm{e}} = \frac{1}{2}\left(\mathbf{H}^{\mathrm{e}} + \mathbf{H}^{\mathrm{eT}}\right). \tag{5}$$

Here, ${}^{4}\mathbf{C}$ is the fourth order elasticity tensor and $\mathbf{E}^{\mathrm{e}}$ the elastic strain. The evolution of slip is accomplished through a visco-plastic power-law by

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0\left(\frac{\left|\tau^{\alpha} - \tau_b^{\alpha}\right|}{s^{\alpha}}\right)^{\frac{1}{m}}\operatorname{sign}\left(\tau^{\alpha} - \tau_b^{\alpha}\right). \tag{6}$$

Parameters $\dot{\gamma}_0$ and m are positive constants. The back stress τ_b^{α} is obtained by the projection of the internal stress $\boldsymbol{\sigma}^{\mathrm{int}}$ onto slip system α