Computational Materials Science 111 (2016) 443–459

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Computational and theoretical aspects of a grain-boundary model that accounts for grain misorientation and grain-boundary orientation

D. Gottschalk [a], A. McBride [b,*], B.D. Reddy [b,1], A. Javili [c,2], P. Wriggers [a], C.B. Hirschberger [a]

[a] Institute of Continuum Mechanics, Leibniz Universität Hannover, Appelstrasse 11, 30167 Hannover, Germany
[b] Centre for Research in Computational and Applied Mechanics, University of Cape Town, 5th floor, Menzies Building, Private Bag X3, 7701 Rondebosch, South Africa
[c] Chair of Applied Mechanics, University of Erlangen–Nuremberg, Egerlandstr. 5, 91058 Erlangen, Germany

ARTICLE INFO

Article history:
Received 25 June 2015
Received in revised form 18 September 2015
Accepted 19 September 2015
Available online 18 October 2015

Keywords:
A. Grain boundaries
B. Crystal plasticity
C. Finite elements
Gradient plasticity

ABSTRACT

A detailed theoretical and numerical investigation of the infinitesimal single-crystal gradient-plasticity and grain-boundary theory of Gurtin (2008) is performed. The governing equations and flow laws are recast in variational form. The associated incremental problem is formulated in minimisation form and provides the basis for the subsequent finite element formulation. Various choices of the kinematic measure used to characterise the ability of the grain boundary to impede the flow of dislocations are compared. An alternative measure is also suggested. A series of three-dimensional numerical examples serve to elucidate the theory.

1. Introduction

The miniaturisation of mechanical components composed of crystalline material requires a continuum theory that accounts for the role of the grain boundary and for size-dependent effects. The grain-boundary model should incorporate both the *misorientation in the crystal lattice* between adjacent grains, and the *orientation of the grain boundary* relative to the crystal lattice of the adjacent grains. Classical theories of plasticity are unable to describe the well-known size-dependent response exhibited by crystalline material at the micro- and nanometre scale. Numerous extended (gradient and non-local) continuum theories of single-crystal plasticity have been presented in the last two decades to circumvent these limitations. The thermodynamically consistent gradient theory of Gurtin and co-workers and related works (see e.g. [17,22,18,19]) have received particular attention. A variational formulation of the Gurtin [17] framework has been developed in Reddy [32,33]. In Gurtin [17] the defect part of the free energy is parametrized in terms of the (bulk) Burgers tensor, a rigorously defined and physically meaningful measure of the (local) Burgers vector and hence the lattice mismatch (see e.g. [29]). The form of the defect energy was modified by Gurtin [19] to account for a continuous distribution of geometrically necessary dislocations (GNDs). The recent work of Gurtin and Reddy [23] uses a scalar measure of the accumulated slips as the basis for the hardening relation, which takes account of both self- and latent-hardening. Furthermore, the resulting initial boundary-value problem is placed in a variational setting in the form of a global variational inequality. Ertürk et al. [9] show how the theory of Gurtin et al. can be related to the more physically motivated theories due to Bayley et al. [4], Evers et al. [12,11,10].

The gradient theory of Gurtin [19] provides a basis to account for the role of the grain boundary (see [20]). Neumann and Dirichlet-type boundary conditions on the slip and the flux of the vectorial microforce (i.e. the microscopic traction), respectively, can be prescribed and are often assumed homogeneous. The homogeneous Dirichlet condition, known as the micro-hard boundary condition, has been widely used to account for the grain boundary or an interface (see e.g. [11,8,27,28,30]). Clearly this boundary condition ignores the complex geometric structures in the vicinity of the grain boundary.

Central to the theory of Gurtin [20] is the introduction of the *grain-boundary Burgers tensor* to parametrize the grain-boundary free energy. The grain-boundary Burgers tensor is obtained from the mismatch in the plastic part of the displacement gradient around a circuit centred on the grain boundary and contains information on both the misorientation in the crystal lattice

* Corresponding author. Tel.: +27 21 650 3817; fax: +27 21 685 2281.
E-mail addresses: gottschalk@ikm.uni-hannover.de (D. Gottschalk), andrew.mcbride@uct.ac.za (A. McBride), daya.reddy@uct.ac.za (B.D. Reddy), ali.javili@ltm.uni-erlangen.de (A. Javili), wriggers@ikm.uni-hannover.de (P. Wriggers), c.b.hirschberger@gmail.com (C.B. Hirschberger).
[1] Tel.: +27 21 650 3817; fax: +27 21 685 2281.
[2] Tel.: +49 (0)9131 85 28502; fax: +49 (0)9131 85 28503.

http://dx.doi.org/10.1016/j.commatsci.2015.09.048
0927-0256/

between adjacent grains, and the orientation of the grain boundary. Furthermore, the definition of grain-boundary Burgers tensor is consistent with that of the Burgers tensor in the bulk.

The grain-boundary Burgers tensor can be expressed in terms of the *intra-* and *inter-grain interaction moduli*. The inter-grain interaction moduli account for mismatch in the slip systems adjacent to the grain boundary and the orientation of the grain boundary. They provide a physically meaningful characterisation of the interaction of neighbouring slip systems with the extremes described as *non-interactive* and *maximally interactive*.

Recently, van Beers et al. [35] have proposed and numerically implemented a theory similar to that of Gurtin [20] for incorporating grain boundaries into the gradient crystal plasticity theory of Evers et al. [11]. A key feature of the theory is the use of a geometrically-motivated vectorial measure to parametrize the grain-boundary free energy. We will show in this work that under *planar conditions* (as investigated numerically by van Beers et al. [35]) the models of Gurtin [20] and van Beers et al. [35] produce identical interaction moduli. In similar work, Özdemir and Yalçinkaya [31] implemented the grain-boundary theory of Gurtin [20]. A series of finite element simulations of planar bi-crystals (single and double slip) illustrated features of the grain-boundary model.

Gudmundson [15] and Fredriksson and Gudmundson [14,13] propose an interface theory in which both the interface moment traction and the plastic slip can be discontinuous at the grain boundary. The model introduces an interfacial free energy that depends on the plastic strain on both sides of the interface. Critically however, the model does not account directly for the mismatch in the adjacent grains or the orientation of the grain boundary. Related works include those by Aifantis and Willis [1,2]. Ekh et al. [7] propose a "micro-flexible" grain boundary which provides a degree of resistance to plastic flow dependent upon the misorientation of the adjacent grains (see [3], for an extension that accounts for thermal effects). They do not consider the orientation of the grain boundary. Wulfinghoff et al. [38] account for grain boundaries within a gradient-plasticity theory by postulating a grain-boundary yield condition and flow rule. The theory does not account for the mismatch in the adjacent grains or the orientation of the grain boundary. Voyiadjis et al. [36] developed and numerically implemented a gradient-plasticity model for the polycrystalline problem which accounts for the role of grain boundaries via the mismatch in the accumulated plastic strain.

Recasting the problem of single-crystal gradient plasticity as a variational formulation makes it amenable to analysis (see [33]). The variational formulation does not have an associated minimisation problem, but the corresponding time-discrete incremental problem does. The variational formulation developed in Reddy [33] is extended here to include the grain boundary and a viscoplastic flow law. The associated incremental minimisation problem is shown to be equivalent to the time-discrete variational problem and provides the point of departure for the numerical implementation within the finite element method. The software AceGen [26] is used to describe the finite element interpolation, and to compute the residual and (algorithmically consistent) tangent contributions directly from the prescribed functional associated with the incremental minimisation problem, using automatic differentiation at the level of the quadrature point. This approach ensures quadratic convergence of the algorithm and greatly simplifies the implementation. Details of the numerical implementation are given.

Gurtin [20] proposes two thermodynamically admissible plastic flow relations for the grain boundary (denoted Gurtin I and II). The flow relations define the structure of the dissipative microscopic stress in the grain boundary microscopic force balance. The flux of dislocations from the grains drives the microscopic force balance. In the first proposal, the grain boundary Burgers tensor is used to parametrize the flow relations, while in the second it is the slip. The first approach accounts for the interaction of slip systems adjacent to the grain boundary. This approach also allows for a recombination of the plastic distortion contributions from adjacent sides via the definition of the grain boundary Burgers tensor. The second approach does not directly account for the structure of the adjacent grains or the orientation of the grain boundary in the plastic flow relation. Both approaches account for the geometric structure of the adjacent grains and the grain boundary via the flux terms from the grains.

A series of three-dimensional numerical examples elucidate the grain-boundary theory. The examples demonstrate single slip in a bi-crystal and multi-slip in a polycrystal where each of the 27 grains is a face-centred-cubic crystal structure. The polycrystal example in particular demonstrates various features of the Gurtin [20] theory that are not obvious from the theory or the single slip examples. The Gurtin I model for the plastic flow relation is unable to capture the widely-used micro-hard condition in multi-slip problems, even when using an artificially high value for grain boundary slip resistance. The Gurtin II model can capture the range of responses between the micro-free and micro-hard conditions. Motivated by a plastic flow relation that accounts for the structure of the grain boundary and captures the micro-hard and micro-free limits and the range between, a modified measure of the grain-boundary Burgers tensor is analysed and implemented. In the modified formulation, the micro-hard limit is recovered for large-angle grain boundaries, and the micro-free for perfectly aligned crystal structures on either side of the grain boundary.

The structure of this work is as follows. The kinematics of the gradient crystal plasticity formulation in the bulk and on the grain boundary are reviewed in Section 2. The kinematic measures of the mismatch at the grain boundary proposed in Gurtin [20] and van Beers et al. [35] are then compared. Particular attention is paid to the inter-grain interaction moduli. The kinetics of the problem and the various restrictions to the theory assumed are presented in Section 3. The governing relations and the plastic flow law are presented in Sections 4 and 5. An alternative measure of the kinematic mismatch at the grain boundary is given. The variational formulation of the problem and the associated incremental formulation are developed in Section 6. This is followed by details of the numerical implementation within the finite element framework. The finite element model is then used to simulate a series of representative numerical examples in Section 8. Finally, conclusions are made and various extensions proposed.

1.1. Notation and basic relations

Direct notation is adopted throughout. Occasional use is made of index notation, the summation convention for repeated indices being implied. When the repeated indices are lower-case italic letters, the summation is over the range $\{1,2,3\}$. Upper-case italic indices can refer to arbitrary adjacent grains $\{A,B\}$. The summation convention is not employed for grains. The scalar product of two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ is denoted $\boldsymbol{a}\cdot\boldsymbol{b}=[\boldsymbol{a}]_i[\boldsymbol{b}]_i$. The scalar product of two second-order tensors $\boldsymbol{A}$ and $\boldsymbol{B}$ is denoted $\boldsymbol{A}:\boldsymbol{B}=[\boldsymbol{A}]_{ij}[\boldsymbol{B}]_{ij}$. The composition of two second-order tensors $\boldsymbol{A}$ and $\boldsymbol{B}$, denoted $\boldsymbol{AB}$, is a second-order tensor with components $[\boldsymbol{AB}]_{ij}=[\boldsymbol{A}]_{im}[\boldsymbol{B}]_{mj}$. The tensor product of two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ is a second-order tensor $\boldsymbol{D}=\boldsymbol{a}\otimes\boldsymbol{b}$ with $[\boldsymbol{D}]_{ij}=[\boldsymbol{a}]_i[\boldsymbol{b}]_j$. The action of a second-order tensor $\boldsymbol{A}$ on a vector $\boldsymbol{b}$ is a vector with components $[\boldsymbol{a}]_i=[\boldsymbol{A}]_{im}[\boldsymbol{b}]_m$. The curl of a second-order tensor $\boldsymbol{A}$ is a second-order tensor with components $[\mathrm{curl}\boldsymbol{A}]_{ij}=\epsilon_{irs}\partial A_{js}/\partial x_r$, where $\boldsymbol{\epsilon}$ is the third-order permutation tensor. An arbitrary quantity in the bulk is denoted $\{\bullet\}$ and analogously $\{\bar{\bullet}\}$ denotes an arbitrary quantity on the grain boundary.