International Journal of Solids and Structures 51 (2014) 1434–1441

Contents lists available at ScienceDirect

International Journal of Solids and Structures

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

Continuous modeling of the structure of symmetric tilt boundaries

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ARTICLE INFO

Article history:
Received 5 July 2013
Received in revised form 13 December 2013
Available online 4 January 2014

Keywords:
Grain boundaries
Disclinations
Dislocations
Nonlocal elasticity
Continuum mechanics

ABSTRACT

In polycrystals, the discontinuity of lattice rotation occurring across symmetric tilt boundaries is accommodated by the periodic arrangement of atoms in structural units. A crossover between this atomistic description and a continuous representation of tilt boundaries is carried out by designing periodic arrays of appropriately chosen smooth disclination dipoles. A comprehensive description of the boundary structure in terms of elastic strain, curvature and energy fields is then derived from a continuous theory of dislocation and disclination density fields, by allowing the initial distributions to relax in their own stress/couple stress fields. The resulting fields are obtained at nanoscale from finite element approximations of the theory. They compare remarkably well with predictions from molecular statics and experimental data. Beyond this description of grain boundaries as continua, the theory naturally provides a basis for coarse-grained spatio-temporal continuous descriptions of polycrystals.

1. Introduction

In crystalline solids such as ice, rocks and metallic materials, grain boundaries are thin sheets of material where the lattice rotates from a crystal orientation to the next one within a few nanometers. Because they treat these layers as infinitely thin interfaces, polycrystalline simulations based on conventional continuum mechanics fail to account for their structure and energy. Conversely, atomistic simulations provide detailed descriptions of the structure of grain boundaries and good estimates of their energy, but coarse-graining to polycrystalline samples remains elusive. In this paper, our intent is to show that a nonlocal continuum mechanics model based on crystal defect fields (disclinations and dislocations) defined at interatomic scale can consistently account for the grain boundary structure and energy, while retaining the potential for being an effective tool in designing scale transitions from atomistic configurations to polycrystals.

Our modeling paradigm, motivated by the remarkable achievements of the Peierls model in elucidating basic dislocation physics (Peierls, 1940), is to account for lattice incompatibility by focusing on densities of crystal defects (dislocations and disclinations) defined continuously at interatomic scale, rather than the atoms themselves. Several attempts in this direction have already been developed, though apparently not implemented numerically (see the review paper McDowell (2008) and references therein). By similarly specifying continuously the displacement and rotation vector fields below interatomic distances, the theory considers the material as capable of transmitting stresses and couple stresses at this scale. Because it accounts for the lattice incompatibility due to crystal defects, the theory is able to describe the associated internal stress and couple-stress fields. As recently shown by Upadhyay et al. (2013), non-locality of the elastic response and length scales characteristic of this behavior hinge upon the breaking of lattice symmetry occurring in the defected areas of the lattice. Plasticity derives from the transport of dislocation and disclination densities through the lattice. The transport equations supply an undisputable kinematic structure for the spatio-temporal dynamics of the crystal defect densities. Using thermodynamical guidance, appropriate constitutive relationships for plasticity can be provided in terms of driving forces vs. dislocation/disclination velocities to substantiate this dynamical structure. Thus completed, the theory allows formulating a boundary value problem for the defects densities and displacement fields, with standard boundary conditions on the displacement and traction vector fields (Fressengeas et al., 2011). In the present work, approximate solutions to this problem in small bi-crystalline samples are generated by using finite element methods similar to those previously employed in the pure dislocation dynamics case (Roy and Acharya, 2005; Varadhan et al., 2006).

In order to show the ability of the above framework at recovering grain boundary structure and energy, symmetrical tilt boundaries are chosen for simplicity. The paper then proceeds in two steps. Firstly, disclination density distributions are arbitrarily chosen to model the boundaries in a manner such that the elastic curvature incompatibility is similar to that obtained from their atomistic representation. Taupin et al. (2013) suggested that periodic arrays of smooth wedge disclination dipoles defined at

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0020-7683/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ijsolstr.2013.12.031

interatomic scale can be adequate counterparts to the structural units composing the symmetrical tilt boundaries in these models. This method will be followed in the present work. Secondly, the assumed defect distributions are allowed to relax and re-arrange by transport in their own self-stress and couple stress fields, until their elastic energy stabilizes and a self-organized structure emerges. The non-locality of the elastic response in the core region appears to be essential in this process. Thus, it is thoroughly analyzed in this paper, within the constitutive framework recently set out in Upadhyay et al. (2013), but in a bi-dimensional setting adequate for the study of symmetrical tilt boundaries.

The paper is organized as follows. Notations are settled in Section 2. The elasto-plastic theory of defects introduced in Fressengeas et al. (2011) and a bi-dimensional model for symmetrical tilt boundaries are briefly recalled in Section 3. The nonlocal elastic constitutive laws valid in the core of the boundaries are derived in Section 4. The construction of tilt boundaries with wedge disclination densities and comparison of the results with molecular statics predictions and experiments are shown in Section 5. Section 6 discusses the continuous nature of the present results, and provides hints on how coarse-graining to polycrystalline samples of the present nanoscale theory could be constructed. Conclusions follow.

2. Notations

A bold symbol denotes a tensor. When there may be ambiguity, an arrow is superposed to represent a vector: $\vec{\mathbf{V}}$. The symmetric part of tensor $\mathbf{A}$ is denoted $\mathbf{A}^{sym}$. Its skew-symmetric part is $\mathbf{A}^{skew}$ and its deviatoric part is $\mathbf{A}^{dev}$. The tensor $\mathbf{A}\cdot\mathbf{B}$, with rectangular Cartesian components $A_{ik}B_{kj}$, results from the dot product of tensors $\mathbf{A}$ and $\mathbf{B}$, and $\mathbf{A}\otimes\mathbf{B}$ is their tensorial product, with components $A_{ij}B_{kl}$. A: represents the trace inner product of the two second order tensors $\mathbf{A}:\mathbf{B}=A_{ij}B_{ij}$, in rectangular Cartesian components, or the product of a higher order tensor with a second order tensor, e.g., $(\mathbf{A}:\mathbf{B})_{ij}=A_{ijkl}B_{kl}$. The cross product of a second-order tensor $\mathbf{A}$ and a vector $\mathbf{V}$, the **div** and **curl** operations for second-order tensors are defined row by row, in analogy with the vectorial case. For any base vector $\mathbf{e}_i$ of the reference frame:

$$(\mathbf{A}\times\mathbf{V})^t\cdot\mathbf{e}_i=(\mathbf{A}^t\cdot\mathbf{e}_i)\times\mathbf{V}, \tag{1}$$

$$(\mathbf{div}\,\mathbf{A})^t\cdot\mathbf{e}_i=\mathbf{div}(\mathbf{A}^t\cdot\mathbf{e}_i), \tag{2}$$

$$(\mathbf{curl}\,\mathbf{A})^t\cdot\mathbf{e}_i=\mathbf{curl}(\mathbf{A}^t\cdot\mathbf{e}_i). \tag{3}$$

In rectangular Cartesian components:

$$(\mathbf{A}\times\mathbf{V})_{ij}=e_{jkl}A_{ik}V_l, \tag{4}$$

$$(\mathbf{div}\,\mathbf{A})_i=A_{ij,j}, \tag{5}$$

$$(\mathbf{curl}\,\mathbf{A})_{ij}=e_{jkl}A_{il,k}. \tag{6}$$

where e_{jkl} is a component of the third-order alternating Levi–Civita tensor $\mathbf{X}$. A vector $\vec{\mathbf{A}}$ is associated with tensor $\mathbf{A}$ by using its trace inner product with tensor $\mathbf{X}$:

$$(\vec{\mathbf{A}})_k=-\frac{1}{2}(\mathbf{A}:\mathbf{X})_k=-\frac{1}{2}e_{ijk}A_{ij}. \tag{7}$$

In the component representation, the spatial derivative with respect to a Cartesian coordinate is indicated by a comma followed by the component index. A superposed dot represents a material time derivative.

3. Continuum mechanics of crystal defects

In a continuum mechanics framework, the material displacement field vector $\mathbf{u}$ is defined continuously in the absence of fracture, at any point of an elasto-plastic body, possibly below interatomic distances. The total distortion tensor, defined as the gradient of the displacement $\mathbf{U}=\mathbf{grad}\,\mathbf{u}$, is a curl-free compatible tensor:

$$\mathbf{curl}\,\mathbf{U}=0. \tag{8}$$

This equation is sufficient to assure the existence of a single-valued continuous displacement field $\mathbf{u}$, solution to the equation $\mathbf{U}=\mathbf{grad}\,\mathbf{u}$, up to a constant translation. In a small deformation setting, the strain tensor $\boldsymbol{\epsilon}$ is the symmetric part of the distortion $\mathbf{U}$, the rotation tensor $\boldsymbol{\omega}$ is its skew-symmetric part and the associated rotation vector $\vec{\boldsymbol{\omega}}$ reads:

$$\vec{\boldsymbol{\omega}}=-\frac{1}{2}\boldsymbol{\omega}:\mathbf{X}=\frac{1}{2}\mathbf{curl}\,\mathbf{u}. \tag{9}$$

Using $\boldsymbol{\epsilon}$ and $\vec{\boldsymbol{\omega}}$, Eq. (8) becomes:

$$\mathbf{curl}\,\boldsymbol{\epsilon}+div(\vec{\boldsymbol{\omega}})\mathbf{I}-\mathbf{grad}^t\vec{\boldsymbol{\omega}}=0, \tag{10}$$

where $\mathbf{I}$ is the identity tensor. The curvature tensor $\boldsymbol{\kappa}=\mathbf{grad}\vec{\boldsymbol{\omega}}$ is also a compatible curl-free tensor. It is decomposed into an elastic component, $\boldsymbol{\kappa}_e$, and a plastic component, $\boldsymbol{\kappa}_p$, such that:

$$\boldsymbol{\kappa}_e=\mathbf{grad}\,\vec{\boldsymbol{\omega}}_e, \tag{11}$$

$$\boldsymbol{\kappa}_p=\mathbf{grad}\,\vec{\boldsymbol{\omega}}_p, \tag{12}$$

$$\boldsymbol{\kappa}=\mathbf{grad}\,\vec{\boldsymbol{\omega}}=\boldsymbol{\kappa}_e+\boldsymbol{\kappa}_p. \tag{13}$$

As remarked by deWit (1970), $(\boldsymbol{\kappa}_e,\boldsymbol{\kappa}_p)$ may not be compatible tensors, if the possibility of multi-valued elastic and plastic rotations $\vec{\boldsymbol{\omega}}_e$ and $\vec{\boldsymbol{\omega}}_p$, *i.e.*, a discontinuity of the elastic and plastic rotations over some surface, is acknowledged. In such cases, a non-zero tensor $\boldsymbol{\theta}$ such that

$$\boldsymbol{\theta}=-\mathbf{curl}\,\boldsymbol{\kappa}_p=\mathbf{curl}\,\boldsymbol{\kappa}_e \tag{14}$$

can be defined. $\boldsymbol{\theta}$ is the disclination density tensor. It is a continuous tensorial rendition of the elastic/plastic rotation discontinuity. The latter is also measured by the Frank vector $\boldsymbol{\Omega}$, *i.e.*, the closure defect of a circuit C, obtained by integrating the incompatible elastic curvatures along C

$$\boldsymbol{\Omega}=\int_C\boldsymbol{\kappa}_e\cdot\mathbf{dr}=\int_S\boldsymbol{\theta}\cdot\mathbf{n}dS, \tag{15}$$

where S is the surface of unit normal $\mathbf{n}$ delimited by the circuit C. As the rotation vectors $(\vec{\boldsymbol{\omega}}_e,\vec{\boldsymbol{\omega}}_p)$ are multi-valued, the elastic and plastic distortion tensors $\mathbf{U}_e$ and $\mathbf{U}_p$ are undefined. Substituting the elastic and plastic curvatures $(\boldsymbol{\kappa}_e,\boldsymbol{\kappa}_p)$ for $(\mathbf{grad}\vec{\boldsymbol{\omega}}_e,\mathbf{grad}\vec{\boldsymbol{\omega}}_p)$ allows splitting Eq. (10) into elastic and plastic components

$$\mathbf{curl}\,\boldsymbol{\epsilon}_e=+\boldsymbol{\alpha}+\boldsymbol{\kappa}_e^t-tr(\boldsymbol{\kappa}_e)\mathbf{I}, \tag{16}$$

$$\mathbf{curl}\,\boldsymbol{\epsilon}_p=-\boldsymbol{\alpha}+\boldsymbol{\kappa}_p^t-tr(\boldsymbol{\kappa}_p)\mathbf{I}. \tag{17}$$

Eqs. (16) and (17) relate the elastic/plastic strains associated with the presence of Nye's dislocation density tensor $\boldsymbol{\alpha}$ in the concurrent presence of incompatible elastic/plastic curvatures. A point-wise measure of the translation discontinuity due to the presence of dislocations is the Burgers vector. It contains a possible contribution from disclinations and reads:

$$\mathbf{b}=\int_C(\boldsymbol{\epsilon}_e-(\boldsymbol{\kappa}_e^t\times\mathbf{r})^t)\cdot\mathbf{dr}=\int_S(\boldsymbol{\alpha}-(\boldsymbol{\theta}\times\mathbf{r})^t)\cdot\mathbf{n}dS \tag{18}$$

Note that Eqs. (14) and (16) may be utilized to estimate the disclination and Nye's dislocation density tensors from orientation maps provided by EBSD experiments, respectively (Beausir and Fressengeas, 2013). In the absence of body forces, the momentum and moment of momentum equations are:

$$\mathbf{div}\,\mathbf{T}=0, \tag{19}$$