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Representation of dislocation cores using Nye tensor distributions

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Abstract

This paper demonstrates how the cores of atomistically simulated dislocations in Cu and Al can be represented by a distribution of infinitesimal dislocations described by appropriate components of the Nye tensor. Components calculated from atomic positions in the dislocated crystal are displayed as contour plots on the plane normal to the dislocation line. The method provides an accurate and instructive means for characterizing dislocation core structures and calculating the total Burgers vector.

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1. Introduction

An important aspect of atomistic studies of lattice dislocations is the observation and detailed visual representation of dislocation core structures. Presently, the most common procedure for dislocation visualization is based on the differential displacement (DD) map method proposed by Vitek et al. [1,2]. Various research groups have used other visualization methods, for example contour plots of invariants of the local strain tensor [3,4], color-coding of atoms according to their potential energy or the number of missing/additional neighbors [5,6], the centrosymmetry parameter [7], etc. Most of these methods are not specific to dislocations and reveal all other distorted regions as well, including stacking faults and point defects. Furthermore, the DD and strain invariant methods require a prior knowledge of the Burgers vector of the dislocation. In contrast, atomistic simulations are often accompanied by the generation of new dislocations whose Burgers vectors may not be known a priori. It is desirable to have a procedure for an automated calculation of Burgers vectors of dislocations without resorting to a circuit construction.

Bilby, Bullough and Smith (BBS) [8] developed the concept of continuously dislocated continuum. Applying this concept to an individual dislocation [9], the atomic misfit within the dislocation core can be represented by infinitesimal dislocations whose distribution is described by the Nye tensor [10]. In the method proposed in this work, atomic coordinates obtained from atomistic simulations and the known perfect-lattice orientation are used to evaluate the lattice distortion tensor on atoms, approximate it by a continuous function of coordinates, and compute the distribution of Nye tensor components over the plane normal to the dislocation line. Contour plots of such distributions provide a more vivid and informative description of the dislocation core structure than other methods do. The following sections give a brief description of the method and apply it to screw and edge dislocations in Cu. A more detailed discussion of the method with additional applications will be published elsewhere [11].

2. The Nye tensor and lattice distortion

A dislocation with a total Burgers vector **b** is described by a distribution of infinitesimal dislocations, each having a differential Burgers vector d**b** [12]. The Nye tensor $\boldsymbol{\alpha}$ describing

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the distribution of the infinitesimal dislocations is defined by [10]

$$\mathrm{d}\mathbf{b} = \boldsymbol{\alpha} \cdot \mathrm{n}\,\mathrm{d}A, \tag{1}$$

where $\mathbf{n}$ is the unit vector normal to an area, dA, enclosed by an infinitesimal Burgers circuit. Integrating over a surface A bounded by a closed circuit C' enclosing the entire distribution of $\boldsymbol{\alpha}$, recovers the Burgers vector of the dislocation:

$$\mathbf{b} = \int_A (\boldsymbol{\alpha} \cdot \mathbf{n})\,\mathrm{d}A. \tag{2}$$

Even if $\mathbf{b}$ is parallel to only one coordinate axis, the infinitesimal dislocations can have Burgers vector components parallel to the other axes as long as the integral of these components over A vanishes.

Alternatively, $\mathbf{b}$ can be obtained from a Burgers circuit construction. The closed Burgers circuit C' in the dislocated crystal consists of lattice vectors d$\mathbf{x}'$ such that

$$0 = \sum_{C'} \mathrm{d}\boldsymbol{x}'. \tag{3}$$

Transforming the vectors d$\mathbf{x}'$ into their images, d$\mathbf{x}$, in the perfect crystal and summing them algebraically along the associated path C gives the negative of $\mathbf{b}$:

$$\mathbf{b} = -\sum_{C} \mathrm{d}\boldsymbol{x}. \tag{4}$$

The lattice deformation that connects the vectors d$\mathbf{x}$ and d$\mathbf{x}'$ can be described by a lattice correspondence tensor $\mathbf{G}$,

$$\mathrm{d}\mathbf{x} = \mathrm{d}\mathbf{x}' \cdot \mathbf{G}, \tag{5}$$

which is the Eulerian deformation gradient; $\mathbf{G}$ is the transpose of Bilby's tensor $\mathbf{E}$ [13]. Replacing the summation in Eq. (4) by integration along C' and applying Stokes' theorem we have

$$\mathbf{b} = -\int_A (\nabla \times \mathbf{G}) \cdot \mathbf{n}\,\mathrm{d}A. \tag{6}$$

Recognizing that the integrand in Eq. (6) is the differential Burgers vector d$\mathbf{b}$, we finally obtain the expression for the Nye tensor:

$$\boldsymbol{\alpha} = -(\nabla \times \mathbf{G}). \tag{7}$$

The following section illustrates how calculations of $\boldsymbol{\alpha}$ can be performed numerically on data specifying atomic positions in a dislocated crystal.

3. Computer implementation and applications

We express atomic coordinates relative to an orthonormal right-handed Cartesian system $\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$, so that $\mathbf{g}_3$ is parallel to the dislocation line while $\mathbf{g}_1$ and $\mathbf{g}_2$ are parallel to suitable low-index crystallographic directions in the perfect lattice. We construct a set of n perfect-lattice vectors ("bonds") $\mathbf{P}^{(\beta)}$ ($\beta = 1, 2, \ldots, n$) connecting an atom to its n nearest neighbors. This set will be used as a reference for establishing the lattice correspondence.

To identify the local crystallographic directions around every atom in the dislocated crystal we first identify nearest neighbors of every atom as atoms lying within a sphere of radius $(1/2)(R_1 + R_2)$, where R_1 and R_2 are the first and second coordination radii in the perfect lattice. Within the dislocation core the number of such neighbors, n', can generally be different from n. Let $\mathbf{Q}^{(\gamma)}$ ($\gamma = 1,2, \ldots, n'$) be the radius vectors of the neighbors in the dislocated crystal. For each neighbor γ, we compute the angles $\varphi^{(\gamma\beta)}$ between $\mathbf{Q}^{(\gamma)}$ and all reference vectors $\mathbf{P}^{(\beta)}$. The reference vector $\mathbf{P}^{(\gamma)}$ with the smallest angular deviation, $|\varphi^{(\gamma\beta)}|$, is identified as the one corresponding to $\mathbf{Q}^{(\gamma)}$, so that $\mathbf{Q}^{(\gamma)}$ is considered as a distortion of $\mathbf{P}^{(\gamma)}$. This procedure establishes a correspondence between all distorted vectors $\mathbf{Q}^{(\gamma)}$ and reference vectors $\mathbf{P}^{(\gamma)}$ for every atom in the block. While this correspondence is unique and the angular deviations are very small away from the dislocation core, inside the dislocation core some deviations can be high.

The general problem of establishing a lattice correspondence for a crystalline defect does not always have a unique solution. The defect core structure can be distorted so severely that the very notion of a correspondence may loose its significance. Additionally, point symmetry can make a correspondence non-unique. The following algorithm is applied to handle non-unique situations. If two perfect-lattice bonds form equal angles with a given deformed bond $\mathbf{Q}^{(\gamma)}$, the latter is excluded from the calculation of $\mathbf{G}$ for the given atom. If one perfect-lattice bond is identified as corresponding to two different deformed bonds for the same atom, we choose the bond whose length is closer to R_1 and disregard the other one. Furthermore, bonds whose angular deviation exceeds a critical value $\varphi_{\max}$ are excluded from $\mathbf{G}$ calculations. For the FCC metals, we find that $\varphi_{\max} = 27^\circ$ gives the most satisfactory results.

To construct the lattice correspondence tensor $\mathbf{G}$ for a given atom, we us the relations (cf. Eq. (5))

$$\mathbf{P}^{(\gamma)} = \mathbf{Q}^{(\gamma)} \cdot \mathbf{G}, \tag{8}$$

which apply for $\gamma = 1, 2, \ldots, n''$, where n'' is the actual number of bond vectors after rejections. Since $n'' > 3$ and each vector consists of three components, this system of equations is overdetermined for the nine components of $\mathbf{G}$. It is, therefore, solved by a mean-squares optimization method. Although the value of $\mathbf{G}$ thus obtained is assigned to the central atom, it actually characterizes the deformation of the entire coordination group around it. The volume associated with this shell defines the "material point" corresponding to the continuum theory. This definition dictates the limit of spatial resolution of this method, which is approximately the first-neighbor distance. The involvement of an excessive number of bonds in this calculation makes it numerically stable: if

some of the bonds have to be rejected as discussed above, there are enough other bonds to produce a reasonable estimate of **G**.

To calculate the Nye tensor, the required spatial derivatives of **G** near each atom are computed using a finite difference approximation. For a particular component IM of tensor **G** at an atom 0, $G^{(0)}_{\mathrm{IM}}$, we define a column vector **A**(IM) as $A(\mathrm{IM})_k \equiv \partial_k G^{(0)}_{\mathrm{IM}}$ for $k = 1, 2, 3$. Let $\Delta G^{(\gamma)}_{\mathrm{IM}} = G^{(\gamma)}_{\mathrm{IM}} - G^{(0)}_{\mathrm{IM}}$ be the difference between the values of G_{IM} at a neighboring atom γ and at the central atom 0. Defining an $(n'' \times 1)$ column vector $\Delta\mathbf{G}_{\mathrm{IM}}$ composed of the values of $\Delta G^{(\gamma)}_{\mathrm{IM}}$ and **Q** as an $(n'' \times 3)$ matrix whose rows are the vectors $\mathbf{Q}^{(\gamma)}$ for $\gamma = 1, 2, \ldots, n''$, the finite-difference equations for all n'' neighbors can be expressed in matrix form

$$\Delta\mathbf{G}_{\mathrm{IM}} = \mathbf{Q} \cdot \mathbf{A}(\mathrm{IM}). \tag{9}$$

This system of equations is solved by the mean-squares method for the three Cartesian components of **A**(IM). The gradients thus obtained represent quantities averaged over the first coordination shell of an atom. By repeating this procedure for each of the nine components of **G**, we construct the tensor of derivatives $T_{imk} = \partial_k G_{in}$. Finally, the Nye tensor is obtained from Eq. (7),

$$\alpha_{jk} = -\varepsilon_{jim} T_{imk} \tag{10}$$

(ε_{jim} being the permutation symbol) and assigned to the atom in question.

The distribution of a particular component of $\boldsymbol{\alpha}$ is represented by a contour plot projected on the plane normal to the dislocation line $\mathbf{g}_3$. The contour plot is superimposed onto the deformed atomic structure. To compute a particular component b_j of the Burgers vector, we perform a numerical integration of α_{j3} on the projection plane over a rectangular area in which the absolute value of α_{j3} is greater than a specified small number.

Figs. 1–2 show examples of contour plots of the Nye tensor for dislocations in Cu. Atomic interactions in Cu are modeled by embedded-atom potentials developed in [14]. The dislocations are created in a large cylindrical simulation block with periodic boundary conditions along the dislocation line and fixed boundary conditions in the other two directions. The atoms are initially displaced from their perfect-lattice positions according to the local continuum anisotropic elastic solution for the strain field of a straight dislocation [15], followed by molecular dynamics runs at several descending temperatures and finally a static relaxation. The Burgers vector of all dislocations is $(1/2)[\bar{1}\,1\,0]$. We only show the relevant part of the $\boldsymbol{\alpha}$ distributions and leave out the large surrounding areas around the dislocation. Distances in the plots are measured in Å and $\boldsymbol{\alpha}$ is measured in Å^{-1}.

Fig. 1 reveals a dissociation of the screw dislocation in Cu into Shockley partials separated by a distance of about 8 Å.

Fig. 1(b) shows that the right partial has a negative edge component (α_{13}) while the left one has a positive component.

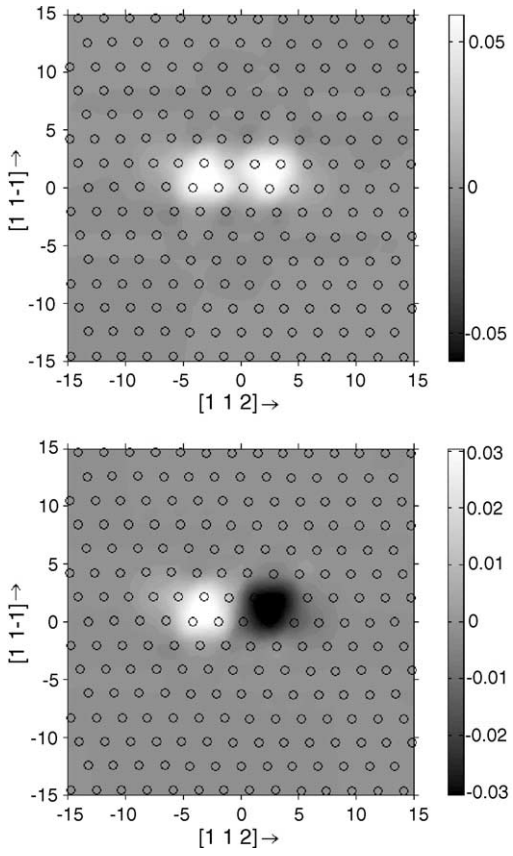

Fig. 1. (a) α_{33} (screw) component. (b) α_{13} (edge) component. Calculated Nye tensor distribution for screw dislocation in Cu.

The integration of the α_{33} plot yields the total Burgers vector of 2.635 Å in good agreement with ideal value 2.556 Å, while the integration of the α_{13} plot gives practically zero as expected. Similar results are obtained for the edge dislocation as shown in Fig. 2. As expected, the dissociated width is about a factor of three larger than for the screw dislocation. The peaks of the α_{13} and α_{33} components of the Nye tensor determine the positions of the Shockley partials and indicate the signs of their edge and screw components.

The total Burgers vector recovered from these plots (2.574 Å) is in excellent agreement with the ideal value. Furthermore, all components of the partials obtained by integrating the Nye tensor distributions over the relevant peak areas compare very well with the ideal Burgers vectors known from the lattice geometry.

Similar calculations for Al using the embedded atom potential [16] show that dissociation into partials is much smaller as expected from its higher stacking fault energy. Even in this case, however, the dissociation is clearly revealed by plotting the edge component α_{13} that immediately identifies the Shockley partials and the signs of their edge components. As with copper, we are able to recover the Burgers vector of both screw and edge dislocations with high accuracy [11].

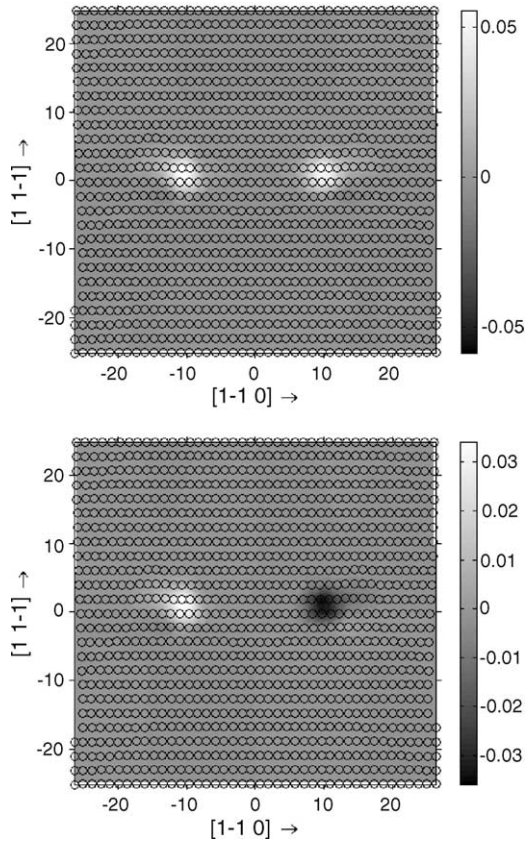

Fig. 2. (a) α_{13} (edge) component. (b) α_{33} (screw) component. Calculated Nye tensor distribution for equilibrium edge dislocation in Cu.

4. Summary

The method proposed here provides a powerful tool for the representation of dislocation core structures. Plots of the components of the Nye tensor in a plane normal to the dislocation line accurately reveal all the details of the dislocation core spreading or dissociation. In contrast to some of the previous methods, Nye tensor calculations do not require prior knowledge of the Burgers vector of the dislocation. Integrating Nye tensor components over appropriate regions of the plane permits accurate determination of the Burgers vector without constructing the Burgers circuit. The Burgers vectors of partial dislocations formed by dissociation of a full dislocation can also be determined if their separation is large enough to avoid significant overlap of the cores. Another advantage of using the Nye tensor is that it only has nonzero values in dislocation cores and is insensitive to compatible lattice distortion fields arising from other lattice defects or external sources. In combination with the atomic resolution of the method, it should be ideal for analyzing fine features of dislocation core spreading and its evolution under applied stresses or during dislocation motion. A recent application of the method to the visualization of the HRTEM image of the core of a screw dislocation in Mo has been made by Mendis et al. [17].

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