Characterization and visualization of the lattice misfit associated with dislocation cores

C.S. Hartley a,*, Y. Mishin b

b School of Computational Sciences, George Mason University, 4400 University Drive, Fairfax, VA 22030-4444, USA

Received 26 August 2004; received in revised form 12 November 2004; accepted 18 November 2004
Available online 24 December 2004

Abstract

Atomic misfit associated with a crystal dislocation is manifested by displacements of atoms from their positions in the perfect lattice. The discrete character of the crystal lattice and the nature of interatomic bonds distribute this misfit over the plane normal to the dislocation line. The Nye tensor, which describes the distribution of the resultant Burgers vector across a plane normal to the dislocation line, provides an excellent means of describing the spatial variation of the misfit. Relevant components of the Nye tensor are calculated from atomic positions in the dislocated crystal, represented by contour plots, and contrasted with the corresponding quantities obtained from a local continuum model. The comparison demonstrates that spatial distributions of components of the Nye tensor provide an accurate and instructive means of representing dislocation core structures. A numerical integration of these distributions permits an accurate calculation of the Burgers vector without constructing a Burgers circuit.

© 2004 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Keywords: Dislocation structure; Simulation; Modeling

1. Introduction

The structure of a dislocation core has a profound impact on the dislocation energy, mobility and ultimately on the mechanical properties of materials. Therefore atomic-level studies of dislocation core structure, spreading, dissociation and similar transformations are of extreme importance for the understanding of mechanical behavior of materials. Computer modeling of dislocations can be performed using either first-principles methods [1] or semi-empirical interatomic potentials ("atomistic simulations") [2]. An important aspect of such studies is the observation and detailed visual representation of dislocation core structures. This can be a challenging task, especially for complex core structures. While an edge dislocation can be readily identified as a termination of a lattice plane when viewing the crystal structure along the dislocation line, a screw dislocation cannot be easily revealed this way since its misfit is dominated by atomic displacements parallel to the dislocation line.

Presently, the most common procedure for dislocation visualization is based on the differential displacement (DD) map method proposed by Vitek et al. [3,4]. A DD plot shows relative displacements of nearest-neighbor (NN) atoms due to a dislocation superimposed on a plot of atomic positions. Relative displacements are shown by arrows centered at midpoints between NN atoms. An arrow points from one atom to another, its length is proportional to a chosen Cartesian component of the displacement, and its direction reflects the sign of the displacement. For simple core structures, a DD plot for one displacement component can be sufficient to provide most of the relevant information about the
extent and symmetry of the core spreading. For example, for a screw dislocation the component parallel to the dislocation line is used. Even in this simple case, however, a single DD plot would overlook atomic displacements normal to the dislocation line that always exist and can actually be revealed by high-resolution transmission electron microscopy (HRTEM) [5]. For more complex situations, particularly those involving core dissociations with the formation of stacking faults, all three displacement components need to be plotted and examined together in order to understand the dissociation scheme. A detailed reconstruction of the actual dislocation core structure from DD plots can be a difficult task.

Various research groups have used other visualization methods. By comparing deformed and ideal atomic positions, the local strain tensor can be evaluated in a finite-difference approximation and its first or second invariant can be represented by contour plots [6]. The choice of the invariant depends on the particular dislocation type (e.g., edge versus screw) and sometimes both the first and second invariants need to be plotted to clearly reveal the symmetry of the core spreading or the dissociation scheme. In some cases, representation of dislocations with contour plots of strain invariants can be more intuitive than with DD maps [7]. When working with atomistic potentials, stress tensors on individual atoms can be computed and contour plots can also represent their invariants. In large-scale molecular-dynamics (MD) simulations, dislocations are often identified by plotting positions of atoms whose energy exceeds a critical value [8]. Alternatively, atoms whose coordination number is different from that in the perfect lattice can be plotted to reveal dislocation lines [9]. Kelchner et al. [10] proposed to visualize dislocations with a centrosymmetry parameter that provides a measure of local departure from centrosymmetry in centrosymmetric crystals.

It should be pointed out that the excess energy, broken bonds, departure from centrosymmetry, as well as local stresses and strains are not specific to dislocations. Rather, they reveal all distorted regions of a crystal, be that a dislocation, a stacking fault or a point defect. In addition, calculations of atomic energies and stresses are only feasible with pair and embedded-atom-type potentials [11] and are more problematic when dealing with electronic-structure calculations. Furthermore, MD simulations of plastic deformation, fracture and other processes are often accompanied by the generation of new dislocations whose Burgers vectors are not known a priori. While they can be determined by drawing appropriate Burgers circuits, it is desirable to have a robust procedure for automated calculations of Burgers vectors of dislocations without resorting to a circuit construction.

The following treatment, based on the concept of the continuously dislocated continuum as described by Bilby, Bullough and Smith (BBS) [12] and Bilby [13], develops a method of analyzing the atomic misfit around a single dislocation in a crystal to obtain components of the Nye tensor [14] on a plane normal to the dislocation line. Atomic positions in a dislocated crystal are obtained by appropriate atomistic simulation methods. The atomic coordinates and the known perfect-lattice orientation are used to evaluate differential displacements of atoms and approximate them by continuous functions of coordinates. This is equivalent to replacing the discrete array of atoms in the dislocated crystal by a non-local continuum in which the misfit due to the dislocation is spread out over the plane normal to the dislocation rather than concentrated along the dislocation line [15]. Components of the Nye tensor then become distribution functions of the Burgers vector components of infinitesimal dislocations. Contour plots that display the values of these components provide a more vivid and informative description of the misfit produced by a dislocation than other methods mentioned earlier. This method does not require prior knowledge of the Burgers vector of a dislocation. Furthermore, a numerical integration of the Nye tensor distribution over an appropriate region normal to the dislocation line permits determination of the unknown Burgers vector of a dislocation with accuracy that is more than sufficient for the characterization of new dislocations emerging during large-scale simulations.

In Section 2 of the paper the concept of the Nye tensor is reviewed and its mathematical definition is formulated in terms convenient for computation. The computer implementation of Nye tensor calculations is described in Section 3. The method is applied in Section 4 to screw and edge dislocations in Cu and Al, used here as model materials. Finally, in Section 5 advantages and limitations of our method are discussed with recommendations concerning its application.

2. The Nye tensor and lattice deformation

A Burgers circuit is a closed path of arbitrary size and shape in the dislocated crystal, beginning at a point, S, and ending at the same point, F, enclosing one or more dislocations intersecting an area A. The circuit is taken in the right-hand (RH) sense relative to a unit vector normal to A. When transferred to a crystallographically equivalent circuit in the perfect lattice (an associated path in Bilby's terminology [13]), S and F do not coincide and the circuit fails to close. The closure failure, measured by the vector \( \mathbf{b} \equiv \mathbf{FS} \) in the perfect lattice, defines the resultant Burgers vector (RBV) of the dislocation array using the FS/RH convention [12,13]. If the circuit in the dislocated crystal contains a single dislocation, the RBV is called the true Burgers vector (TBV) of the dislocation. The TBV for a single dislocation is al-
ways a lattice vector in the perfect crystal, independent of the size of the circuit.

When a lattice containing a single dislocation is approximated by a local continuum, the dislocation is concentrated along a line. Crystallographically equivalent circuits not enclosing the dislocation line will close in both the perfect and dislocated lattice. Replacing this model by a non-local continuum effectively distributes the singularity associated with the dislocation line over an area normal to the dislocation line. The total dislocation can then be considered to have dissociated into a distribution of parallel dislocations, each having infinitesimal strength [16]. These infinitesimal dislocations can be described by distribution functions normalized so that the total Burgers vector associated with any Burgers circuit enclosed by the dislocation is equal to the Burgers vector of the dislocation. A Burgers circuit enclosing material that does not include the entire set of distribution functions may have a closure failure in the perfect crystal equal to a fraction of the Burgers vector.

Following [13], designate a set of covariant basis vectors of the perfect lattice by \( \mathbf{i}_a \). At every point, \( \mathbf{P} \), of the dislocated lattice \( \mathbf{e}_a \) related to those in the perfect crystal by a local deformation tensor, \( \mathbf{F}(\mathbf{P}) \), such that

\[
\mathbf{e}_a = \mathbf{F}_a^i(\mathbf{P})\mathbf{i}_i
\]

(1)

with the inverse transformation given by

\[
\mathbf{i}_a = (\mathbf{F}^{-1})^i_a\mathbf{e}_i
\]

(2)

where \( \mathbf{F}^{-1} \) is the inverse of \( \mathbf{F} \). Greek and Latin suffixes are employed to distinguish vectors and tensors in the perfect and dislocated crystal, respectively. Summation from 1 to 3 over repeated indices is implied. In the following development, the specification \( \mathbf{P} \) will be dropped with the understanding that the values of quantities in the dislocated crystal and the perfect crystal are evaluated at corresponding material points. Expressing the components of the lattice basis vectors of the perfect and dislocated crystals in terms of a common Cartesian coordinate system with basis vectors \( \mathbf{g}_a \) allows us to express the components of the deformation tensor in the same form as Eqs. (1) and (2) [17]. Let the \( L^x_a = \mathbf{i}_a \cdot \mathbf{g}^x \) and \( L^y_a = \mathbf{g}^x \cdot \mathbf{e}_a \) be matrices that specify the Cartesian components of the basis vectors. Then

\[
\mathbf{L} = \mathbf{L}^T \cdot (\mathbf{F}^{-1})^T
\]

(3)

relates basis vectors in the perfect and dislocated lattices with \( \mathbf{F} \) expressed in terms of its components referred to Cartesian axes. The superscript \( T \) indicates the transpose of a tensor. In the subsequent discussion, the deformation tensor \( (\mathbf{F}^{-1})^T \) is denoted as \( \mathbf{G} \) and termed “the lattice correspondence tensor”. It is the transpose of Bilby’s lattice correspondence function, \( \mathbf{E} \) [13].

The RBV of a differential Burgers circuit enclosing a non-zero distribution of infinitesimal dislocations is related to the Nye tensor \( \mathbf{x} \) by

\[
\mathbf{db} = \mathbf{x} \cdot \mathbf{n} d\mathbf{s},
\]

(4)

where \( \mathbf{n} \) is a unit vector normal to the area, \( d\mathbf{s} \), enclosed by the circuit. Denoting by \( \mathcal{A} \) the surface bounded by a circuit enclosing the entire distribution of \( \mathbf{x} \),

\[
\mathbf{b} = \int_{\mathcal{A}} (\mathbf{x} \cdot \mathbf{n}) d\mathbf{s}
\]

(5)

gives the TBV of the dislocation. Note that even if the TBV of a dislocation is parallel to only one coordinate axis, there can exist distributions of infinitesimal dislocations having Burgers vector components parallel to the other axes as long as the integral of these components over \( \mathcal{A} \) vanishes.

We will now follow [12,13,18] to express the Nye tensor in terms of the lattice correspondence tensor. A Burgers circuit, \( \mathcal{C} \), in the dislocated crystal that encloses material for which the distribution function of infinitesimal dislocations is non-zero consists of lattice vectors \( d\mathbf{x}' \), such that

\[
0 = \sum_{\mathcal{C}} d\mathbf{x}'.
\]

(6)

Transforming the vectors \( d\mathbf{x}' \) into their images, \( d\mathbf{x} \), in the perfect crystal and summing them algebraically along the associated path, \( \mathcal{C} \), gives the negative of the TBV of the dislocation

\[
\mathbf{b} = -\sum_{\mathcal{C}} d\mathbf{x}.
\]

(7)

The same deformation that connects the lattice basis vectors in the perfect and dislocated crystals (cf. Eq. (3)) relates the vectors \( d\mathbf{x} \) and \( d\mathbf{x}' \),

\[
d\mathbf{x} = d\mathbf{x}' \cdot \mathbf{G}.
\]

(8)

Then by Eqs. (7) and (8), replacing the sum in Eq. (7) by an integral, we have

\[
\mathbf{b} = -\int_{\mathcal{C}} d\mathbf{x}' \cdot \mathbf{G}.
\]

(9)

Applying Stokes’ theorem to Eq. (9) gives

\[
\mathbf{b} = -\int_{\mathcal{A}} (\nabla \times \mathbf{G}) \cdot \mathbf{n} d\mathbf{s}.
\]

(10)

The integrand in Eq. (10) is the differential TBV, \( db \).

Comparing Eq. (10) with Eq. (4), we obtain the expression

\[
\mathbf{x} = -(\nabla \times \mathbf{G})
\]

(11)

for the Nye tensor.

Eshelby’s model of a continuous distribution of dislocations on a plane [16] is related to the components of the Nye tensor by the following argument. Consider a distribution of infinitesimal dislocations parallel to \( \mathbf{g}_3 \),
concentrated on a single slip plane normal to \( \mathbf{g}_2 \). The vector \( \mathbf{g}_1 \) lies in the slip plane normal to the lines of the dislocation and forms a RH set with \( \mathbf{g}_2 \) and \( \mathbf{g}_3 \). To calculate the distribution of misfit, compute the differential displacement, \( \Delta \mathbf{u}(x_1) \), between atoms above and below the slip plane as a function of distance parallel to \( \mathbf{g}_1 \). The RBV, \( \delta \mathbf{B} \), due to dislocations lying in an infinitesimal strip of width \( |\delta x_1| \) is (no summation on \( k \))

\[
\delta B_k(x_1) = B_k \eta_{(k)}(x_1) \delta x_1 = \left( \frac{\partial \Delta u}{\partial x_1} \right)_{\mathbf{g}_1} \delta x_1, \tag{12}
\]

where \( \eta_{(k)}(x_1) \) is the number per unit length of infinitesimal dislocations located at \( x_1 \) having Burgers vector components parallel to \( \mathbf{g}_k \). Considering an element of area normal to \( \mathbf{g}_1 \), \( \delta \mathbf{B} = h|\delta x_1| \), where \( h \) is the distance between adjacent slip planes employed in the calculation of \( \Delta \mathbf{u}(x_1) \), Eq. (4) gives

\[
z_{(k)}(x_1) = \frac{1}{h} \left( \frac{\partial \Delta u}{\partial x_1} \right)_{\mathbf{g}_1} |\delta x_1| \tag{13}
\]

relating the components of the Nye tensor to the distribution functions.

Previous applications of this idea [16,19] have assumed that Burgers vectors of infinitesimal dislocations were parallel to the RBV of the entire array. However, if an RBV component of infinitesimal dislocations vanishes for the array, \( \delta z_{(k)} \) cannot be separated into a product of an RBV component and an associated distribution function for that component. Nevertheless, local components of the Nye tensor can be regarded as distribution functions for infinitesimal Burgers vectors by noting that

\[
z_{(k)}(x_1) = \frac{1}{h} \left( \frac{\partial \Delta u}{\partial x_1} \right)_{\mathbf{g}_1}. \tag{14}
\]

Local components of the Nye tensor that do not contribute to the RBV of the array will integrate to zero when Eq. (5) is evaluated over the entire plane normal to the dislocation lines. The preceding discussion and Eq. (14) correct the relationship presented in Eq. (30) of [15]. The following section illustrates how data specifying atomic positions in a dislocated crystal can be treated to obtain local components of the Nye tensor.

3. Computer implementation

3.1. Creating a dislocation

We construct a cylindrical simulation block that initially contains a perfect crystal lattice with a desired orientation relative to a RH orthonormal Cartesian system. We choose the cylinder axis parallel to \( \mathbf{g}_3 \), and \( \mathbf{g}_1 \) and \( \mathbf{g}_2 \) parallel to suitable low-index crystallographic directions. The boundary conditions are fixed in the \( \mathbf{g}_1 \) and \( \mathbf{g}_2 \) directions and periodic in the \( \mathbf{g}_3 \) direction. An inner region of the block containing free (dynamic) atoms is surrounded by a mantle of fixed atoms that remain “frozen” during MD and static simulations. The thickness of the fixed region is at least twice the cutoff radius of atomic interactions. Depending on the dislocation type, the block contains 1.5–2×10^4 atoms. The thickness of the block in the \( \mathbf{g}_3 \) direction is limited to two lattice periods. For convenience, the \( \mathbf{g}_2 \) direction is chosen to be normal to a slip plane of the dislocation to be studied. In preparation for further calculations, 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 \( (n \) is the first neighbor coordination number, e.g., \( n = 12 \) for FCC lattice). The set of vectors \( \mathbf{P}^{(\beta)} \) will be used as a reference for establishing the lattice correspondence.

We create a single dislocation parallel to \( \mathbf{g}_3 \) with a desired Burgers vector \( \mathbf{b} \). To this end, both fixed and free atoms are displaced from their initial positions according to the local continuum anisotropic elastic solution for the strain field of a straight dislocation [20] using known elastic constants of the material. We ensure that the dislocation line is placed between atomic rows to avoid singular values at atomic positions. Atomic positions in the dislocated crystal obtained in this manner are called “nonequilibrium”. To bring the dislocation to equilibrium at 0 K, we run MD simulations for 10 ps at several descending temperatures between 500 and 100 K, followed by a static relaxation (total energy minimization). Atomic positions in the dislocated crystal obtained by this procedure are called “equilibrium”. The MD simulation is needed to help the system overcome activation barriers that may exist on its way to equilibrium. Since the equilibration process is accompanied by spreading of the dislocation core, the strain field around the dislocation changes. Because the atoms residing in the fixed region remain in their initial positions and only free atoms move, some incompatibility can arise at the boundary between the free and fixed regions. This incompatibility can be made small by choosing a large enough radius of the free region. The latter condition is presumably met in our simulations, but in any case our goal is to demonstrate the proposed methodology rather than to achieve an ultimate convergence.

3.2. Determining the lattice correspondence tensor

Although in principle Eq. (3) can be solved to give the lattice correspondence tensor, the choice of appropriate basis vectors near the dislocation core is often problematic. To mitigate this difficulty and to increase the numerical stability of the computation, the lattice correspondence tensor is calculated by a scheme that employs all first neighbors of an atom.
The first step is to identify local crystallographic directions around every atom. For every atom in the dislocated lattice, we identify its nearest neighbors as atoms lying within a search sphere of radius \( R_s = 1/2(R_1 + R_2) \), where \( R_1 \) and \( R_2 \) are the first and second coordination radii in the perfect lattice. (Although in the BCC structure \( R_1 \) and \( R_2 \) are closer to each other than in FCC, this choice of \( R_s \) works well also for screw dislocations in BCC Fe and Mo (to be published elsewhere). We expect this choice of \( R_s \) to be suitable for hexagonal close packed crystals as well.) Within the dislocation core the number of such neighbors, \( n' \), can generally be different from that in the perfect lattice, \( n \). Let \( Q(\gamma) \) \((\gamma = 1, 2, \ldots, n')\) be the radius vectors of the neighbors in the dislocated crystal. For each neighbor, \( \gamma \), we compute the angles \( \phi^{(\gamma)} \) between \( Q^{(\gamma)} \) and all reference vectors \( P^{(0a)} \).

The reference vector \( P^{(0a)} \) with the smallest angular deviation, \( |\phi^{(\gamma)}| \), is identified as the one corresponding to \( Q^{(\gamma)} \). In other words, the interatomic bond \( Q^{(\gamma)} \) is considered as a deformation of the perfect-lattice bond \( P^{(0a)} \).

This procedure establishes a correspondence between all distorted vectors \( Q^{(\gamma)} \) and reference vectors \( P^{(0a)} \) for every atom in the block. While away from the dislocation core this correspondence is unique and the angular deviations are very small, inside the dislocation core some deviations can be as high as 30°.

It should be emphasized that the general problem of establishing a lattice correspondence for a crystalline defect does not always have a unique solution. First of all, the defect core structure can be distorted so severely compared to perfect lattice that the very notion of a correspondence may lose its significance. Secondly, point symmetry can make a correspondence non-unique. For example, an intrinsic stacking fault (ISF) in an FCC crystal can be obtained by three symmetrically equivalent but physically different relative translations of two half-crystals in \((211)\) directions parallel to a \(\{111\}\) plane. Having only atomic coordinates for an ISF one can never determine the initial perfect-lattice state and thus establish a unique lattice correspondence. This example is relevant to situations where a dislocation dissociates into Shockley partials separated by an ISF. Even though the strain field produced by the partials breaks the exact symmetry of the ISF structure, calculations of the lattice correspondence within the ISF region are still problematic.

The following algorithm is applied to handle non-unique situations. If two perfect-lattice bonds form equal angles with a given deformed bond \( Q^{(\gamma)} \), the latter is simply excluded from the calculation of \( G \) 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 \( \phi_{\text{max}} \) are excluded from \( G \) calculations. For the FCC metals studied in this work, we find that \( \phi_{\text{max}} = 27° \) gives the most satisfactory results. Results presented in Section 4 demonstrate that the rejection of problematic bonds does not affect the Burgers vector calculations and leads to very informative plots of core structures.

The lattice correspondence tensor \( G \) is constructed for each atom. According to Eq. (8), the relations

\[
P^{(\gamma)} = Q^{(\gamma)} \cdot G
\]

apply for \( \gamma = 1, 2, \ldots, n'' \), where \( n'' \) is the actual number of vectors after rejections. Since \( n'' > 3 \) and each vector consists of three components, this system of equations is overdetermined for the nine components of \( G \). The set of \( 3n'' \) equations relating the components of \( G \) to those of \( P^{(\gamma)} \) and \( Q^{(\gamma)} \) can be written in matrix form as

\[
P = Q \cdot G,
\]

where \( P \) and \( Q \) are \((n'' \times 3)\) matrices whose rows correspond to the index of the vector \( (\gamma) \) and columns, to the components of each vector along the reference Cartesian axes. The mean-squares solution of Eq. (16) has the form [21]

\[
G = Q^T P,
\]

where

\[
Q^T = (Q^T \cdot Q)^{-1} \cdot Q^T
\]

is the generalized inverse of \( Q \), also called the Moore–Penrose matrix [22]. Although this value of \( G \) is assigned to the central atom, it actually characterizes deformation of the entire coordination group around it. Thus, it is an average deformation gradient within the first coordination shell around an atom. The involvement of the relatively large \((O(n))\) number of bonds in this calculation makes it numerically stable. If some of the bonds have to be disregarded for the reasons discussed above, there are enough other bonds to produce a reasonable estimate of \( G \). The limit of resolution of this method is approximately a sphere centered on each atom and having a radius equal to the first neighbor distance. The volume associated with this sphere defines the “point” with which all continuum quantities are associated.

3.3. Nye tensor calculation

To obtain the Nye tensor \( \mathbf{z} \) from \( G \) for each atom and its nearest neighbors, the required spatial derivatives of \( G \) in the vicinity of each atom are computed using a finite difference approximation. Choose a particular tensor component of \( G \) at an atom, \( G^{(0)}_{\text{IM}} \), where the capital Latin suffixes indicate particular Cartesian coordinates and \( (0) \) indicates the atom for which \( G \) is defined. Define a \((3 \times 1)\) column vector \( \mathbf{A(\text{IM})} \) as \( A(\text{IM})_k \equiv \delta_k G^{(0)}_{\text{IM}} \) for \( k = 1, 2, 3 \). Also

\[
\Delta G^{(\gamma)}_{\text{IM}} = G^{(\gamma)}_{\text{IM}} - G^{(0)}_{\text{IM}}
\]
is the difference between the values of the component \( G_{IM} \) at a neighboring atom, \( \gamma \), and at the central atom, 0. Define a \((n'' \times 1)\) column vector \( \Delta G_{IM} \) composed of the values of \( \Delta G_{\gamma IM} \) for \( \gamma = 1, 2, \ldots, n'' \). Then the finite-difference equations for all nearest neighbors can be expressed as the matrix equation

\[
\Delta G_{IM} = Q \cdot A(IM).
\]  

This system of equations is overdetermined for the three Cartesian components of \( A(IM) \). As before, the values of the components that minimize the squares of the residuals of Eq. (20) are given by

\[
A(IM) = Q^+ \cdot \Delta G_{IM},
\]

where \( Q^+ \) is given by Eq. (18). The values of the derivatives thus obtained are assigned to the central atom. As for the \( G \)-tensor itself, they 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 \( T_{imk} = \partial_k G_{im} \). Finally, the Nye tensor is obtained from Eq. (11),

\[
\gamma_{jk} = -\epsilon_{jim} T_{imk},
\]

(\( \epsilon \) being the permutation symbol) and assigned to the atom in question. As a side product of these calculations, other quantities that characterize the lattice deformation can be computed and plotted, such as the Eulerian finite strain tensor, \( E^* \), the rotational part of \( E^* \), etc. [17].

The distribution of a particular component of \( \gamma \) or any other quantity is represented by a contour plot projected on the plane normal to the dislocation line (and thus normal to \( g_3 \)). To construct a contour plot, the values of the quantity assigned to individual atoms are interpolated to a fine uniform grid using a triangular interpolation method. The contour plot is superimposed onto the deformed atomic structure. In view of the periodicity along the dislocation line, we only show projections of atoms contained within one period. To compute a particular component \( b_j \) of the Burgers vector, we perform a numerical integration of \( \gamma_{j3} \) on the projection plane over a rectangular area in which the absolute value of \( \gamma_{j3} \) is greater than a specified small number.

4. Application to dislocations in Cu and Al

We model atomic interactions in Cu and Al by embedded-atom potentials developed in [23,24]. The potentials were constructed by fitting to experimental and first-principles data for a large set of properties of these metals. In particular, the elastic constants are reproduced in excellent agreement with experiment [21,22]. The ISF energies predicted by the potentials are 44 and 166 mJ/m\(^2\), respectively [19]). Figs. 1–4 represent contour plots of various components of the Nye tensor for selected dislocations.
The Burgers vector of all dislocations is \( \frac{1}{2} \langle -1 1 0 \rangle \). The magnitude and sense of a Nye tensor component \( a_{ij} \) is indicated by a color scale covering the range from \(-|a_{ij}|_{\text{max}} \) to \(|a_{ij}|_{\text{max}} \), where \(|a_{ij}|_{\text{max}} \) is the maximum value of \(|a_{ij}| \) over the plot. We only show the relevant part of the \( a \) distribution and leave out the large surrounding areas around the dislocation. The distances in the plots are measured in Å and \( a \) is measured in Å\(^{-1}\).

Fig. 1(a) displays the \( z_{33} \) distribution for a non-equilibrium (undissociated) screw dislocation in Cu. In our geometry, \( z_{33} \) represents the screw component of the dislocation. Since the atoms are displaced according to local continuum elasticity theory, \( z_{33} \) is, in fact, a delta-function. The computation procedure employed here yields a sharp peak whose exact shape depends on the placement of the dislocation line but whose width always remains comparable to the interatomic distance \( R_1 \). This width defines the spatial resolution of our method, namely, about 2.5–3 Å. As expected from local
continuum elasticity theory, the $\alpha_{13}$ and $\alpha_{23}$ components are identically zero. Integration over the peak area gives us a Burgers vector of 2.521 Å in excellent agreement with the ideal value 2.556 Å (Table 1).

Fig. 1(b) and (c) shows the distributions of $\alpha_{13}$ and $\alpha_{13}$ for the same dislocation after it has been brought to equilibrium using the relaxation procedure described earlier. The plots reveal a dissociation of the dislocation into Shockley partials separated by a distance of about 8 Å. Fig. 1(c) allows us to determine that the right partial has a negative edge component ($\alpha_{13}$) while the left one a positive component. As expected, the integration of the $\alpha_{33}$ plot yields an accurate estimate of the total Burgers vector (Table 1) while the integration of the $\alpha_{13}$ plot gives practically zero. (If the integration results in a Burgers vector component below $10^{-3}, 10^{-2}$ Å, we consider this component as zero since it is comparable to the accuracy of our calculations. The zero values indicated in the appropriate lines of Tables 1 and 2 should be understood in this sense.) The $\alpha_{23}$ component is practically zero, hence its plot is not shown here.

Similar results are obtained for an edge dislocation as shown in Fig. 2. As expected, the dissociated width of the edge dislocation is about a factor of three larger than that of the screw dislocation. From the location of the peaks of the $\alpha_{13}$ and $\alpha_{33}$ components of the Nye tensor we can determine both the positions of the Shockley partials and the signs of their edge and screw components. As expected, the $\alpha_{23}$ component is found to be practically zero. Table 1 illustrates that the total Burgers vector recovered from these plots is in excellent agreement with the ideal value.

As a further test, we have computed the edge and screw components of the partials by integrating the Nye tensor distributions over the relevant peak areas. Table 2 shows that the results compare very well with the ideal Burgers vectors known from the lattice geometry. This agreement demonstrates the ability of our method to characterize even partial dislocations on a quantitative level, at least if those are separated well enough to decouple the relevant integrals.

Fig. 3(a) and (b) presents the results of similar calculations for a screw dislocation in Al. As expected from its high ISF energy, the distance between partial dislocations in the equilibrium configuration is much smaller than in Cu. While the plot of the screw component $\alpha_{33}$ shows only some elongation of the core along the (111) plane, by plotting the edge component $\alpha_{13}$ we immediately identify the Shockley partials and determine the signs of their edge components. Thus, even in this case our method clearly reveals the dissociation. As shown in Table 1, in all cases we are able to recover the resultant Burgers vector of the total dislocation with high accuracy for both aluminum and copper.

Finally, numerous calculations have been performed to demonstrate that our representation is specific to dislocations and insensitive to point defects. As an example, Fig. 4 displays the screw components of the partials of a dissociated edge dislocation in Al together with a lattice vacancy. The vacancy was created at a site marked by the arrow followed by a static relaxation of the block. As expected, the Nye tensor remains practically zero around the vacant site while clearly revealing the Shockley partials. This was commonly observed for both vacancies and interstitials placed at various lattice positions.

5. Discussion and conclusions

The concept of the Nye tensor was originally developed to characterize the resultant Burgers vector of dislocation ensembles [12–14] but was later applied to describe the lattice misfit associated with a single dislocation having a non-compact core [15]. This latter idea is the basis of a method first applied by Cooper et al. [25] and further developed and extended in this work for the characterization of dislocation core structures. We notice that Daw et al. [26] also proposed to employ the continuum dislocation distribution theory [27] to characterize individual computer-simulated dislocations. Their method was applied to an edge dislocation in Ni.

The method provides a powerful tool for the description of misfit in the vicinity of a dislocation core obtained by various simulation procedures. Plots of the components of the Nye tensor in a plane normal to the dislocation line accurately reveal all details of dislocation core spreading or dissociation. Nye tensor calculations do not require prior knowledge of the Burgers vector of the dislocation. Furthermore, by integrating suitable components of the Nye tensor over appropriate regions of the plane normal to the dislocation line, the

---

**Table 1**

Comparison of the ideal Burgers vector with that for non-equilibrium and equilibrium screw and edge dislocations in Cu and Al calculated from the Nye tensor distributions (Å)

<table>
<thead>
<tr>
<th></th>
<th>Cu</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Screw</td>
<td>Edge</td>
</tr>
<tr>
<td>Ideal</td>
<td>2.556</td>
<td>2.556</td>
</tr>
<tr>
<td>Non-equilibrium</td>
<td>2.521</td>
<td>2.613</td>
</tr>
<tr>
<td>Equilibrium</td>
<td>2.635</td>
<td>2.574</td>
</tr>
</tbody>
</table>

**Table 2**

Comparison of ideal Burgers vectors of Shockley partial dislocations with those calculated from the Nye tensor distributions for an equilibrium edge dislocation in Cu (Å)

<table>
<thead>
<tr>
<th></th>
<th>Cu</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Right</td>
</tr>
<tr>
<td>Ideal</td>
<td>[1.278 0 0.738]</td>
</tr>
<tr>
<td>Computed</td>
<td>[1.292 0 0.748]</td>
</tr>
</tbody>
</table>
Burgers vector of the dislocation can be determined with high accuracy. The Burgers vectors of partial dislocations formed by dissociation of the dislocation can also be determined if their separation is large enough to neglect their overlap.

This technique should prove useful in distinguishing among predictions of dislocation core structures arising from various simulation methods. In addition, the values of the Nye tensor obtained by atomic simulations can be used as source functions to calculate the perturbations in the dislocation strain field near the core due to the misfit distribution arising from the discrete lattice [15], thus creating an analytical link between discrete atomic models and a non-local continuum model of the dislocation. We anticipate that the method can also be useful for analyzing experimental dislocation core structures obtained by HRTEM.

Another advantage of using the Nye tensor is that it only has nonzero values when misfit due to dislocations is present and is insensitive to compatible lattice deformations arising from other lattice defects or external sources. In contrast, visualization methods that reveal all lattice strains [2,6,7] include stacking faults, vacancies, interstitials and other sources of strain as well as dislocations. The atomic resolution of this method renders it ideal for analyzing fine features of dislocation core spreading and its evolution under applied stresses or during dislocation motion.

In cases of widely dissociated dislocations, for example in intermetallic compounds [2,6,7,9], it is often desirable to observe the location of the planar faults between the partials. Since there is no Burgers vector content associated with planar faults, they are "invisible" in our method. However, they can be readily revealed by neighbor analysis, color coded, and superimposed on Nye tensor plots.

To construct Nye tensor plots, one needs to know the lattice orientation around the dislocation. In large-scale atomistic simulations, especially when there is a tendency for dislocations to form walls, lattice rotation can be produced and reliable Nye tensor calculations may require a correction for the new lattice orientation. An automated introduction of such corrections would require a specially designed computational procedure. For the same reason, the proposed formulation of the method will not apply to a polycrystalline material. However, if orientations of individual grains are known, the procedure proposed here for establishing the lattice correspondence (Section 3) can be generalized by comparing each set of $Q^{(i)}$ vectors against sets of $P^{(j)}$ vectors corresponding to individual grains and choosing the set with the smallest angular deviation. This is equivalent to assigning each atom to one grain or another. Although some ambiguity may be associated with this procedure, it can still prove useful for analyzing grain boundary structures and dislocations located in or near grain boundaries. These and other generalizations of the method can be the subject of future work.

Acknowledgements

The authors wish to acknowledge support of this research by the Air Force Office of Scientific Research through Grant No. FA9550-04-1-0017. We also appreciate helpful discussions with K. Hemker and B. Mendis.

References