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Using a scalar parameter to trace dislocation evolution in atomistic modeling

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ABSTRACT

A scalar γ-parameter is proposed from the Nye tensor. Its maximum value occurs along a dislocation line, either straight or curved, when the coordinate system is purposely chosen. This parameter can be easily obtained from the Nye tensor calculated at each atom in atomistic modeling. Using the γ-parameter, a fully automated approach is developed to determine core atoms and the Burgers vectors of dislocations simultaneously. The approach is validated by revealing the smallest dislocation loop and by tracing the whole formation process of complicated dislocation networks on the fly.

1. Introduction

Atomistic modeling such as molecular dynamics simulations has become a powerful tool which allows us to unambiguously examine deformation processes of crystalline materials from an atomistic viewpoint [1]. When the applied loading is approaching the strength of materials during simulations, small loops or segments of dislocations will nucleate and then gradually grow up [2–5]. This evolution process of dislocations usually dominates the deformation behaviors of materials. Therefore, it is desirable to develop dislocation visualization methods to reveal the underlying mechanisms of deformation in atomistic modeling.

Dislocations can be visualized by excess energy analysis [6], common neighbor analysis [7], and other filtering tools [8] because they cause variations of atomic energy and positions. However, these filtering tools provide no information about the Burgers vectors to characterize dislocations. There are two types of methods to obtain the Burgers vectors of dislocations. One is through the Burgers circuit mapping, and various ways of construction and mapping of the Burgers circuit have been proposed [9–13]. The other is by numerical integration of the Nye tensor over an area perpendicular to the dislocation line [14–17]. This integration is relatively time-consuming since it needs an interpolation method to get the accurate shape of spatial distribution of the Nye tensor [14,17]. It is apparent that the integration could become problematic for closely spaced dislocations because of the overlap of their Nye tensor field. On the other hand, except the case with straight dislocations [18], the Nye tensor cannot be used to detect independently core atoms of curved dislocations because the value of its nine elements could change dramatically with the dislocation line direction. This can be seen from the work of Begau et al. [17], in which a filtering tool rather than the Nye tensor was utilized to detect core atoms of curved dislocations.

It is the goal of this paper to develop a simple approach on the basis of the Nye tensor calculation only, which is capable of detecting atoms in dislocation cores without aid of any filtering tool, and at the same time, determining their Burgers vectors by the property of a scalar γ-parameter we proposed rather than the integration of the Nye tensor mentioned above. In this work, a γ-parameter is first proposed on the basis of the Nye tensor. Then, using this scalar parameter, a simple approach is developed and implemented into atomistic modeling. Several examples are selected to demonstrate the properties of the γ-parameter and the ability of our approach. Finally, advantages and limitations of our approach are discussed.

2. Theoretical derivations

A dislocation is characterized mainly by its Burgers vector that can be described by the Nye tensor [19,20]. Suppose that a single dislocation with a Burgers vector $\boldsymbol{b}$ (henceforth called dislocation

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$\boldsymbol{b}$) exists in a continuum media. Its line could be straight or curved, denoted by "L". Its Burgers vector $\boldsymbol{b}$ is defined as

$$\boldsymbol{b} = -\oint_C \boldsymbol{G}d\boldsymbol{y} \tag{1}$$

where C is a closed circuit around the dislocation line L, $\boldsymbol{G}$ is the lattice distortion tensor, the same as that defined in Ref. [14], and $d\boldsymbol{y}$ is an infinitesimal step along the Burgers circuit C. When the Stokes' theorem is applied to Eq. (1), we have

$$\boldsymbol{b} = \int_A \boldsymbol{\alpha}\boldsymbol{n}ds \tag{2}$$

Here A, ds, and $\boldsymbol{n}$ are the area bounded by the circuit C, an area element and the unit normal vector of the area element, respectively. $\boldsymbol{\alpha}$ is the well-known Nye tensor, the tensor of dislocation density. The nine components of $\boldsymbol{\alpha}$ can be calculated according to

$$\alpha_{ij} = -\varepsilon_{jkl}\partial g_{il}/\partial x_k \tag{3}$$

where i, j, k and $l = 1$–3, the permutation tensor $\varepsilon_{jkl} = (j-k)(k-l)(l-j)/2$, and the Einstein summation convention is employed. In Eq. (3), α_{ij} and g_{il} are the component of $\boldsymbol{\alpha}$ and $\mathbf{G}$, respectively. Eqs. (1)–(3), equivalent to Eqs. (9)–(11) in Ref. [14], are briefly outlined here for completeness.

The Nye tensor near the line L of the dislocation $\boldsymbol{b}$ is a function of the line direction and the Burgers vector [19]. Let P be a point of intersection of the dislocation line L and the area A, and $\boldsymbol{l}$ be a unit direction vector of the line L at P. Following Kröner's Eq. (32) in Ref. [21], the Nye tensor at the point P can be written as

$$\boldsymbol{\alpha} = \boldsymbol{b}\boldsymbol{l}^T\delta(\rho) \tag{4}$$

Here the superscript "T" represents the transpose of a vector. $\delta(\rho)$ is a delta function which is infinite along the dislocation line and zero otherwise, and ρ is the distance to the point P. Dislocation cores are assumed to have a negligible width in Eq. (4). This is an idealized situation because dislocation cores are more or less dispersed [22]. Eq. (4) implies that

$$\boldsymbol{\alpha} \propto \boldsymbol{b}\boldsymbol{l}^T \tag{5}$$

In order to employ $\boldsymbol{\alpha}$ to visualize curved dislocations, it is necessary to propose a new parameter independent to the line direction $\boldsymbol{l}$. For this purpose, a matrix $\boldsymbol{Y}$ is built by the equation:

$$\boldsymbol{Y} = \boldsymbol{\alpha}\boldsymbol{\alpha}^T(\propto \boldsymbol{b}\boldsymbol{b}^T) \tag{6}$$

The term in the parenthesis is derived from Eq. (5). It is seen from Eq. (6) that all the elements in $\boldsymbol{Y}$, including the γ-parameter defined later, depend only on the Burger vector, but not a function of the dislocation line direction $\boldsymbol{l}$. Furthermore, the matrix $\boldsymbol{b}\boldsymbol{b}^{\mathrm{T}}$ in Eq. (6) will contain only one nonzero element if $\boldsymbol{b}$ becomes parallel to a coordinate axis. Then, the corresponding nonzero element in $\boldsymbol{Y}$ (the γ-parameter) is obtained to reveal curved dislocations. This can be achieved by coordinate system transformation, as presented in the following.

Two types of orthogonal coordinate systems are utilized throughout this work. One is the coordinate system (henceforth represented by $\{\boldsymbol{x}_i\}$) of the simulation box with three axes that are denoted by the unit vectors $\boldsymbol{x}_1$, $\boldsymbol{x}_2$, and $\boldsymbol{x}_3$, and the other is established for each type of Burgers vectors. Assume that the Burger vector $\boldsymbol{b}$ has n known values, e.g. they are usually $\langle 1\,1\,1\rangle/2$ and $\langle 0\,0\,1\rangle$ translation vectors in a body centered cubic (bcc) crystal, that is, $\boldsymbol{b} = \boldsymbol{b}_k$ ($k = 1\ldots n$). Each $\boldsymbol{b}_k$ has a coordinate system $\{{}^k\boldsymbol{x}_i\}$ with the condition that ${}^k\boldsymbol{x}_3$ should be chosen to be parallel to $\boldsymbol{b}_k$, as sketched in Fig. 1. In order to distinguish them from different coordinate systems, the vectors and matrices have a left superscript "k" when defined in $\{{}^k\boldsymbol{x}_i\}$, while they have no such superscripts in $\{\boldsymbol{x}_i\}$.

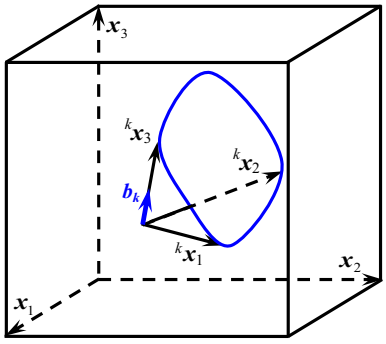

Fig. 1. Two types of coordinate systems for dislocation visualization. One is the coordinate system of the simulation box with three axes $\boldsymbol{x}_1$, $\boldsymbol{x}_2$ and $\boldsymbol{x}_3$, and the other has three axes ${}^k\boldsymbol{x}_1$, ${}^k\boldsymbol{x}_2$ and ${}^k\boldsymbol{x}_3$. The latter is designed expressly (${}^k\boldsymbol{x}_3 \| \boldsymbol{b}_k$) for visualization of all dislocations with a Burgers vector $\boldsymbol{b}_k$ in the simulation box. Only one dislocation loop $\boldsymbol{b}_k$ is sketched for clarity.

In the coordinate system $\{{}^k\boldsymbol{x}_i\}$, Eq. (6) becomes

$${}^k\boldsymbol{Y} = {}^k\boldsymbol{\alpha}({}^k\boldsymbol{\alpha})^T \tag{7}$$

The tensors ${}^k\boldsymbol{\alpha}$ can be calculated from $\boldsymbol{\alpha}$ by

$${}^k\boldsymbol{\alpha} = ({}^k\mathbf{A})\boldsymbol{\alpha}({}^k\mathbf{A})^T \tag{8}$$

where the components of ${}^k\mathbf{A}$ is defined as

$$a_{ij} = ({}^k\boldsymbol{x}_i)^T\boldsymbol{x}_j \tag{9}$$

The transformation of a second-rank tensor can be found in Chapter I in Ref. [23]. Because $\boldsymbol{b}_k$ is set to lie along ${}^k\boldsymbol{x}_3$, only the last element of the matrix $\boldsymbol{b}_k\boldsymbol{b}_k^T$ is nonzero. Therefore, according to Eq. (6), the last element of ${}^k\boldsymbol{Y}$ (at column 3 and row 3),

$${}^k\gamma = ({}^k\alpha_{31})^2 + ({}^k\alpha_{32})^2 + ({}^k\alpha_{33})^2 \tag{10}$$

is chosen to reveal dislocations, which is called γ-parameter in this study. Substituting Eq. (8) into Eq. (7), it is not difficult to obtain that

$${}^k\gamma = \sum_{j=1}^{3}(a_{31}\alpha_{1j} + a_{32}\alpha_{2j} + a_{33}\alpha_{3j})^2 \tag{11}$$

From Eq. (11) it is seen that that the γ-parameter is a function of a_{31}, a_{32} and a_{33}, and thus it depends only on ${}^k\boldsymbol{x}_3$, which is selected to be parallel to $\boldsymbol{b}_k$, but not on ${}^k\boldsymbol{x}_1$ and ${}^k\boldsymbol{x}_2$. Therefore, ${}^k\boldsymbol{x}_1$ and ${}^k\boldsymbol{x}_2$ can be freely selected in calculation of the γ-parameter. Both Eqs. (10) and (11) shows that the γ-parameter is always nonnegative.

The γ-parameter can be utilized to determine the Burger vector simply by coordinate transformation. Without loss of generality, let us choose $\boldsymbol{b} = \boldsymbol{b}_{\mathrm{m}}$ to provide an example. When $\boldsymbol{b} = \boldsymbol{b}_{\mathrm{m}}$, by use of Eqs. (6) and (7), one can get

$${}^k_m\boldsymbol{Y} \propto \begin{bmatrix} ({}^k_m b_1)^2 & ({}^k_m b_1)({}^k_m b_2) & ({}^k_m b_1)({}^k_m b_3) \\ ({}^k_m b_2)({}^k_m b_1) & ({}^k_m b_2)^2 & ({}^k_m b_2)({}^k_m b_3) \\ ({}^k_m b_3)({}^k_m b_1) & ({}^k_m b_3)({}^k_m b_2) & ({}^k_m b_3)^2 \end{bmatrix} \tag{12}$$

Here the left subscript "m" means that ${}^k\boldsymbol{Y}$ occurs near a dislocation $\boldsymbol{b}_m$. $\boldsymbol{b}_m$ is denoted by ${}^k\boldsymbol{b}_m$ in $\{{}^k\boldsymbol{x}_i\}$. Assume that ${}^k\boldsymbol{b}_m = [\,{}^k_m b_1 \quad {}^k_m b_2 \quad {}^k_m b_3\,]^T$, where ${}^k_m b_1$, ${}^k_m b_2$ and ${}^k_m b_3$ are real numbers. The length of ${}^k\boldsymbol{b}_m$ is calculated as $d_m = \sqrt{({}^k_m b_1)^2 + ({}^k_m b_2)^2 + ({}^k_m b_3)^2}$. Correspondingly, the γ-parameter in Eq. (10) can be written as

$${}^k_m\gamma = ({}^k_m\alpha_{31})^2 + ({}^k_m\alpha_{32})^2 + ({}^k_m\alpha_{33})^2 \tag{13}$$

It is apparent that both k and m take on the values 1 to n in Eqs. (10)–(13).