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Improvement of nonlocal Peierls-Nabarro models

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ABSTRACT

We review the major efforts that improve the accuracy of Peierls-Nabarro (PN) model in predicting core structure and Peierls stress, and recognize that the nonlocal atomic interactions in the core region should be accounted for in calculating the dislocation energy. Although some efforts have been devoted to taking the nonlocal interaction into account, further improvement is needed to simplify the computational complexity and resolve the inconsistency between the continuum model and the discrete nature of the lattice. Here we developed a two-dimensional (2D) and a three-dimensional (3D) nonlocal semi-discrete variational Peierls-Nabarro (SVPN) models by incorporating the nonlocal atomic interactions into the semi-discrete variational Peierls framework. The nonlocal SVPN models are applied to dislocations with extended core in copper and compact core in iron. Molecular dynamics simulations are performed to validate the model predictions. We found that the nonlocal SVPN model (both 2D and 3D) significantly improves the prediction accuracy for dislocation core structure and Peierls stress. Moreover, the results show that the 2D and 3D models give similar predictions of the Peierls stress and dislocation core structure, when the atomic relaxation in the normal direction is allowed in the 2D model to describe the interatomic interactions in the slip plane.

1. Introduction

Crystal plasticity is accommodated by dislocation slips and localized shear transformations (such as twinning and phase transformation) that are accomplished by the movement twinning dislocations/disconnections or steps. The mobility of these linear defects to a great extent determines mechanical properties of materials. Therefore, accurate prediction of Peierls stress for a dislocation (the minimum external stress to move a straight dislocation) is vital to understand the mobility of the dislocation. Much effort has been devoted to measure and estimate the Peierls stress associated with dislocations by using theory, modeling, and experiments [1–4]. Molecular statics/dynamics simulations that are capably of calculating atomic interactions in full three dimensions were extensively used to study dislocation behaviors including nucleation, motion, and reactions [5–7]. However, it is limited for complex system because of the unavailability of the empirical potentials for molecular statics/dynamics simulations. Atomistic calculations using first principles density function theory have no dependence on potentials while have the limited simulation volumes. Thus it is rarely used to study the motion of dislocations.

Continuum elasticity theory well describes the long-range elastic strain of a dislocation for length scales beyond a few lattice spacing, but it breaks down in the region surrounding the dislocation center (referred to as the dislocation core). The early crystallographic model developed by Peierls and Nabarro (PN) [8,9] (referred to as original PN model) was the first one to describe crystallographic character of a dislocation core in the frame of continuum elasticity theory based on the assumption of one dimensional sinusoidal law for atomic interactions across the slip plane, and its analytical solution gave the core structure and Peierls stress for the first time. This method is naturally associated to the inconsistency between the continuum model and the discrete nature of the lattice [10,11]. There has been a great deal of interest in describing accurately the core structure of a dislocation at the atomic scale because the structure and properties of dislocation core control the mobility of the dislocation, which accounts for the intrinsic ductility or brittleness of solids. To capture the core structure of a dislocation, several improvements [11–15] have been proposed in past decades. Vitek [12,13] proposed a more physically realistic way to describe atomic interactions by replacing the sinusoidal force with the gradient of the γ-surface (the

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model is thus referred to as the γ-PN model), and from the maximum slope of which, the Peierls stress of dislocations with both narrow and wide core can be directly estimated [16,17]. Schoeck [14,15] further generalized the γ-PN model to a two dimensional one. The γ-PN models have been frequently adopted to investigate dislocation properties [18–21] for its efficiency in obtaining the two dimensional dislocation core. Inconsistency between the continuum and discrete treatment of the dislocation in the γ-PN model was overcome by the semi-discrete variational Peierls framework (referred to as SVPN model) [11]. In SVPN model, discrete nature of the lattice was accounted for in calculating the dislocation energy, and the dislocation profile was allowed to fully relax in three dimensions as the dislocation moves in lattice under the external applied stress [11].

All these improvements were made within the locality assumption, i.e., the misfit energy in the region of dx depends only on the γ-surface at that local atomic site, which was implied in that the γ-surface was calculated using a uniform disregistry vector. However, the large gradient in the dislocation profile has been demonstrated using atomistic simulations but not incorporated into PN models. Schoeck [22] and Miller et al. [23] modified the misfit energy in the slip plane by considering the large displacement gradient effects in the core region in order to account for the nonlocal effects. Their applications were limited due to the complicated nonlocal mathematical formulation or the difficulty in assessing the nonlocal parameters. In this work, we developed an improved two-dimensional (2D) nonlocal SVPN model by incorporating the nonlocal atomic interactions into the SVPN model, wherein the form of the nonlocal interaction energy term was inspired from the nonlocal kernel derived by Miller et al. [23] but extended to two dimensions in a simpler form, and the nonlocal coefficient is computed directly from the dislocation core structure. Moreover, we extended the improved 2D nonlocal SVPN model to a three-dimensional (3D) one by explicitly introducing the vertical component of the disregistry vector in the dislocation energy. Finally, we tested our 2D and 3D nonlocal SVPN models for dislocations in iron and copper, by comparing predictions for the core structure and Peierls stress with MD simulations.

2. Typical PN models

2.1. Local PN models

In the original PN model [8,9,24], dislocation energy is composed of two parts, the elastic energy stored in the two half continuum linear elastic solid separated by the dislocation slip plane, and the atomic misfit energy in the slip plane to account for the nonlinear interatomic interaction, which is confined in the slip plane. The dislocation profile or the disregistry, $\delta(x)$ (relative displacement of the atom pairs across the shear plane), should minimize the total energy. Correspondingly, the total energy is a functional of the dislocation profile,

$$E[\delta(x)] = E_{elastic} + E_{misfit} = K\iint \frac{d\delta(x')}{dx'}\frac{\delta(x)}{x-x'}dxdx' + \int \gamma[\delta(x)]dx \quad (1)$$

where the two terms on the right hand are the elastic energy and the misfit energy respectively. K depends on the dislocation type, and equals to $\mu/(4\pi)$ for a screw dislocation and $\mu/(4(1-\nu)\pi)$ for an edge dislocation assuming isotropic elasticity, where μ is the shear modulus and ν is the Poisson's ratio. $\gamma[\delta(x)]$ is the misfit potential to describe the interatomic interaction across the slip plane, gradient of which is the atomic restoring force. The dislocation profile is obtained by minimizing the total energy. Then Peierls stress is determined as the maximum slope of the misfit energy variation as the dislocation profile is rigidly translated in crystal for one lattice period.

Three major simplifications were made in the original PN model. (i) One dimensional sinusoidal form for the periodical misfit potential $\gamma[\delta(x)]$ was assumed to describe the interatomic interactions. (ii) Inconsistency exists in calculating the misfit energy, which was obtained by continuously integrating the $\gamma[\delta(x)]$ in Eq. (1) to obtain the dislocation profile $\delta(x)$, but to determined Peierls stress it was obtained by discretely summing up $\gamma[\delta(x_i)]$ at atomic sites x_i. (iii) Dislocation profile was rigidly translated in the lattice without relaxation in determining the Peierls stress.

To better describe the interatomic interactions, the concept of the γ-surface (the generalized stacking fault energy (GSF energy) surface firstly proposed by Vitek [12,13]) was used. Joos et al. [16,17] firstly modified the magnitude of the sinusoidal misfit potential according to the maximum gradient of the γ-surface. Later, Schoeck [14,15] directly replaced the sinusoidal misfit potential in Eq. (1) with the γ-surface, and the PN model was thus generalized to a 2D one (referred to as γ-PN model), the dislocation energy is written as,

$$E[\vec{\delta}(x)] = E_{elastic} + E_{misfit} = \iint \frac{d\vec{\delta}(x')}{dx'}\frac{H}{x-x'}\vec{\delta}(x)dxdx' + \int \gamma[\vec{\delta}(x)]dx \quad (2)$$

where the dislocation profile $\vec{\delta}(x)$ is a 2D vector spreading in the slip plane. The symmetric Stroh tensor H in the elastic energy term can account for the elastic anisotropy according to anisotropic elastic theory [25,26]. The 2D disregistry profile is solved by variational methods. Peierls stress is calculated based on the variation of the misfit energy (by discretely summing the GSF energy $\gamma[\delta(x_i)]$ at atomic sites x_i instead of continually integrating the GSF energy) with respect to the rigid translation of the dislocation profile in lattice. Due to the availability of γ-surface from first principles calculations, the γ-PN model has been widely applied to investigate dislocation properties such as dislocation dissociation, grain boundary dislocations and even dislocation properties under high pressure [18–21].

The inconsistency between the discrete nature of the lattice and the continuum treatment of the 2D disregistry vector in integrating the dislocation energy, is conquered by SVPN model [11]. The elastic energy and misfit energy in SVPN model were calculated by linearly interpolating the dislocation profile according to the position of the atomic rows x_i. By doing so, discrete nature of the lattice was accounted for. Moreover, the dislocation profile is treated as a 3D disregistry vector (two in-plane components plus the normal component) to describe the dislocation core. Therefore, the dislocation profile $\vec{\delta}(x)$ is discretized as $\delta_k(x_i)$, $k = 1, 2, 3$ denoting the dislocation profile along x-, y- and z-direction respectively, where y is the normal direction. The total energy is thus rewritten as

$$\begin{aligned} E[\vec{\delta}(x_i)] &= E_{el} + E_{misfit} - E_{app} \\ &= \sum_{i,j}\chi_{ij}\left[K_e\left(\rho_1(x_i)\rho_1(x_j) + \rho_2(x_i)\rho_2(x_j)\right) + K_s\rho_3(x_i)\rho_3(x_j)\right] \\ &\quad + \sum_i \gamma[\vec{\delta}(x_i)]\Delta x - \sum_{i,k}\frac{x_{i+1}^2 - x_i^2}{2}\left(\rho_k(x_i)\tau_k\right) \end{aligned} \quad (3)$$

The discrete coefficient χ_{ij} is

$$\begin{aligned} &\chi_{ij} = \tfrac{3}{2}\phi_{i+1,i}\phi_{j+1,j} + \psi_{i,j} + \psi_{i+1,j+1} - \psi_{i+1,j} - \psi_{i,j+1} \\ &\phi_{i,j} = x_i - x_j, \psi_{i,j} = \tfrac{1}{2}\phi_{i,j}^2 \ln|\phi_{i,j}| \end{aligned} \quad (4)$$

The first two energy terms correspond to the elastic energy and misfit energy in the discrete forms, similar to those in Eq. (1) for