

Research Article

Surface Effects on the Properties of Screw Dislocation in Nanofilms

Lili Liu,^{1,2} Zhenya Meng,² Gang Xu,¹ Chenglin He,¹ Xiaozhi Wu,^{2,3} and Rui Wang²

¹Department of Physics, Chongqing Three Gorges University, Chongqing 404100, China

²Institute for Structure and Function, Chongqing University, Chongqing 401331, China

³College of Materials Science and Engineering, Chongqing University, Chongqing 400044, China

Correspondence should be addressed to Xiaozhi Wu; xiaozhiwu@cqu.edu.cn

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The image dislocation method is used to construct the governing equation of dislocations in nanofilms. The classical Peierls-Nabarro equation can be recovered when the thickness of nanofilm is taken to be infinite. In order to determine the core width and Peierls stress of dislocations, the unstable stacking fault energies of Al and Cu nanofilms are calculated via the first-principle methods. It is found that surface effect can increase the Peierls stresses of screw dislocations in Al and Cu nanofilms.

1. Introduction

Thin film materials are of great importance in modern technology. They have a wide range of applications in engineering systems, such as highly integrated electronic circuits and microelectromechanical devices. It is widely accepted that defects such as dislocations play a key role in determining the mechanical properties of materials [1]. The classical Peierls-Nabarro (P-N) dislocation model has been the most widely used model of dislocations in bulk materials [2, 3]. Although powerful in its simplicity, it cannot deal with the dislocations in nanofilm with free surfaces [4, 5]. Accounting for the free surface on the physical properties of dislocations in nanofilm is important, as the ratio of surface to volume is high. The effects of free surface on the dislocation properties cannot be neglected anymore; the dislocation behavior in thin films is different from that in bulk materials [6, 7]. Recently, Lee and Li constructed a half-space P-N model for dislocations near a free surface and they claimed that the mobility of the dislocation will be increased near the free surface [8, 9]. Cheng et al. investigated Peierls stress of a screw dislocation below a free surface via a self-consistent semidiscrete variational P-N model using image dislocation method [10]. It is found that the free surface increases the Peierls stress and in consistence with the results obtained by molecular dynamics simulation

[11, 12]. In this letter, the image dislocation method is used to investigate the dislocation core structure and Peierls stress in nanofilm with double free surfaces. The image dislocations are introduced to satisfy the free surface boundary condition; namely, the stress field acting on the surface should vanish [13]. The governing equation for dislocations in nanofilm is constructed according to the procedure for P-N equation provided by Joós et al. [14, 15]. Furthermore, the unstable stacking fault (USF) energies of Al and Cu nanofilms are also calculated by first-principle methods to discuss the effect of surface [16].

2. Dislocations Properties in Nanofilms

To facilitate the presentation we adopt the following conventions in all that follows (see Figure 1). In a Cartesian set of coordinates xyz , the xoz plane is the slip plane and y -axis is normal to the slip plane. The z -axis is the direction of the screw dislocation and the direction of the Burgers vector. In an isotropic crystal and elastic continuum theory, the screw dislocation in bulk material produces a stress field σ_{yz} along its Burgers vector [1]

$$\sigma_{yz} = \frac{\mu b}{2\pi} \frac{x}{x^2 + y^2}. \quad (1)$$

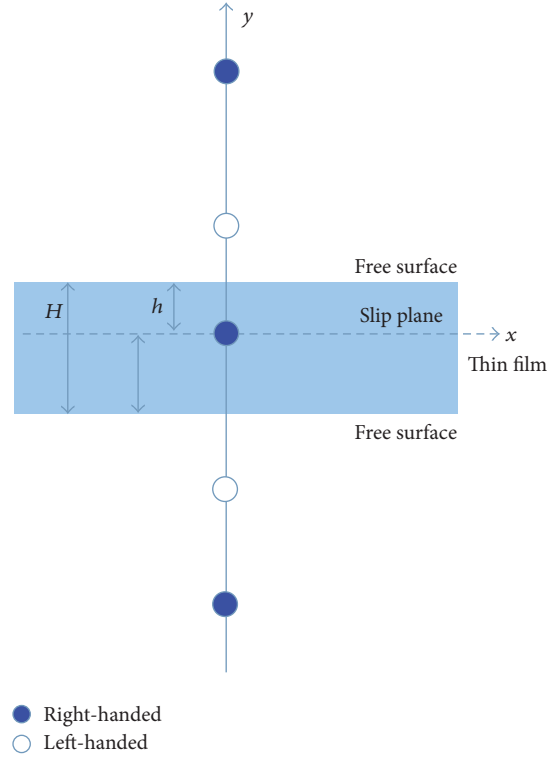


FIGURE 1: An array of imaginary dislocations of the original screw dislocation in the thin film. The slip plane of the original screw dislocation is parallel to the surfaces of the thin film and the effects of the surfaces can be described by the array imaginary dislocations. H is the thickness of nanofilms, and h | $(H - h)$ shows the position of slip plane.

μ is the shear modulus. In order to take into account the surface effect on the screw dislocation properties, a screw dislocation with thickness H at a distance h below the upper free surface is considered in a nanofilm (see Figure 1). In the typical way to count for the image effect, the two image screw dislocations with the opposite Burgers vector $b' = -b$ are distributed along a horizontal line at a distance h above the upper free surface and $(H - h)$ below the lower free surface. These two image dislocations superpose new stresses which are equal and opposite to the already existing stresses on the upper and lower surfaces, respectively. However, the above (below) image screw dislocation leaves a residual stress acting on the lower (upper) free surface, so that an additional image is required, which in turn requires another image and so on. The result is an infinite set of image screw dislocations. The stress field of original screw dislocation in thin film combined with the surface effect can be equally produced by this infinite set of screw dislocations. Then, the stress field on the $y = 0$ plane can be written as

$$\begin{aligned} \sigma_{yz} = & \frac{\mu b}{2\pi} \frac{1}{x} + \frac{\mu b'}{2\pi} \frac{x}{x^2 + (2h)^2} + \frac{\mu b'}{2\pi} \frac{x}{x^2 + (2H - 2h)^2} \\ & + \frac{\mu b}{2\pi} \frac{x}{x^2 + (2H)^2} + \frac{\mu b}{2\pi} \frac{x}{x^2 + (2H)^2} \\ & + \frac{\mu b'}{2\pi} \frac{x}{x^2 + (2h)^2} + \frac{\mu b'}{2\pi} \frac{x}{x^2 + (2H - 2h)^2} \end{aligned}$$

$$\begin{aligned} & + \frac{\mu b}{2\pi} \frac{x}{x^2 + (4H)^2} + \frac{\mu b}{2\pi} \frac{x}{x^2 + (4H)^2} \\ & + \frac{\mu b'}{2\pi} \frac{x}{x^2 + (4H + 2h)^2} + \frac{\mu b'}{2\pi} \frac{x}{x^2 + (6H - 2h)^2} \\ & + \dots \end{aligned} \quad (2)$$

It is helpful to rearrange the terms

$$\begin{aligned} \sigma_{yz} &= \frac{\mu b}{2\pi} \left[\sum_{n=-\infty}^{+\infty} \frac{x}{x^2 + (2nH)^2} - \sum_{n=-\infty}^{+\infty} \frac{x}{x^2 + (2nH + 2h)^2} \right] \end{aligned} \quad (3)$$

Using identities,

$$\begin{aligned} \sum_{n=-\infty}^{+\infty} \frac{1}{q^2 + n^2} &= \frac{\pi}{q} \coth \pi q, \\ \sum_{n=-\infty}^{+\infty} \frac{1}{q^2 + (n + p)^2} &= \frac{\pi}{q} \frac{\sinh 2\pi q}{\cosh 2\pi q - \cos 2\pi p}. \end{aligned} \quad (4)$$

One obtains

$$\begin{aligned} \sigma_{yz} &= \frac{\mu b}{4H} \left[\coth \frac{\pi x}{2H} - \frac{\sinh (\pi x/H)}{\cosh (\pi x/H) - \cos (2\pi h/H)} \right] \end{aligned} \quad (5)$$

In the above equation $b' = -b$ is used. It is interesting to find that $\sigma_{yz} = 0$ when $h = 0$. The first-term of (3) represents the shear stress on $y = 0$ plane of array right-handed screw dislocations siting $0, \pm 2H, \pm 4H, \dots$. The second-term of (3) represents the shear stress on $y = 0$ plane of an array left-handed screw dislocations siting $2h, 2H - 2h, 2H + 2h, \dots$. It is also

easy to verify that $\sigma_{yz} = 0$ on $y = h$ and $y = -(H - h)$ planes; that is to say the free surface boundary condition is satisfied.

Like in the P-N model, an infinitesimal distribution of Burgers vector is introduced $db = \rho(x)dx$ with $\rho(x) = du(x)/dx$ [14, 15]. The governing equation for the screw dislocation in thin film can be obtained by

$$\frac{\mu}{4H} \int_{-\infty}^{+\infty} \left[\coth \frac{\pi(x-x')}{2H} - \frac{\sinh(\pi(x-x')/H)}{\cosh(\pi(x-x')/H) - \cos(2\pi h/H)} \right] \frac{du(x')}{dx'} dx' = f(u). \quad (6)$$

The restoring force $f(u)$ can be obtained from the gradient of the generalized stacking fault (GSF) energy γ_u , which can be obtained from the first-principle calculation [16]. The USF energy, the maximum of the GSF energy, is the key role to control the properties of dislocation, such as the dislocation mobility and nucleation [17]. Therefore, the form of sinusoidal restoring force used here can be given as follows:

$$\gamma(u) = \frac{\gamma_{us}}{2} \left(1 - \cos \frac{2\pi u}{b} \right) \quad (7)$$

with γ_{us} being the USF energy. Then, we have the restoring force

$$f(u) = \frac{\partial \gamma(u)}{\partial u} = \frac{\pi \gamma_{us}}{b} \sin \frac{2\pi u}{b}. \quad (8)$$

There is a little difference comparing with the original sinusoidal restoring force $(\mu b/2\pi d) \sin(2\pi u/b)$ used in the original P-N model. The maximum restoring force $\mu b/2\pi d$ is substituted by $\pi \gamma_{us}/b$ for actual materials.

Dislocation equations can be deduced from (6) in two limitations: (i) dislocation in semi-infinite material with seldom surface ($H \rightarrow \infty$), (ii) dislocation in bulk material without surface ($H \rightarrow \infty$ and $h \rightarrow \infty$), and (iii) dislocation in the middle of the nanofilms ($h = H/2$).

(i) When $H \rightarrow \infty$, the first-term of (6) becomes the usual P-N integral for an isolated screw dislocation, and the second-term of (6) becomes the integral for imaginary screw dislocation at a distance h below the free surface. Hence, the dislocation equation can easily yield

$$\frac{\mu}{2\pi} \int_{-\infty}^{+\infty} \left[\frac{1}{x-x'} - \frac{x-x'}{(x-x')^2 + (2h)^2} \right] \frac{du(x')}{dx'} dx' = f(u). \quad (9)$$

This equation is the same as previous dislocation equation obtained by Cheng et al. for semi-infinite material with seldom free surface [10].

(ii) When $H \rightarrow \infty$ and $h \rightarrow \infty$, one obtains the classical P-N dislocation equation in bulk

$$\frac{\mu}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x-x'} \frac{du(x')}{dx'} dx' = f(u). \quad (10)$$

(iii) When $H = 2h$, we can get dislocation equation in the middle of the nanofilms

$$\frac{\mu}{2H} \int_{-\infty}^{+\infty} \frac{1}{\sinh(\pi(x-x')/H)} \frac{du(x')}{dx'} dx' = f(u). \quad (11)$$

In this letter, for the dislocation equation (6) the dislocation solution can be written as

$$u(x) = \frac{b}{\pi} \arctan \left[\frac{H}{\pi \zeta} \sinh \left(\frac{\pi x}{H} \right) \right] + \frac{b}{2} \quad (12)$$

with $\zeta = \eta \zeta_0$ and $\zeta_0 = d/2$. η is the core width parameter of screw dislocation in thin film. Equation (12) tends to the original Peierls solution $u(x) = (b/\pi) \arctan(x/\zeta_0) + b/2$, when $H \rightarrow \infty$ [14]. It is interesting to find that (12) is the suitable approximation solution of these equations with $\eta \approx 1$ for original sinusoidal force law $(\mu b/2\pi d) \sin(2\pi u/b)$ in simple cubic lattice. In this letter, the suitable approximation can be interpreted as the relative error from the sinusoidal law of force, and the relative error in the core region decreases with thickness of nanofilm. This also means that the core width of screw dislocation is nearly independent on the thickness of nanofilm. The classic Peierls solution is also used to solve these equations, but asymptotic behavior of the stress and restoring force is not consistent far from dislocation.

Generally, a narrow dislocation core implies a relatively high Peierls stress. In this letter, the Peierls stresses are evaluated through the calculation of the misfit energy E taken as the sum of the local misfit energies between pairs of atomic planes [14]

$$E(x_0) = \sum_{n=-\infty}^{+\infty} \gamma[u(nb - x_0)]. \quad (13)$$

The minimum stress required to overcome the energy barrier $E(x_0)$ is then defined as the Peierls stress σ_p

$$\sigma_p = \max \left\{ \frac{dE(x_0)}{dx_0} \right\}. \quad (14)$$

Surface effect contains two parts: one introduces the stress field of image dislocation that changes the form of dislocation equation and the other results in the changing of GSF energy. Thus, it means that the primary role to dislocation properties

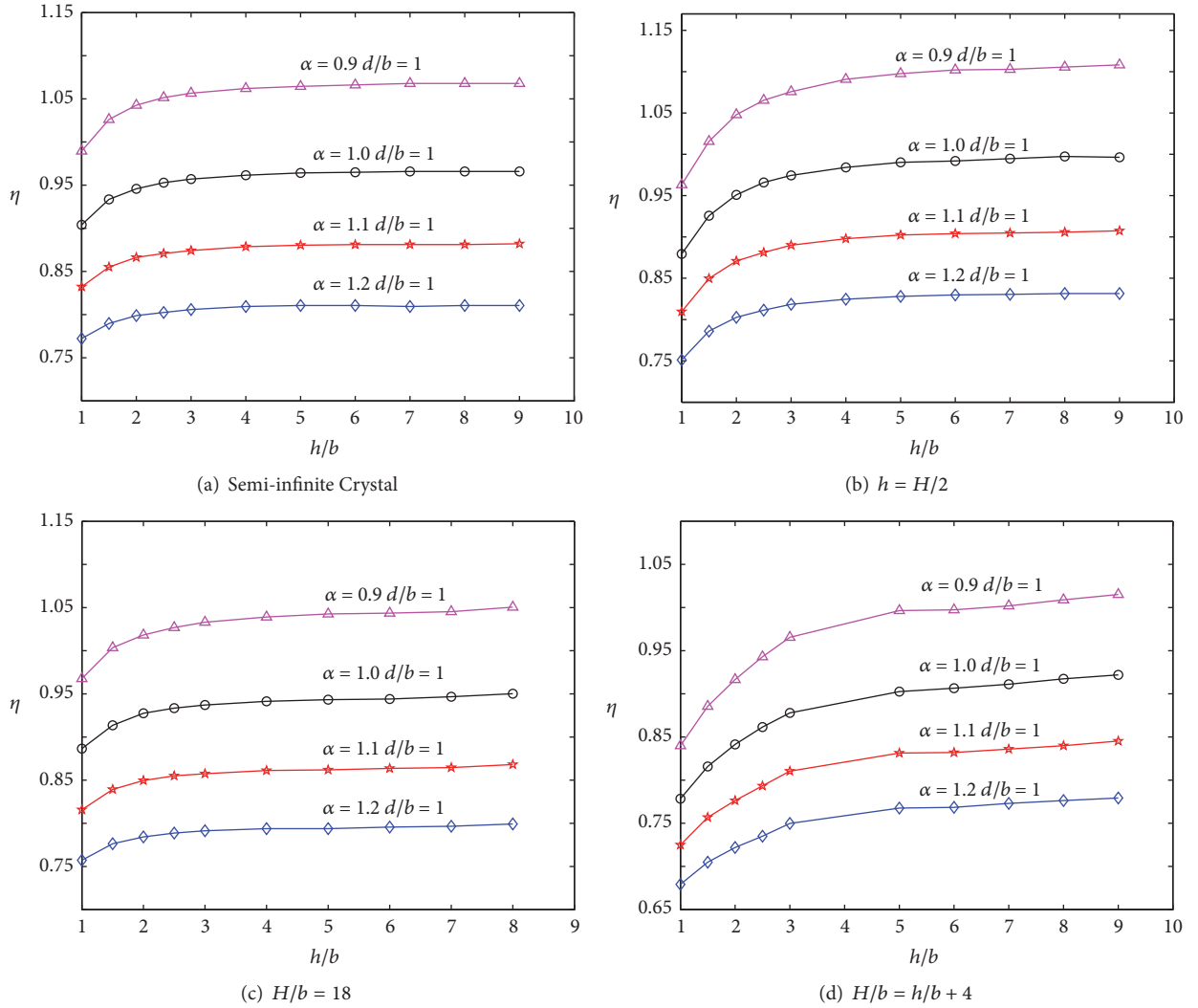


FIGURE 2: Variation of core structure parameter η with respect to the dislocation's distance to the surface for various normalized unstable stacking fault energy for screw dislocations.

is originated from the GSF energy and the effect of stress field of image dislocations is small.

To research how the core width (ξ) of screw dislocation changes with the interplanar atomistic spacing (d/b), the core structure parameters (η) are plotted with respect to its distances to the free surface (h/b) for different α and d/b in Figures 2 and 3, respectively. In our study, $\gamma_{us} = \alpha \cdot \mu b^2 / 2\pi^2 d$ instead of $\gamma_{us} = \mu b^2 / 2\pi^2 d$, with α in the range of 0.8~1.2. The range of d/b studied is 0.7~1.4 in real crystals, and the range for h/b studied is 1~9, because the surface effect becomes less significant only when the dislocation is more than 9 layers of atoms away from the free surface. This result is consistent with Cheng et al. [10] in semi-infinite crystal (see Figure 2(a)). Unlike Cheng et al. [10], we are more concerned with surface effects on the properties of screw dislocation in nanofilms. The core structure parameter (η) in nanofilms is influenced by h as well as the nanofilms thickness (H). Therefore, three kinds of models are constructed in order to investigate the

interaction between the dislocation and double free surfaces: (1) screw dislocation in the middle ($h = H/2$) of the nanofilms; (2) nanofilms thickness $H/b = 18$; (3) the height of the distance below the surface $(H-h)/b = 4$. It is found that, similar to the results for the semi-infinite crystal, the core structure parameter (η) decreases when the screw dislocation in nanofilms gets closer to the surface with the same α and d/b ; it means that screw dislocation near the surface causes a narrower dislocation core (Figures 2(b)–2(d)). The increase of α will also lead to the reduction of the core structure parameter (η) with the same h/b and d/b , but the core structure parameter (η) increases with increasing d/b with the same h/b and α (see Figure 3).

In order to investigate the effect of free surface on the Peierls stress, the variation of σ_p/σ_p^0 of a screw dislocation with respect to its distance (h) to the free surface for different α and d/b is shown in Figures 4 and 5, respectively, where σ_p/σ_p^0 is the amplification factor for the Peierls stress. As

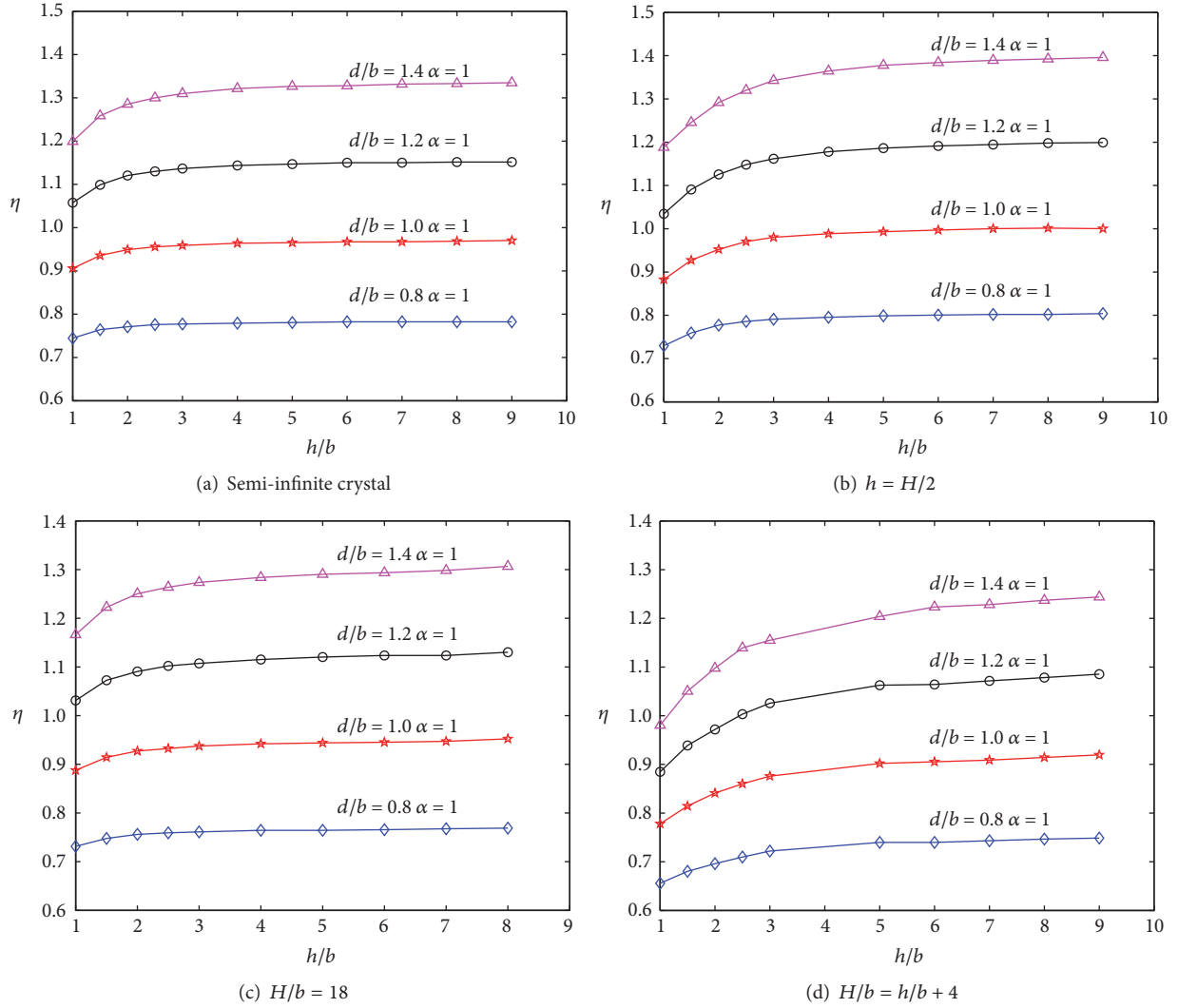


FIGURE 3: Variation of core structure parameter η with respect to the dislocation's distance to the surface for various interplanar atomistic spacing (d/b) for screw dislocations.

shown in these figures, we can find that the amplification factor (σ_p/σ_p^0) of screw dislocation decreases with respect to h with the same d/b and α ; it is shown that our results agree well with conclusion of Cheng et al. [10]. When we increase the interplanar atomistic spacing (d/b), surprisingly contrary to what Cheng et al. concluded, it is found that σ_p/σ_p^0 increases, rather than decreasing with the same h and α (see Figure 5). We believe that interplanar atomistic spacing (d/b) has a better influence on Peierls stress than surface effect.

In this letter, we focus on the dislocation core structure and Peierls stresses of $(1/2)\langle 110 \rangle\{111\}$ screw dislocations in Al and Cu nanofilms. The lattice constants and elastic constants are shown in Table 1. The shear moduli μ of Al and Cu nanofilms can be determined from their elastic constants C_{11} , C_{12} , and C_{44} via the equation $\mu = 3C_{44}(C_{11} - C_{12})/(4C_{44} + C_{11} + C_{12})$ [18]. The USF energies of Al and Cu nanofilms for different thickness are listed in Table 2. The USF energy

TABLE 1: The lattice constants a , Burgers vector b and distance between slip planes d (in units of Å), elastic constants C_{11} , C_{12} , and C_{44} (in units of GPa), and shear modulus μ of Al and Cu.

Materials	a	b	d	C_{11}	C_{12}	C_{44}	μ
Al	4.039	2.856	2.332	112.5	60.9	39.6	18.5
Cu	3.637	2.572	2.100	164.7	126.6	72.2	14.2

decreases with the thickness of nanofilms, and the USF energies are the smallest for bulk Al and Cu. This trend is in accordance with the results obtained by Datta et al. [19].

The core structure parameter is determined by substituting the dislocation solution equation (12) into the dislocation equation via comparing the maximum restoring force (see Figure 6). The dislocation densities are shown in Figure 7, and the core width of dislocations in nanofilms becomes

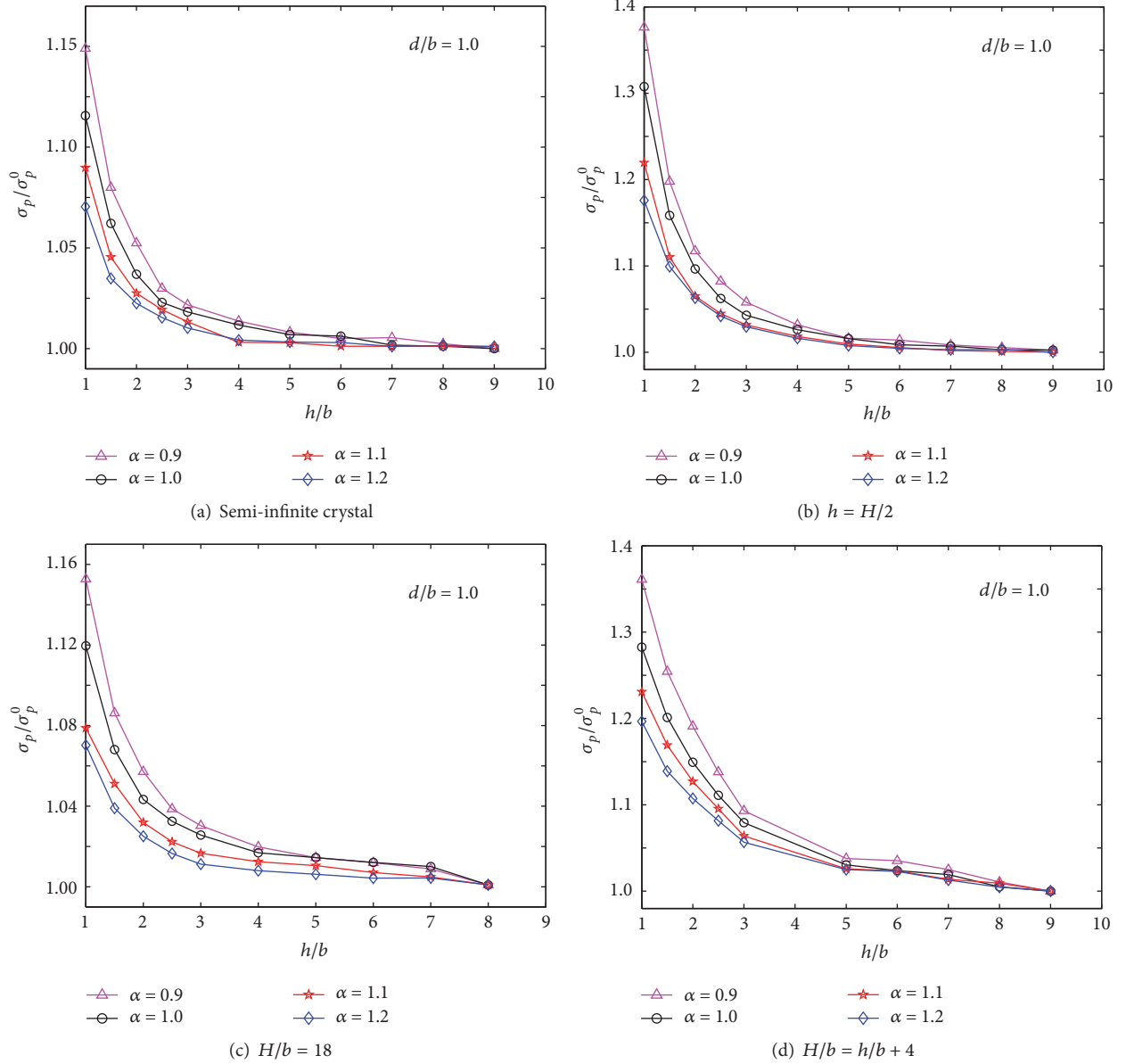


FIGURE 4: Variation of the amplification factors of Peierls stress for a screw dislocation with respect to its distance to the surface for various normalized unstable stacking fault energy.

TABLE 2: The unstable stacking fault energy γ_{us} (in units of mJ/m^2), core structure parameter η , core width ξ (in units of b), and Peierls stress σ_p (in units of μ) of the $(1/2)\langle 110 \rangle\{111\}$ screw dislocations in Al and Cu nanofilms.

Nanofilms	Al				Cu			
	γ_{us}	η	ξ	σ_p	γ_{us}	η	ξ	σ_p
3 6	379.8	0.64	0.644	0.172	503.7	0.350	0.351	6.295
3 9	356.2	0.69	0.693	0.147	498.4	0.357	0.357	6.109
6 9	343.7	0.73	0.721	0.131	498.1	0.361	0.361	6.033
Bulk	339.4	0.79	0.792	0.118	495.7	0.371	0.391	5.850

narrower than that in bulk (see Table 2 and Figure 7). Peierls stress decreases with the thickness of nanofilms.

Weinberger simulated the Peierls stress of an edge dislocation in molybdenum with modified Finnis-Sinclair potential to check the thickness dependence of the Peierls stress [11]. It is found that Peierls stress rises with decreasing thickness when thickness is below 8 nm, and Peierls stress for large thicknesses converges to around 20 MPa (Peierls stress of dislocations in bulk Mo). Our results are in agreement with the conclusions of Weinberger [11]. However, Lee and Li show that Peierls stress of a surface screw dislocation may be about 5–15% less than that in bulk materials based on a half-space P-N model [8]. Gars and Markenscoff accounted the effect of free surface on the Peierls stress by using the variable-core dislocation model [6]. The trend is the same as obtained by Lee and Li, but the order of magnitude is different, due to the surface effects on the variable width. The opposite results

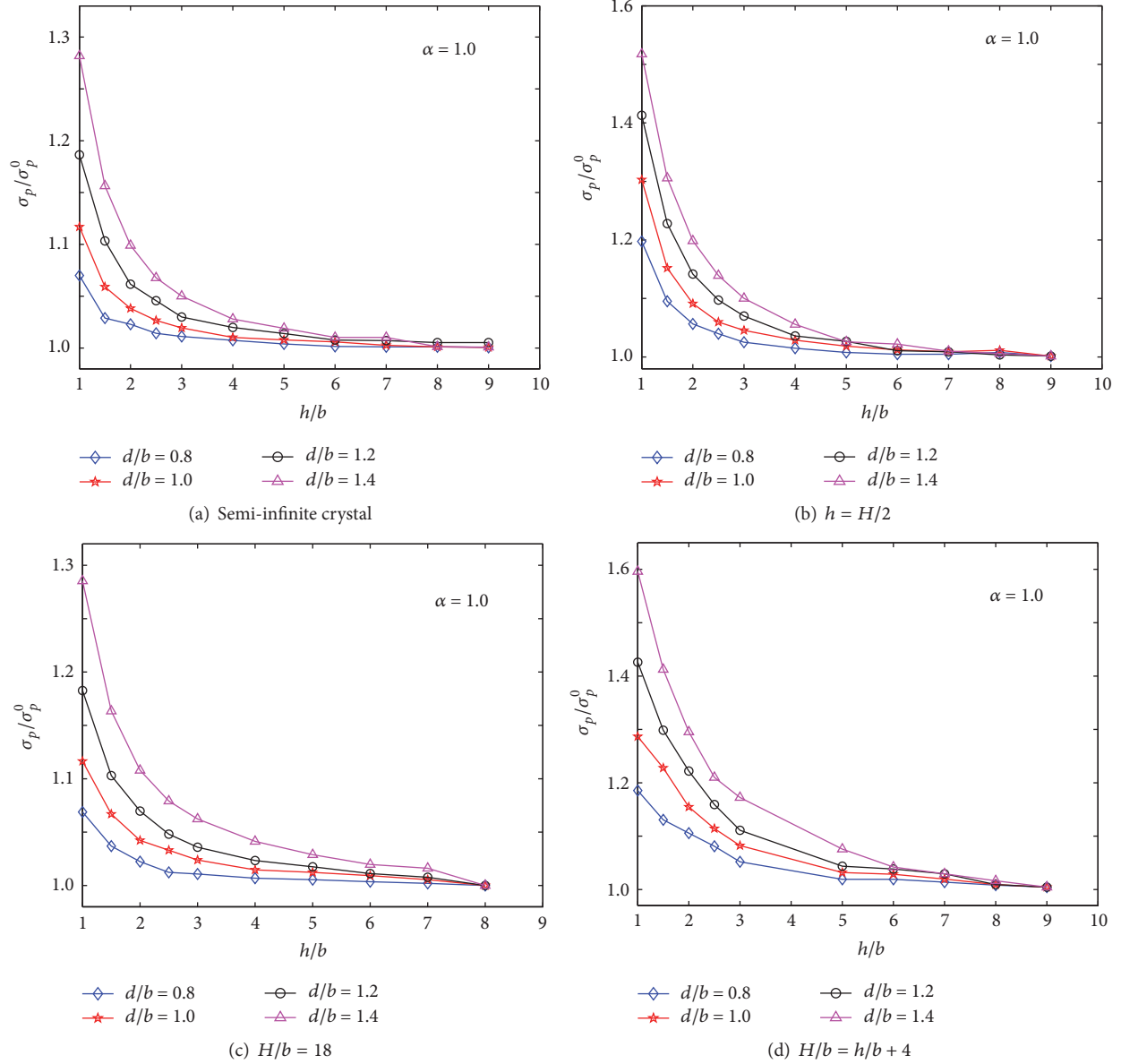


FIGURE 5: Variation of the amplification factors of Peierls stress for a screw dislocation with respect to its distance to the surface for various interplanar atomistic spacing (d/b).

originated from the missing change of dislocation profile under the free surface, as pointed out by Cheng et al. [10]. This shortage can be covered by the new dislocation solution presented here for dislocations in nanofilms.

3. Conclusions

In summary, we have constructed the governing equation of screw dislocations in nanofilms using the image dislocation method. The classical Peierls-Nabarro equation can be recovered when the thickness of nanofilm is taken to be infinite. We have studied the effects of USF energies, the spacing between the dislocation and the surface (h), and the interplanar atomic spacing (d/b) on both Peierls stress

and core structure parameter, respectively. The core structure and Peierls stress of dislocations in Al and Cu nanofilms are determined by the governing equation combined with the USF energies obtained by the first-principle methods. It is found that surface effect can increase the Peierls stresses of screw dislocations in Al and Cu nanofilms.

Competing Interests

The authors declare that they have no competing interests.

Acknowledgments

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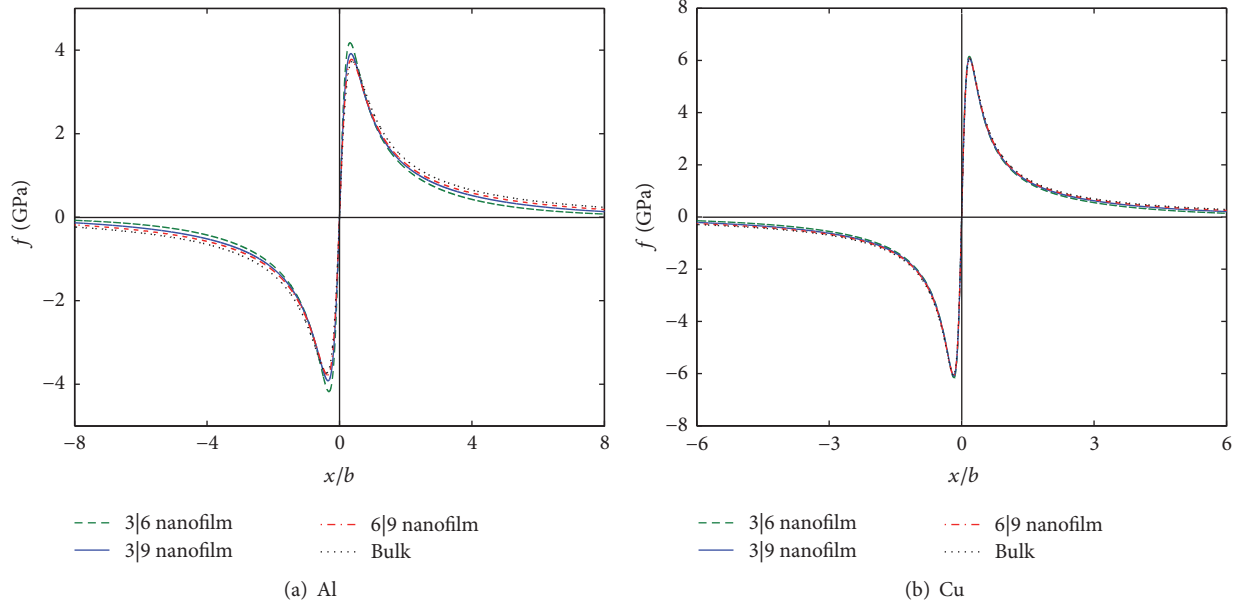


FIGURE 6: Stress fields of the $(1/2)\langle 110 \rangle \{111\}$ screw dislocations in Al and Cu nanofilms for different $h \mid (H - h)$.

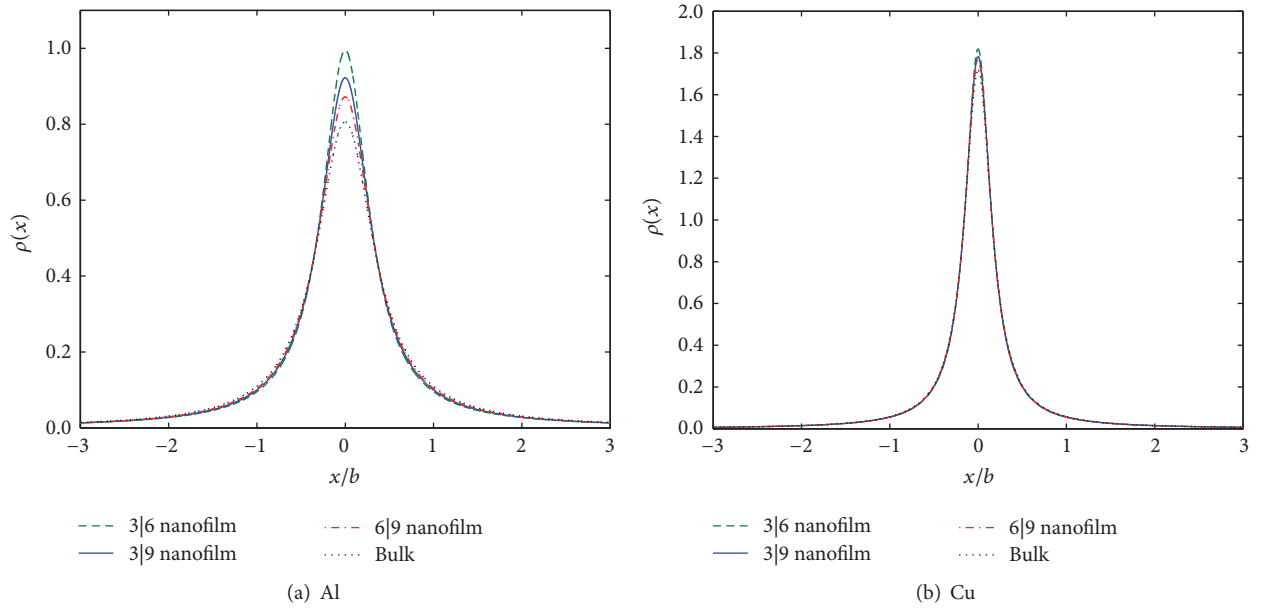


FIGURE 7: Dislocation densities of the $(1/2)\langle 110 \rangle \{111\}$ screw dislocations in Al and Cu nanofilms for different $h \mid (H - h)$.

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