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A half-space Peierls–Nabarro model and the mobility of screw dislocations in a thin film

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Abstract

In this paper, a half-space Peierls–Nabarro (HSPN) model is proposed to re-examine the mobility of a screw dislocation along a thin film/substrate (half-space) interface. In this configuration, the screw dislocation is subjected to an image force due to the free surface, and we are concerned with the interaction between the dislocation and the free surface. Unlike the original Peierls–Nabarro (P–N) model, the HSPN model takes into account the effect of the image force, which leads to modifications on analytical expression of the Peierls barrier stress. The modified Peierls stress is a function of the thin film thickness, which allows us to accurately predict the mobility of a dislocation in the interface between the thin film and the substrate. Based on the proposed HSPN model, we have found that the Peierls stress of a surface screw dislocation may be about 5–15% less than that in bulk materials.
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Keywords: Dislocation; Image force; Peierls stress; Misfit energy; Thin films

1. Introduction

The thin film is one of the most important nanoscale structures in modern technology. It is the primary configuration for integrated circuits, computer memories, microelectrical mechanical sensors and other nanoscale devices.

Most commercialized thin film devices are made of epitaxial thin films, where lattice misfit between the substrate and the thin film is common. The main stress relaxation mechanism for such a misfit is provided by the presence of dislocations either inside the thin film or in the interface [1,2], even though the mismatch strain may not be relieved. In other words, it is thermodynamically favorable for the presence of dislocations inside the thin film, which in turn affects the quality as well as functionality of thin film devices. There have been intensive researches and studies conducted on dislocation mechanics in thin films in the past few decades, e.g. Refs. [3–10] among many others. For comprehensive information, readers are referred to an excellent monograph by Freund and Suresh [11].

One of the milestones of thin film mechanics is Matthews and Blakeslee's seminal work, in which the authors [1,2,12,13] used the energy argument to successfully predict the critical thickness of the thin film that is dislocation-free. When finding the critical thickness, the expression of dislocation energy is needed to be included in the total energy of the system. Rigorously speaking, this energy ought to include both self energy as well as the core energy, but the core energy is often either neglected or roughly estimated [4,14]. Since the core energy can be as high as 20% of the total dislocation energy, today most refined thin film dislocation models include dislocation core energy in the calculation of critical thickness, e.g. a threading dislocation model developed by Freund [5]. In some thin film models, even though the domain of the thin film/substrate system is bounded, the core energy is often estimated by using the stress field of bulk materials as an approximation. This may affect the accuracy in the prediction of the critical thickness.

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To have a more realistic estimate on the core energy and its effect on the critical thickness, the core energy in the thin film was re-examined by Beltz and Freund [15], in which the Peierls–Nabarro (P–N) model was used to calculate the misfit energy, and hence the critical thickness of the thin film. Similar approaches, which use the P–N model to calculate the core energy, have been adopted by others as well, e.g. Wang et al. [16] in the case of piezoelectric thin films.

In the P–N model, the mobility of a dislocation is measured by the Peierls–Nabarro barrier stress [17,18], or the Peierls stress in short,

$$\sigma_{\mathrm{p}} = \frac{2\mu}{1-v}\exp\left(-\frac{4\pi d}{2(1-v)b}\right) \tag{1}$$

where μ is the shear modulus and v is the Poisson's ratio. This expression is obtained by summing the misfit atomic energy stored inside a glide plane [19]. A more realistic measure of the dislocation core energy and hence the Peierls stress of the dislocation can be provided by atomistic simulations [20,21]. However, as numerical experiments, atomistic simulations provide no analytical solution, and their results depend on the choice of the atomistic potentials that describe the atomic and ionic interaction [19]. Even though the P–N model has limitations, e.g. an unrealistic sinusoidal traction–displacement relation and the absence of thermal effect [22,23], it nevertheless provides unique analytical expressions for both core energy and Peierls stress, and thus provides the benchmark solution for the dislocation mobility.

Since the P–N model is formulated for an interface between two half-spaces, it is only applicable for dislocation motions in bulk materials. The interaction between a free surface and a dislocation, which is important for the thin film configuration, is, however, incompatible with the original P–N model. It is believed that the image force due to the free surface will interact with the dislocation in a thin film, which in turn alters the misfit energy landscape, and cause variance in core energy built-up. This important effect, to the best of the authors' knowledge, has not been adequately taken into account in most dislocation mobility estimates in thin films, and most of the dislocation mobility estimates in thin films are still based on the original P–N model.

Recent atomistic simulations [24,25] have revealed that the image force indeed affects significantly the magnitude of the core energy, especially for dislocations near the free surface of a thin film. In particular, this has an important effect on the mobility of surface dislocations. The objective of this work is to re-examine the mobility of a dislocation in a thin film by using a half-space P–N model (HSPN) that takes into account the image force effect, in the hope of providing theoretical guidance on the mobility of surface or near-surface dislocations.

The attempt to include an interface effect into the P–N model is not new. A similar dislocation/free-surface interaction model was proposed before by Pacheco and Mura [26] (denoted as "PM model" in this paper). The present model, however, is different from the PM model in that the latter is for a screw dislocation in a two-phase material rather than in a half-space. A comparison between these two models will be discussed later in the paper.

The proposed HSPN model adopts most assumptions and approximations used in the standard P–N model described by Hirth and Lothe [19] and Joos and Duesbury [27]. Moreover, it further assumes that a single image dislocation can be spread out and can be represented by an image dislocation distribution, located above the original dislocation with a distance of twice the thin film thickness and having a Burgers vector opposite to the original dislocation. By doing so, the zero traction boundary condition on the free surface is then satisfied for the HSPN model.

The main scope of this work is to develop an HSPN model, which could become useful for analysis of dislocation motions in thin films. We first describe the HSPN model in Section 2 and then calculate both the misfit energy and the Peierls stress in the interface between the thin film and the substrate in Section 3. Finally in Section 4, we compare the differences between the HSPN model with the original P–N model. The main emphasis will be on the amplification factors that depend on the thickness of the thin film.

2. The half-space Peierls–Nabarro (HSPN) model

2.1. The HSPN model

We consider a screw dislocation with a Burgers vector, $\mathbf{b} = b\mathbf{e}_z$, in the direction [0 0 1] of a crystal, which is embedded in the interface between a layer of thin film and a substrate (see Fig. 1) with the same elastic shear modulus μ. It is well known that the stress of a single dislocation will cause stress singularity at the origin of the dislocation. To remove this stress singularity, we distribute the dislocation along the x-axis with the Burgers vector density [17,18]

$$b'(x) = \frac{\mathrm{d}\Delta u_z}{\mathrm{d}x} \tag{2}$$

where $\Delta u_z = u_z^- - u_z^+$ is the relative displacement between the thin film u_z^+ ($\forall y > 0$) and the substrate u_z^- ($\forall y < 0$).

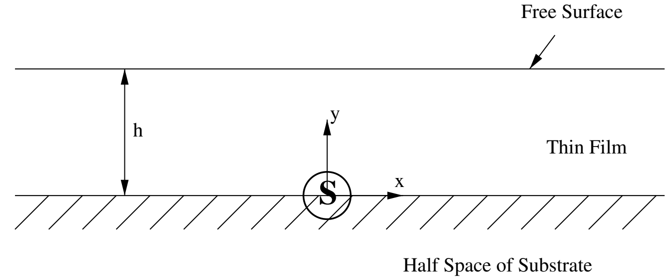

Fig. 1. A screw dislocation at the interface between a substrate and a thin film.

In the proposed HSPN model, we assume that the following assumptions of the original P–N model in an unbounded domain still hold:

- the traction–displacement relation obeys the sinusoidal force law inside the glide plane;
- the material remains elastic outside this glide plane;
- the temperature effect is neglected; and
- the translation of the dislocation is rigid so that there is no change of the geometric core structure in the process.

However, because of the free surface at $y = h$, the dislocation-induced displacement field is different from that of an unbounded domain, such that the antisymmetric property of u_z $(u_z^+ = -u_z^-)$, which is usually assumed for the case of the unbounded domain, no longer holds. To isolate the effect of the free surface, we split the displacements u_z into two parts, u_z^∞ and u_z^b. The former denotes the displacements caused by the distributed screw dislocations in the unbounded domain and the latter denotes the elastic displacements caused by the free surface at the boundary $y = h$. We assume that the free surface can only cause a continuous displacement field across the interface at $y = 0$, and hence there is no discontinuity in $u_z^b(x)$, i.e. $\Delta u_z^b = 0$. The Burgers vector density can then be expressed as

$$b'(x) = \frac{\mathrm{d}\Delta u_z^\infty}{\mathrm{d}x} \tag{3}$$

The above argument is based on the hypothesis that the Burgers vector distribution, or the dislocation core structure, is not affected by the boundary, or independent from material configurations. We can view the Burgers vector distribution as an imposed eigen-strain, which remains self-contained, or autonomous, regardless of the existence of the free surface. In other words, we assume that the geometric core structure of a screw dislocation is unchanged, independent from the free surface [11]. With this assumption, the HSPN model is essentially a P–N model incorporated with the free-surface effect.

By applying the sinusoidal law [17], the restoring force due to the displacement of a screw dislocation at the glide plane is

$$\sigma_{yz}^\infty(x,0) = \tau_{\max}\sin\frac{2\pi\Delta u_z^\infty}{b} \tag{4}$$

where

$$\tau_{\max} = \frac{\mu b}{2\pi d} = \frac{Db}{2w_\mathrm{h}} \tag{5}$$

is chosen for the elastic limit to apply in small deformation theory. The symbol $D = \mu/2\pi$ is the normalized shear modulus with respect to 2π, $w_\mathrm{h} = d/2$ is the half-width of the dislocation and d is the thickness of the non-Hookean slab joining the thin film and the substrate. The superscript ∞ indicates that the stress does not include the stress due to the free surface. Since the core structure of the dislocation is assumed unchanged with the existence of the free surface, the thickness d, so is the half-width of the dislocation, is independent of the film thickness h.

With the above assumptions, we can then utilize the original P–N solution

$$\sigma_{yz}^\infty(x,0) = \frac{Dbx}{x^2 + w_\mathrm{h}^2}, \quad \Delta u_z^\infty(x,0) = \frac{b}{\pi}\tan^{-1}\left(\frac{x}{w_\mathrm{h}}\right)$$
$$b'(x) = \frac{b}{\pi}\frac{w_\mathrm{h}}{x^2 + w_\mathrm{h}^2} \tag{6}$$

by enforcing $\Delta u_z^\infty(\pm\infty) = \pm b/2$ [19]. To find the shear stress corresponding to the misfit in the unbounded domain, we sum the contribution of the distributed dislocation along the glide plane,

$$\sigma_{yz}^\infty(x,y) = D\int_{-\infty}^{\infty} b'(x')\frac{(x-x')\mathrm{d}x'}{(x-x')^2 + y^2} = \frac{Dbx}{x^2 + (|y| + w_\mathrm{h})^2} \tag{7}$$

To take into account the effect of the free surface, we generalize the concept of the image stress due to a single discrete dislocation to that of a distributed image dislocation layer due to a distributed dislocation layer (see Fig. 2). We assume that the image screw dislocation with the opposite Burgers vector ($-\mathbf{b}$) is distributed along a horizontal line above the thin film at the height $y = 2h$ according to the standard P–N procedure. This image screw dislocation distribution causes an image stress in the lower half-space ($y \leqslant h$),

$$\sigma_{yz}^\mathrm{I}(x,y) = \frac{-Dbx}{x^2 + (|y - 2h| + w_\mathrm{h})^2} \tag{8}$$

If we sum the shear stress due to these two screw dislocation distributions, we can obtain the total shear stress:

$$\sigma_{yz}(x,y) = \sigma_{yz}^\infty(x,y) + \sigma_{yz}^\mathrm{I}(x,y) = Dbx\left(\frac{1}{x^2 + (|y| + w_\mathrm{h})^2} - \frac{1}{x^2 + (|y - 2h| + w_\mathrm{h})^2}\right) \tag{9}$$

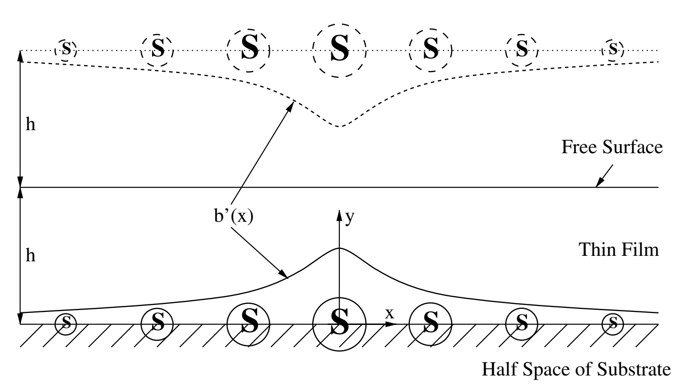

Fig. 2. A distributed screw image dislocations at $y = 2h$ (outside the physical domain).

One can verify that the total shear stress vanishes at $y = h$, i.e. the zero traction at the free surface is indeed satisfied.

We note in passing that since the HSPN model requires a non-vanishing non-Hookean slab joining the thin film and the substrate, the thickness of the thin film for the HSPN model cannot vanish. The minimum thickness for the model to be valid should be $d/2$, i.e. $h_{\min} = d/2$. The dislocation that corresponds to the minimum thickness $h_{\min}$ is understood as a surface dislocation.

2.2. Comparison between HSPN model and PM model

To find the external stress that holds a screw dislocation in equilibrium in a two-phase material formed by joining two dissimilar elastic half-spaces, Pacheco and Mura [26] constructed a Peierls–Nabarro model in which they spread two (real and image) screw dislocations along a plane that is perpendicular to the interface between the thin film and the substrate, based on a similar procedure employed in the P–N model. In the PM model, instead of using two horizontally parallel dislocation distributions (HSPN model), two vertically overlapped dislocation distributions are used to spread the two dislocations (see Fig. 3). Therefore, the PM model is fundamentally different from the HSPN model. In fact, the PM model is pertinent to the dislocation mobility perpendicular to the interface, whereas the HSPN model is concerned with the dislocation mobility along the interface.

Since the thin film/substrate system is anisotropic, the dislocation mobility along the interface is expected to be different from that perpendicular to the interface. Thus, the Peierls stress obtained from the HSPN model will then be different from that obtained from the PM model.

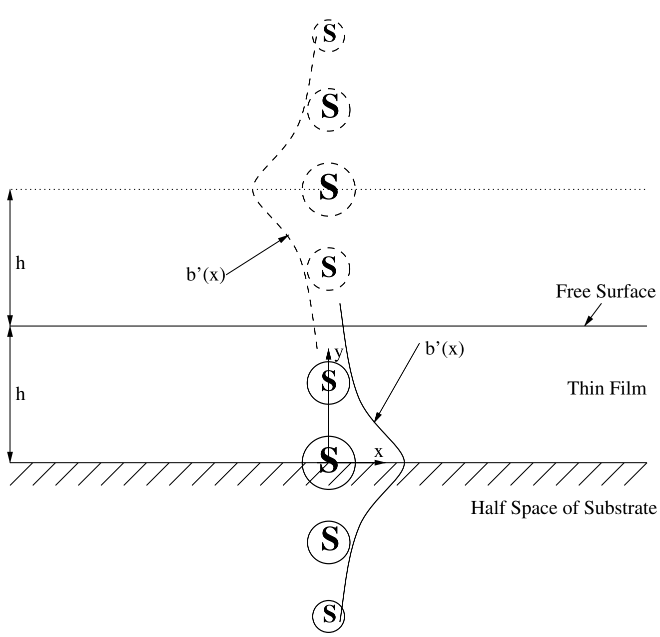

Fig. 3. Schematic diagram of the PM model.

In the PM model, an additional external stress is, however, required to hold the screw dislocation in equilibrium [26]. It may be technically challenging for the summation of the misfit energy density along the plane of dislocation distribution, because the dislocation distribution is asymmetric and there is an interaction between the real dislocation distribution and the image dislocation distribution. We believe that these may render the calculation of the Peierls stress problematical, and hence the mobility of a screw dislocation based on the PM model has not been obtained yet.

On the contrary, the HSPN model does not require any external stress to hold the screw dislocation in equilibrium. It is also relatively tractable for the summation of the misfit energy density along the plane of distribution, which maintains symmetry and involves only the real misfit strains.

3. Misfit energy and Peierls stress

To calculate the misfit energy, we adopt the discrete summation procedure proposed by Joos and Duesbery [27], which has become the standard procedure in calculating the misfit energy. This approach is more physically realistic, because the resulting misfit energy has the correct period, which is especially important for very narrow dislocations, ($d \ll s$) where d is the width of the dislocation and s is the lattice spacing, and the resulting Peierls stress also fits better to the atomistic theory. Note that the Peierls stress for the dislocation in the unbounded domain differs from the expression in Eq. (1) by a factor of 2 in both the exponential and the coefficient, as shown below for an edge dislocation,

$$\sigma_{\mathrm{p}} = \frac{\mu}{1-\nu} \exp\left(-\frac{2\pi d}{2(1-\nu)b}\right) \tag{10}$$

3.1. Misfit energy density in glide plane

The misfit energy can be obtained by summing the misfit energy density over the glide plane. The misfit energy density is calculated by following the standard procedure as well [19], except that the factor of 1/2 is dropped because both the top and bottom crystals of the slip plane are considered [27]. The local misfit shear strain at the glide plane of the screw dislocation is

$$\gamma_{yz}(x,0) = \frac{\phi_z}{d} = \pm\frac{b}{2d} - \frac{\Delta u_z^{\infty}}{d} \tag{11}$$

where ϕ_z is the disregistry that records the lattice misfit between the thin film and the substrate.

The key difference between the HSPN model and the original P–N model is that in the HSPN model the image stress due to the free surface interacts with the dislocation in the thin film. Thus, the misfit energy in the thin film/substrate system has two sources: (1) the contribution due to the misfit stress in the unbounded domain, and (2) the contribution due to the image stress. The misfit energy density, which is the unit misfit energy stored in a volume element of height d, lattice spacing s and unit depth in the z-direction, at the glide plane ($y = 0$) can then be written as

$$\begin{aligned}\Delta W(x) &= sd\int_0^{\gamma_{yz}} \sigma_{yz}(x,0)\,\mathrm{d}\gamma_{yz}\\ &= -s\int_{b/2}^{\Delta u_z^\infty} \sigma_{yz}^\infty(x,0)\,\mathrm{d}\Delta u_z^\infty - s\int_{b/2}^{\Delta u_z^\infty} \sigma_{yz}^{\mathrm{I}}(x,0)\,\mathrm{d}\Delta u_z^\infty\\ &= \Delta W^\infty(x) + \Delta W^{\mathrm{I}}(x) \qquad (12)\end{aligned}$$

This misfit energy density is stored between a pair of atomic planes separated by a distance s. For the sake of comparison, we split the misfit energy density into two parts: $\Delta W^\infty(x)$ and $\Delta W^{\mathrm{I}}(x)$. The former is the conventional misfit energy density, which can be calculated by a standard procedure, i.e.

$$\begin{aligned}\Delta W^\infty(x) &= -s\int_{b/2}^{\Delta u_z^\infty} \sigma_{yz}^\infty(x,0)\,\mathrm{d}\Delta u_z^\infty\\ &= \frac{sDb^2}{4\pi w_{\mathrm{h}}}\left(\cos\frac{2\pi\Delta u_z^\infty}{b} + 1\right) \qquad (13)\end{aligned}$$

The latter is the misfit energy contribution due to the image stress $\sigma_{yz}^{\mathrm{I}}(x,0)$. It is written as

$$\begin{aligned}\Delta W^{\mathrm{I}}(x) &= -s\int_{b/2}^{\Delta u_z^\infty} \sigma_{yz}^{\mathrm{I}}(x,0)\,\mathrm{d}\Delta u_z^\infty\\ &= -\frac{sDb^2 w_{\mathrm{h}}}{8\pi h(h+w_{\mathrm{h}})}\ln\frac{x^2+(2h+w_{\mathrm{h}})^2}{x^2+w_{\mathrm{h}}^2} \qquad (14)\end{aligned}$$

Define two dimensionless parameters that depend on the film thickness h,

$$\rho(h) = \frac{4\pi h}{s}, \quad \kappa(h) = \frac{w_{\mathrm{h}}}{h+w_{\mathrm{h}}} \qquad (15)$$

We can then express the second misfit energy density as

$$\Delta W^{\mathrm{I}}(x) = -\frac{Db^2\kappa(h)}{2\rho(h)}\ln\frac{x^2+(2h+w_{\mathrm{h}})^2}{x^2+w_{\mathrm{h}}^2} \qquad (16)$$

The significance of the parameters ρ and κ will be discussed in a later section.

3.2. Total misfit energy in lattice

Following Nabarro [18], the origin of the dislocation is introduced at the position $x = a$, $0 < a < s$ and the atomic planes at ns, where $n = 0, \pm1, \pm2, \ldots$ will experience a relative displacement $\Delta u_z^\infty(ns - a)$. As usually adopted in the P–N model, in this study we also assume that the core structure of the dislocation remains the same during the translation. Therefore, to calculate the total misfit energy in the lattice, we replace the argument x of the unit misfit energy in Eq. (12) by $ns - a$ and sum the unit misfit energy along the glide plane over the lattice (over n), as shown below,

$$\begin{aligned}W(a) &= \sum_{n=-\infty}^{\infty} \Delta\widetilde{W}(n,a)\\ &= \sum_{n=-\infty}^{\infty} (\Delta\widetilde{W}^\infty(n,a) + \Delta\widetilde{W}^{\mathrm{I}}(n,a))\\ &= W^\infty(a) + W^{\mathrm{I}}(a) \qquad (17)\end{aligned}$$

where the symbol tilde (~) indicates that the energy W takes the arguments n and a instead of x. Similarly, we split the total misfit energy into two parts, $W^\infty(a)$ and $W^{\mathrm{I}}(a)$, in order to compare with the P–N model. The former is the misfit energy due to σ_{yz}^∞,

$$\widehat{W}^\infty(\alpha) = \frac{Db^2}{2} + Db^2\sum_{n=1}^{\infty} \mathrm{e}^{-\xi n}\cos(n\alpha) \qquad (18)$$

where $\xi = 2\pi w_{\mathrm{h}}/s$, $\alpha = 2\pi a/s$ are the two normalized dimensionless quantities. The symbol hat ($\hat{}$) indicates that the energy W takes the argument α instead of a. By expressing the cosine function in terms of exponentials, the above geometric series can be summed up [27] to yield

$$\widehat{W}^\infty(\alpha) = \frac{Db^2}{2}\frac{\sinh\xi}{\cosh\xi - \cos\alpha} \qquad (19)$$

Similarly, $W^{\mathrm{I}}(a)$ is an even function. We can also use the property of Fourier series to obtain

$$\widehat{W}^{\mathrm{I}}(\alpha) = -\frac{Db^2\kappa(h)}{2} - \frac{Db^2\kappa(h)}{\rho(h)}\sum_{n=1}^{\infty}\frac{1}{n}\mathrm{e}^{-\xi n}\left(1-\mathrm{e}^{-\rho(h)n}\right)\cos(n\alpha) \qquad (20)$$

or

$$\widehat{W}^{\mathrm{I}}(\alpha) = -\frac{Db^2\kappa(h)}{2\rho(h)}\ln\left(\frac{\cosh(\xi+\rho(h)) - \cos\alpha}{\cosh\xi - \cos\alpha}\right) \qquad (21)$$

since the series in the sum is a combination of two Mercator series.

By combining both misfit energies, we have the total misfit energy as,

$$\widehat{W}(\alpha) = \frac{Db^2}{2}\left(\frac{\sinh\xi}{\cosh\xi-\cos\alpha} - \frac{\kappa(h)}{\rho(h)}\ln\left(\frac{\cosh(\xi+\rho(h))-\cos\alpha}{\cosh\xi-\cos\alpha}\right)\right) \qquad (22)$$

Since no approximation is made during the summation, the total misfit energy shown in Eq. (22) is valid for dislocations of all sizes.

For narrow dislocations ($\xi \ll 1$), of which the dislocation core is smaller than the lattice constant (size), the leading term ($n = 0$) in the sum of Eq. (17) contributes to the misfit energy most significantly. Hence, the two components of the total misfit energy for narrow dislocations are

$$\begin{aligned}W^{n,\infty}(a) &= \frac{sDb^2}{2\pi}\frac{w_{\mathrm{h}}}{a^2+w_{\mathrm{h}}^2}\\ W^{n,\mathrm{I}}(a) &= -\frac{Db^2\kappa(h)}{2\rho(h)}\ln\left(\frac{a^2+(2h+w_{\mathrm{h}})^2}{a^2+w_{\mathrm{h}}^2}\right)\end{aligned} \qquad (23)$$

where the superscript n indicates that the quantity is for narrow dislocations. For wide dislocations ($\xi \ll 1$), the leading term ($n = 1$) in the sum of Eqs. (18) and (20) contribute to the misfit energy significantly. Thus the two components of the total misfit energy for wide dislocations are

$$\widehat{W}^{\mathrm{w},\infty}(\alpha) = \frac{Db^2}{2}\left(1 + 2\mathrm{e}^{-\xi}\cos\alpha\right)$$
$$\widehat{W}^{\mathrm{w,I}}(\alpha) = -\frac{Db^2}{2}\left(\kappa(h) + \frac{2\kappa(h)}{\rho(h)}\mathrm{e}^{-\xi}\left(1 - \mathrm{e}^{-\rho(h)}\right)\cos\alpha\right) \tag{24}$$

where the superscript w indicates that the quantity is for wide dislocations.

3.3. Peierls stress

For dislocations of all sizes, the lattice friction σ^{∞} due to W^{∞} when the dislocation moves by a distance a is

$$\sigma^{\infty} = -\frac{1}{b}\frac{\mathrm{d}W^{\infty}(a)}{\mathrm{d}a} = \frac{Db\pi}{s}\frac{\sinh\xi\sin\alpha}{(\cosh\xi - \cos\alpha)^2} \tag{25}$$

and the lattice friction σ^{I} due to W^{I} is

$$\sigma^{\mathrm{I}} = -\frac{1}{b}\frac{\mathrm{d}W^{\mathrm{I}}(a)}{\mathrm{d}a} = -\frac{Db\pi}{s}\frac{(\cosh(\xi+\rho(h)) - \cosh\xi)\sin\alpha}{(\cosh(\xi+\rho(h)) - \cos\alpha)(\cosh\xi - \cos\alpha)} \tag{26}$$

Summing these two frictions yields the total lattice friction.

The modified Peierls stress, which is the maximum lattice friction, for the screw dislocation at the interface of thin film/substrate system is then given as

$$\sigma_{\mathrm{p}} = \frac{\mu b}{2s}\left(g_1(\alpha_{\mathrm{m}}) - \frac{\kappa(h)}{\rho(h)}g_2(\alpha_{\mathrm{m}})\right)g_3(\alpha_{\mathrm{m}}) \tag{27}$$

where

$$g_1(\alpha_{\mathrm{m}}) = \frac{\sinh\xi}{\cosh\xi - \cos\alpha_{\mathrm{m}}} \tag{28}$$
$$g_2(\alpha_{\mathrm{m}}) = \frac{\cosh(\xi+\rho(h)) - \cosh\xi}{\cosh(\xi+\rho(h)) - \cos\alpha_{\mathrm{m}}} \tag{29}$$
$$g_3(\alpha_{\mathrm{m}}) = \frac{\sin\alpha_{\mathrm{m}}}{\cosh\xi - \cos\alpha_{\mathrm{m}}} \tag{30}$$

and α_{m} maximizes the lattice friction.

By taking the derivative of the misfit energy shown in Eq. (23) with respect to a, the Peierls stress for the narrow dislocation is

$$\sigma_{\mathrm{p}}^{n} = \left(\frac{2\mu b}{s}\right)\frac{\alpha_{\mathrm{m}}^{n}\xi}{(\alpha_{\mathrm{m}}^{n})^2 + \xi^2}\left(\frac{1}{(\alpha_{\mathrm{m}}^{n})^2 + \xi^2} - \frac{1}{(\alpha_{\mathrm{m}}^{n})^2 + (\rho(h)+\xi)^2}\right) \tag{31}$$

where $\alpha_{\mathrm{m}}^{n} = \zeta\xi$ is the maximizer of the lattice friction. The parameters

$$\zeta = \left(\frac{2}{3 + \lambda + \sqrt{(3+\lambda)^2 + 20\lambda}}\right)^{1/2} \tag{32}$$

and $\lambda = (w_{\mathrm{h}}/(2h + w_{\mathrm{h}}))^2$ are two dimensionless parameters. For different thicknesses of thin film, λ ranges from 0 ($h = \infty$) to 1 ($h = 0$), and ζ ranges from $1/\sqrt{5}(h=0)$ to $1/\sqrt{3}(h=\infty)$.

Similarly, by using the misfit energy shown in Eq. (24), the Peierls stress of wide dislocations is given as

$$\sigma_{\mathrm{p}}^{\mathrm{w}} = \frac{\mu b}{s}\mathrm{e}^{-\xi}\left(1 - \frac{\kappa(h)}{\rho(h)}\left(1 - \mathrm{e}^{-\rho(h)}\right)\right) \tag{33}$$

4. Amplification factors

We now discuss the effect of free surface on the misfit energy and the Peierls stress of the screw dislocation in the thin film/substrate system.

To isolate this effect, an amplification factor *f*, which is defined as the ratio between the HSPN solutions and the conventional P–N solutions, is introduced. The amplification factor is a function of the film thickness h. It provides quantitative information, or a scaling law, on how the misfit energy and the Peierls stress change due to the existence of a free surface. The emphasis here is placed on the asymptotic behavior of this factor as the film thickness h approaches to $h = h_{\mathrm{min}}$. In particular, we are interested in the two special cases: the narrow and the wide dislocations.

4.1. Dislocation of all sizes

The misfit energies given in Eqs. (19) and (22) are periodic functions. They both have maximum values when the dislocation is in the unshifted position, i.e. $a = 0$. In this paper, the amplification factor for misfit energy is defined as the ratio of the maximum misfit energies, and it is given as

$$f_W(h) \equiv \frac{W_{\max}}{W_{\max}^{\infty}} = 1 - \left(\frac{\kappa(h)}{\rho(h)}\right)\frac{\cosh\xi - 1}{\sinh\xi}\ln\left(\frac{\cosh(\xi+\rho(h)) - 1}{\cosh\xi - 1}\right) \tag{34}$$

Whereas the amplification factor for the Peierls stress σ_{p} is defined as

$$f_{\sigma}(h) \equiv \frac{\sigma_{\mathrm{p}}}{\sigma_{\mathrm{p}}^{\infty}} = \frac{\left(g_3(\alpha_{\mathrm{m}})(g_1(\alpha_{\mathrm{m}}) - \frac{\kappa(h)}{\rho(h)}g_2(\alpha_{\mathrm{m}})\right)}{g_3(\alpha_{\mathrm{m}}^{\infty})g_1(\alpha_{\mathrm{m}}^{\infty})} \tag{35}$$

where the scalar $\alpha_{\mathrm{m}}^{\infty}$ is the maximizer of the lattice friction σ^{∞} in Eq. (25), and is given as [27]

$$\alpha_{\mathrm{m}}^{\infty} = \cos^{-1}\left(\frac{1}{2}\left(\sqrt{9 + \sinh^2\xi} - \cosh\xi\right)\right) \tag{36}$$

The maximizer α_{m} is different from $\alpha_{\mathrm{m}}^{\infty}$ in general unless $\xi \gg 1$ for wide dislocations or when the thickness h is approaching infinity (unbounded domain).

Both the factors $f_W(h)$ and $f_{\sigma}(h)$ have the limits that $f_{W/\sigma} \to 1$ if $h \to \infty$ and $f_{W/\sigma} \to 0$ if $h \to 0$. The first limit ensures that the P–N solution is recovered if the dislocation is in the unbounded body ($h \to \infty$). The second limit, however, does not imply a zero misfit energy, nor a zero Peierls stress for a surface dislocation. As explained in Section 2, the HSPN model requires a non-vanishing non-Hookean slab joining the thin film and the substrate, and hence the minimum thickness of the thin film for the HSPN model to be valid should be $d/2$, i.e. $h_{\min} = d/2$. For instance, if the thickness of this slab d is one lattice spacing, i.e. $d = s$, the minimum thickness of the thin film is $h_{\min} = s/2$, and it corresponds to the minimum amplification factors $f_{W,\min} \equiv f_W(h_{\min}) = 0.54$ and $f_{\sigma,\min} \equiv f_\sigma(h_{\min}) = 0.92$. In other words, for a surface screw dislocation, both misfit energy and Peierls stress are not zero. They are about 50% and 10%, respectively, less than those of the same dislocation in the unbounded body if the width, $2w_{\mathrm{h}}$, of the dislocation is about the lattice spacing s.

It is worth noting that a zero thickness h, i.e. without the existence of a thin film, implies a perfect lattice in the system (substrate only). We should expect zero Peierls stress when $h = 0$ since there is no lattice misfit in the system. Therefore, the second limit does give a correct answer of the modified Peierls stress for any non-zero thickness d of the non-Hookean slab.

4.2. Narrow dislocations

For narrow dislocations, the amplification factor for the maximum misfit energy is

$$f_W^n(h) \equiv \frac{W_{\max}^n}{W_{\max}^{n,\infty}} = 1 - \frac{\xi\kappa(h)}{\rho(h)} \ln\left(\frac{\rho(h)+\xi}{\xi}\right) \tag{37}$$

and the amplification factor for the Peierls stress is

$$f_\sigma^n(h) \equiv \frac{\sigma_{\mathrm{p}}^n}{\sigma_{\mathrm{p}}^{n,\infty}} = \frac{16\zeta}{3\sqrt{3}(\zeta^2+1)^2}\left(1 - \frac{\lambda\zeta^2+\lambda}{\lambda\zeta^2+1}\right) \tag{38}$$

where, as derived in Joos and Duesbury [27],

$$\sigma_{\mathrm{p}}^{n,\infty} = \left(\frac{3\sqrt{3}}{8\xi^2}\right)\frac{\mu b}{s} \tag{39}$$

If the thickness h of the thin film is $d/2$, i.e. $h_{\min}$, we have $\rho = 2\xi$, $\kappa = 0.5$, $\lambda = 1/9$ and

$$\zeta = \sqrt{\frac{9}{14+\sqrt{241}}} \simeq 0.55 \tag{40}$$

and the resulting minimum amplification factors are

$$\begin{aligned} f_{W,\min}^n &\equiv f_W^n(h_{\min}) = 1 - \frac{\ln(3)}{4} \simeq 0.73 \\ f_{\sigma,\min}^n &\equiv f_\sigma^n(h_{\min}) = \frac{128\zeta}{3\sqrt{3}(\zeta^2+1)^2(\zeta^2+9)} \simeq 0.86 \end{aligned} \tag{41}$$

Both the minimum amplification factors $f_{W,\min}^n$ and $f_{\sigma,\min}^n$ are independent of ξ. Since we expect the minimum amplification factor $f_{\sigma,\min}^n$ to increase when the size of the dislocation increases, $f_{\sigma,\min}^n = 0.86$ is the minimum amplification factor for the screw dislocation at the surface of the thin film regardless of the value of ξ, i.e. the size of dislocations.

4.3. Wide dislocations

For wide dislocations, the amplification factor for the maximum misfit energy is

$$\begin{aligned} f_W^{\mathrm{w}}(h) &\equiv \frac{W_{\max}^{\mathrm{w}}}{W_{\max}^{\mathrm{w},\infty}} \\ &= 1 - (1+2\mathrm{e}^{-\xi})^{-1}\left(\kappa(h) + \frac{2\kappa(h)}{\rho(h)}\mathrm{e}^{-\xi}(1-\mathrm{e}^{-\rho(h)})\right) \\ &\simeq 1 - \kappa(h) \end{aligned} \tag{42}$$

and the amplification factor for the Peierls stress is

$$f_\sigma^{\mathrm{w}}(h) \equiv \frac{\sigma_{\mathrm{p}}^{\mathrm{w}}}{\sigma_{\mathrm{p}}^{\mathrm{w},\infty}} = 1 - \frac{\kappa(h)}{\rho(h)}(1-\mathrm{e}^{-\rho(h)}) \tag{43}$$

where

$$\sigma_{\mathrm{p}}^{\mathrm{w},\infty} = \frac{\mu b}{s}\mathrm{e}^{-\xi} \tag{44}$$

From the expressions of the amplification factors for wide dislocations, we notice that the reduction in the maximum misfit energy is controlled by the parameter κ (see Eq. (42)), and the reduction in the Peierls stress has an exponential term with the rate of decay described by the parameter ρ (see Eq. (43)).

If the thickness h of the thin film is $d/2$, we have $\kappa = 0.5$. The corresponding minimum amplification factors are

$$\begin{aligned} f_{W,\min}^{\mathrm{w}} &\equiv f_W^{\mathrm{w}}(h_{\min}) = 0.5 \\ f_{\sigma,\min}^{\mathrm{w}} &\equiv f_\sigma^{\mathrm{w}}(h_{\min}) = 1 - \frac{1}{4\xi}(1-\mathrm{e}^{-2\xi}) \end{aligned} \tag{45}$$

We notice that the minimum amplification factor $f_{\sigma,\min}^{\mathrm{w}}$ for wide dislocations is ξ-dependent. The higher the value of ξ, the closer to 1 the value of $f_{\sigma,\min}^{\mathrm{w}}$. Therefore, when the size of the dislocation increases, the boundary effect on the Peierls stress becomes less significant.

To show how the misfit energy and the Peierls stress change as the thickness of the thin film increases, we plot the amplification factors f_W and f_σ versus the normalized thickness h/s in Fig. 4 for different d/s ratios. In these two plots, the middle three curves are plotted by using the exact amplification factors shown in Eqs. (34) and (35). For the other two cases, we use the approximate amplification factors shown in Eqs. (37), (38) and Eqs. (42), (43) for both narrow ($d/s = 0.25$) and wide ($d/s = 4$) screw dislocations, respectively.

Fig. 4a shows that the boundary effect on the misfit energy is quite significant. For the dislocation of core size $d/s = 1$, the reduction in the maximum misfit energy can be as high as about 50% for a surface dislocation. In general, for all sizes of dislocations, the reduction becomes less

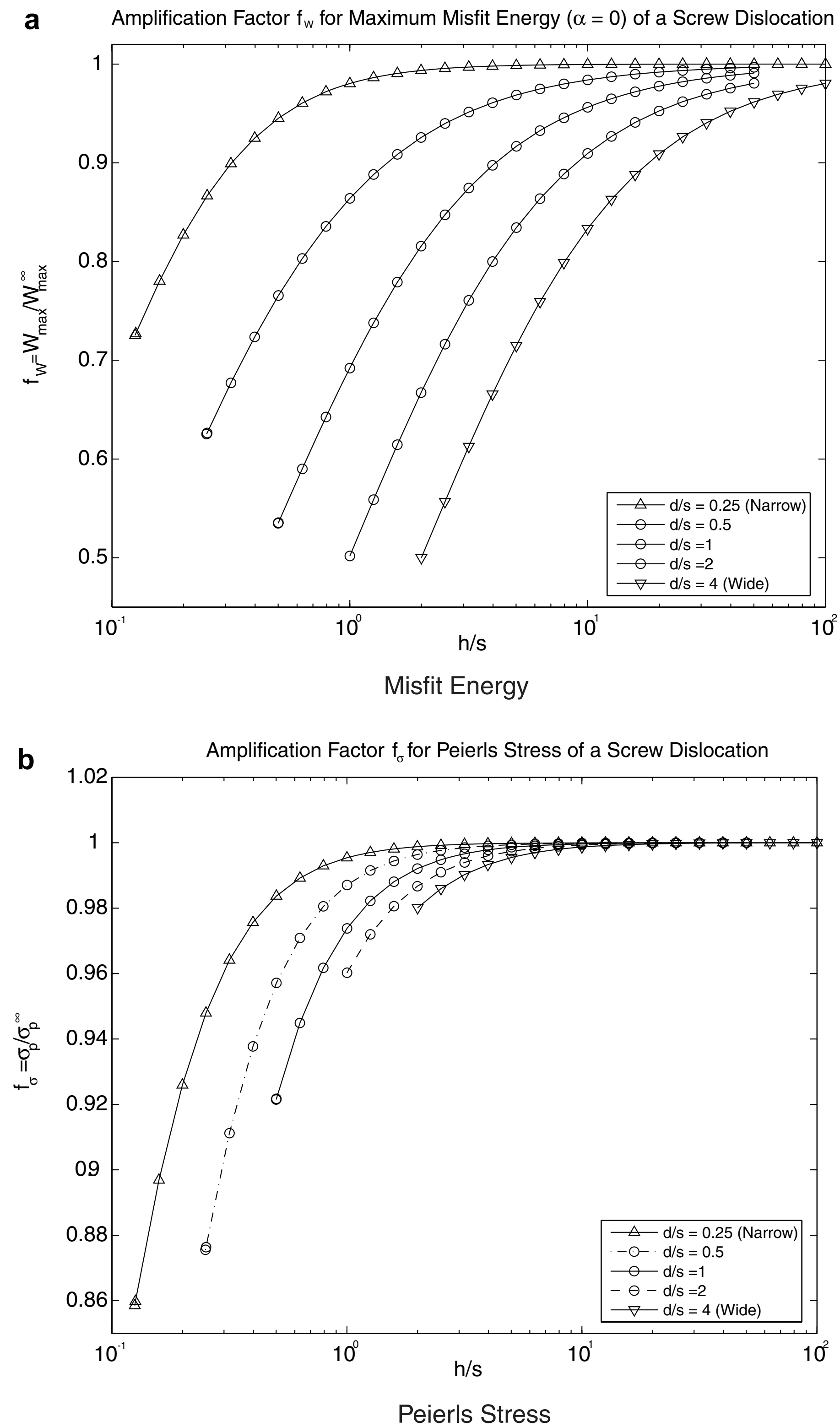

Fig. 4. Amplification factors versus h/s for different d/b ratios.

than 5% only when there are at least 100 layers of atoms between the dislocation and the free surface.

In comparison with the misfit energy, the boundary effect on the Peierls stress of the dislocation is not that significant (see Fig. 4b). For the dislocation with core size $d/s = 1$, if there is at least one layer of atoms ($h/s = 1.5$) between the dislocation and the free surface, the reduction in the Peierls stress is less than 5%.

5. Conclusions

By spreading an image dislocation along an imaginary interface, an HSPN model has been proposed. With this model, close form expressions for both misfit energy and Peierls stress have been obtained for a screw dislocation in a thin film/substrate system.

In comparison with the misfit energy and the Peierls stress of the conventional P–N model, we have derived amplification factors for screw dislocations of all sizes. The approximated amplification factors are also obtained for the two limiting cases: narrow and wide dislocations.

Using the HSPN model, it is shown that the reduction in the misfit energy due to the boundary effect can be as high as 50% for a surface dislocation. This effect becomes less significant only when the dislocation is more than 100 layers of atoms away from the free surface. It is possible that the HSPN model may serve as a good approximation of atomistic simulations.

In this work, we have also studied the dependence of the Peierls stress on the free surface effect via a continuum model. By considering the effect of image dislocations, the Peierls stress is shown to be dependent on the film thickness in the thin film/substrate system. Our results indicate that the free surface effect on the Peierls stress is insignificant when the dislocation is far away from the free surface, which is the classical result of the P–N model. As the screw dislocation approaches the free surface, the Peierls stress reduces exponentially, and the Peierls stress for a surface screw dislocation appears to be about 85 % or more of the value predicted by the classical Peierls stress in the bulk material. This lower bound of the amplification factor is applicable for screw dislocations of all sizes. The reduction of the Peierls stress for the surface dislocation is therefore at most 15%, depending on the size of the dislocation.

The concept and mathematical structure of the HSPN model can be readily extended into the case of edge dislocations. We shall report the HSPN model for edge dislocations in a separated paper.

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