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Analysis of dislocation nucleation from a crystal surface based on the Peierls–Nabarro dislocation model

Guanshui Xu*, Chuanli Zhang

Department of Mechanical Engineering, University of California, Riverside, CA 92521, USA

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Abstract

Dislocation nucleation from a stressed crystal surface is analyzed based on the Peierls–Nabarro dislocation model. The variational boundary integral approach is used to obtain the profiles of the embryonic dislocations in various three-dimensional nucleation configurations. The stress-dependent activation energies required to activate dislocations from their stable to unstable saddle point configurations are determined. Compared to previous analyses of this type of problem based on continuum elastic dislocation theory, the present analysis eliminates the uncertain core cutoff parameter by allowing for the existence of an extended dislocation core as the embryonic dislocation evolves. Moreover, atomic information can be incorporated to reveal the dependence of the nucleation process on the profile of the atomic interlayer potential as compared to continuum elastic dislocation theory in which only elastic constants and Burgers vector are relevant. Finally, the presented methodology can also be readily used to study dislocation nucleation from the surface heterogeneities such as cracks, steps, and quantum structures of electronic devices.

Keywords: Dislocation nucleation; Surface; Activation energy; Peierls–Nabarro dislocation model; Atomic interlayer potential

1. Introduction

The fundamental mechanisms of dislocation nucleation from a crystal surface have been of considerable interest in a wide variety of scientific and engineering problems. One example is the growth of high-quality strained heteroepitaxial layer structures

* Corresponding author. Tel.: 909-787-2497; fax: 909-787-2899.
E-mail address: gxu@engr.ucr.edu (G. Xu).

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for fabrication of high-speed electronics and optoelectronics (e.g. Nix, 1989; Mooney, 1996; Freund, 2000). Since materials of layers are selected primarily on the basis of their electronic characteristics, it is unavoidable to have a mismatch in lattice parameter between the layers or the layer and substrate. This mismatch gives rise to mechanical stress, which in turn could induce evolution of surface morphology (Gao et al., 1999) and/or nucleation of misfit dislocations from the surface (Kamat and Hirth, 1990; Beltz and Freund, 1993, 1994; Wagner, 1999). These dislocations in electronically active regions within devices are either detrimental by degrading the electrical and optoelectrical performance of materials or potentially beneficial by generating self-organized quantum structures relevant to the next generation of devices (e.g. Zunger, 1998). Understanding the formation of dislocations in strained semiconductor layer materials, with an aim toward controlling them, is therefore of central interest in the semiconductor industry.

Two conditions are of particular interest in understanding nucleation of a dislocation from a stressed crystal surface. One is the critical stress under which dislocation nucleation occurs instantaneously at absolute zero. The other is the activation energy required to thermally activate dislocation nucleation at a stress level below this critical value at a finite temperature. In principle, nucleation is controlled by atomic-scale processes and needs to be investigated at the atomic level. Atomistic simulations with appropriate empirical potentials may be used to determine the first condition (Kelchner et al., 1998; Brochard et al., 2000). It is, however, not effective in determining the activation energy because of its serious limitation on resolving unstable saddle point configurations in large systems. As a consequence, most analyses of this problem have been so far based on continuum elastic dislocation theory in which the condition for the formation of a semicircular dislocation loop is worked out based on an approach similar to that used by Cottrell (1953) to estimate the energy required for homogeneous nucleation of a circular dislocation loop in a perfect bulk crystal (Kamat and Hirth, 1990; Beltz and Freund, 1993, 1994; Wagner, 1999). In general, these analyses assume that dislocation loops are in the semicircular shape and the dislocation image force is either ignored or treated approximately. The image force, however, can be rigorously treated in this framework by making use of the general solution of an infinitesimal dislocation loop in a half-space (Bacon and Groves, 1970; Eshelby, 1979), as demonstrated in the analysis of Beltz and Freund (1993). The predicted critical radius of the dislocation loop is on the order of the size of the dislocation core, therefore indicating that the obtained energetics of dislocation nucleation could be unreliable because of the limitation of continuum elastic dislocation theory at the core region. Alternatively, as suggested by Beltz and Freund (1993), this problem may be resolved by using the Peierls–Nabarro dislocation model (Peierls, 1940; Nabarro, 1947). The model is believed to provide a more definitive solution because it eliminates the uncertain core cutoff parameter existing in continuum elastic dislocation theory by allowing for the existence of an extended dislocation core. Beltz and Freund (1994) used this model and analyzed the energy condition for the formation of misfit dislocations. Although their analysis is limited to the formation of a straight dislocation in a plain strain condition, the results, nevertheless, indicate that the analysis based on the Peierls–Nabarro dislocation model is justified because it reveals the dependence of the energetics of

dislocation formation on other materials properties such as the unstable stacking energy in addition to elastic constants.

In the classic Peierls–Nabarro dislocation model of a straight edge dislocation, the profile of the dislocation along the slip plane, corresponding to the relative displacement between two atomic layers, is modeled as a continuous distribution of infinitesimal dislocations (Eshelby, 1949). The simple sinusoidal shear resistance relation is assumed along the slip plane, while the crystal blocks above and below the slip plane are treated as linear elastic media. The balance of the lattice restoring stress and the elastic stress due to all infinitesimal dislocations across the slip plane results in an integrodifferential equation that leads to an analytical solution of the dislocation profile. Since this solution removes the singularity of the classical Volterra dislocation, the Peierls–Nabarro model gives the first indication of the size of the dislocation core and the energy barrier associated with it, albeit with its unrealistic use of the linear elasticity in the highly non-linear and discrete core region (e.g., Hirth and Lothe, 1982).

The Peierls–Nabarro dislocation model has been recently advanced to study dislocation nucleation from cracks (Schoeck and Pueschl, 1991; Rice, 1992). Xu et al. (1995, 1997) have incorporated the Peierls–Nabarro dislocation model into a variational boundary integral method (Xu and Ortiz, 1993) and analyzed dislocation nucleation from cracks in various three-dimensional configurations. Coupled tension and shear interlayer potentials, including surface production due to dislocation nucleation, are also developed accordingly to account for the general stress condition acting on the slip plane at the crack tip. Numerical techniques are developed for effectively determining the unstable saddle point dislocation configurations. Recently, a variational boundary integral method for the general anisotropic elastic solid has also been developed (Xu, 2000) and the energetics of homogeneous nucleation of a dislocation loop under stress in perfect crystals has been analyzed (Xu and Argon, 2000).

In this paper, this model is further extended to analyze nucleation of half dislocation loops from a stressed surface. Instead of using the general elastic solutions of dislocations in the half space, a rather straightforward methodology is presented to rigorously account for the surface effect. The saddle point configurations of embryonic dislocations and their associate thermal activation energies are determined in the same way by energy variational principle. Comparison will be made with previous analyses based on continuum elastic dislocation theory, with emphasis placed on the generic effects of the interlayer atomic potential on dislocation nucleation. We note that the presented methodology can also be readily used for the study of dislocation nucleation from the surface heterogeneities such as cracks, steps, and quantum structures. The comprehensive study of these subjects for particular material systems of technological interest shall be presented in future papers.

2. Variational formulation of the Peierls–Nabarro dislocation model

We begin by considering a general geometry for dislocation nucleation from a surface, as shown in Fig. 1. The angle between the surface and slip plane on which nucleation of dislocation occurs is denoted by α. The symbol ϕ denotes the angle

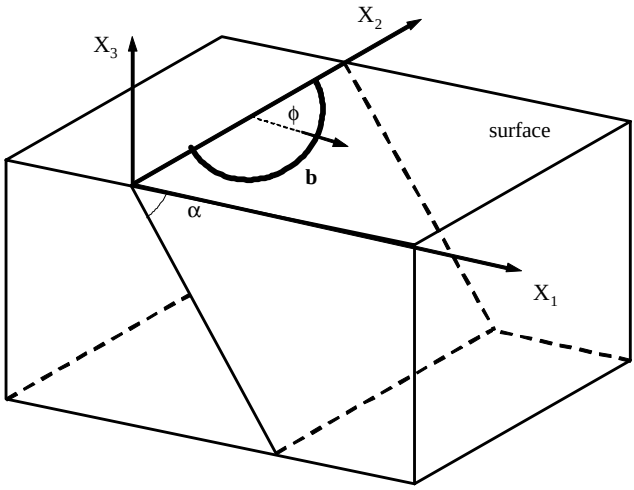

Fig. 1. The configuration for nucleation of a half-dislocation loop from a crystal surface.

between the Burgers vector and the intersection of the slip plane and the surface. Cartesian coordinates are selected so that the x_3-axis is normal to the surface and the x_2-axis is parallel to the intersection of the slip plane and the surface.

In the previously developed variational boundary integral method in which the Peierls–Nabarro dislocation model is incorporated for the analysis of dislocation nucleation from the crack (Xu et al., 1995, 1997), the total energy of the system is expressed by an integral equation in terms of the displacements ascribed on the crack and slip plane on which dislocation nucleation occurs. These displacements, including dislocation profiles on the slip plane, are solved based on a variational minimization process employed by finite element methodology. To use this method to study dislocation nucleation from the surface, the surface effect needs to be considered. One way to solve this problem is to modify the original variational boundary integral method for the infinite solid by employing general solutions of infinitesimal dislocation loops in the half space (Bacon and Groves, 1970; Eshelby, 1979). Alternatively, we propose a straightforward approach that allows for the use of the existing variational boundary integral method for half space problems. In this approach, the surface is modeled as part of a very large crack embedded in an infinite solid. As the size of this crack is selected to be much larger than any relevant size of the dislocation configuration, the problem can then be solved in an equivalent system that is essentially composed of the slip plane and the crack embedded in the infinite solid. This approach and its advantage of solving half-space problems that involve non-planar surfaces are schematically shown in Fig. 2.

Let $\boldsymbol{\delta}(\mathbf{x})$ denote the relative displacement between the adjacent atomic layers along the slip plane and the opening displacement of the crack. The potential energy Π of the system can be expressed as

$$\Pi[\boldsymbol{\delta}(\mathbf{x})] = W[\boldsymbol{\delta}(\mathbf{x})] + V[\boldsymbol{\delta}(\mathbf{x})] - P[\boldsymbol{\delta}(\mathbf{x})], \tag{1}$$

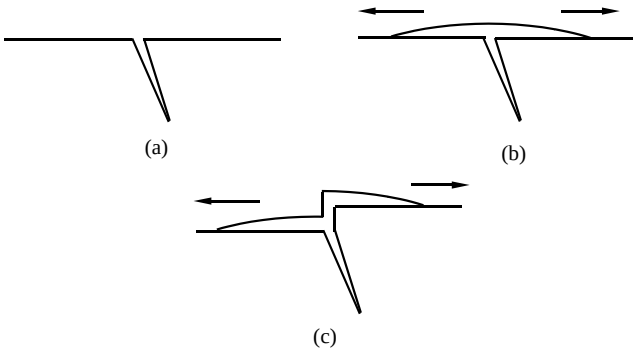

Fig. 2. Schematic illustration of transferring the half-space problems into the problems in an infinite space: (a) a surface crack; (b) the surface and the surface crack can be viewed together as a three dimensional crack embedded in an infinite medium; (c) a surface step can also be viewed as part of a three dimensional crack.

where W is the elastic strain energy associated with the displacement on the crack and slip plane; V the interatomic layer potential energy defined on the slip plane; and P the work of the external applied forces. By modeling the displacement as a continuous distribution of dislocation loops and using the known expression of interaction energy between two dislocation loops (Lothe, 1982), the elastic strain energy for a general anisotropic solid can be obtained as (Xu, 2000)

$$W[\boldsymbol{\delta}(\mathbf{x})] = \frac{1}{16\pi^2}\int_S\int_S \frac{1}{R}\int_0^{2\pi} \mathbf{e}_i \cdot \{[(\mathbf{n}\times\nabla\delta_i)_1\times\mathbf{z}, (\mathbf{n}\times\nabla\delta_j)_2\times\mathbf{z}] - [(\mathbf{n}\times\nabla\delta_i)_1\times\mathbf{z}, \mathbf{z}]\cdot(\mathbf{z},\mathbf{z})^{-1}\cdot[\mathbf{z}, (\mathbf{n}\times\nabla\delta_j)_2\times\mathbf{z}]\}\cdot\mathbf{e}_j \,\mathrm{d}\psi\,\mathrm{d}S_1\,\mathrm{d}S_2, \tag{2}$$

where S represents the slip plane and the crack surface; $(.)_1$ and $(.)_2$ denote two different points on the surfaces S; R is the distance between these two points; $\mathbf{e}_i$, $i=1,2,3$, are Cartesian basis vectors; $\mathbf{n}$ is the normal vector to the crack and slip plane; $\mathbf{z}$ is a unit vector perpendicular to $\mathbf{R}$; and ψ is the angle between $\mathbf{z}$ and an arbitrary chosen reference $\mathbf{z}_0$. The components of the second-rank tensor in the notation $(\mathbf{a},\mathbf{b})$ is defined as $(\mathbf{a},\mathbf{b})_{jk} = a_i c_{ijkl} b_l$, where c_{ijkl} are elastic constants.

The interlayer potential energy is given by

$$V[\boldsymbol{\delta}(\mathbf{x})] = \int_S \Phi[\boldsymbol{\delta}(\mathbf{x})]\,\mathrm{d}S, \tag{3}$$

where $\Phi[\boldsymbol{\delta}(\mathbf{x})]$ is the interlayer potential energy defined on per unit area of the slip plane, which can be developed by considering two blocks of crystals sliding uniformly across the slip plane, as shown in Fig. 3. By assuming that the sliding is restricted in the Burgers vector direction, i.e. the constrained path approximation (Rice, 1992), we may use Δ_r and Δ_t to denote the relative sliding and opening displacement between two adjacent atomic layers; and σ_r and σ_t the corresponding shear and normal resistance between the two blocks of crystals, respectively. As pointed out by Rice, δ_r and δ_t are

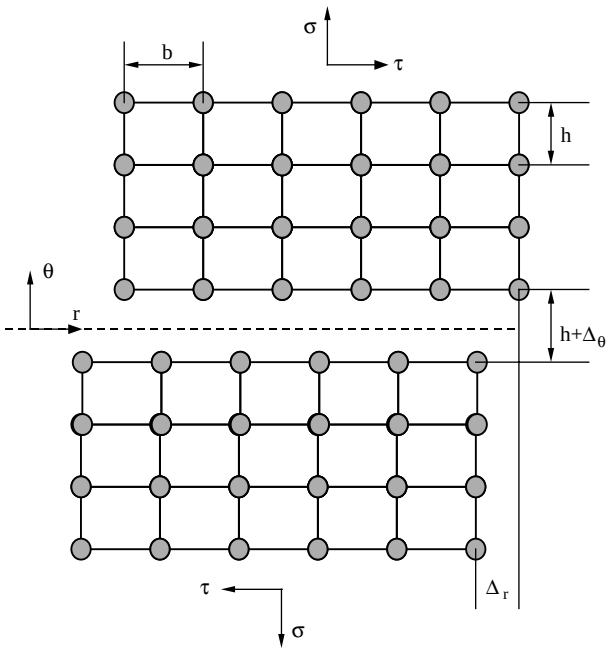

Fig. 3. Block-like lattice sliding and opening between two adjacent atomic planes.

inelastic displacements defined along a cut of zero thickness in an elastic continuum. The total displacements Δ_r and Δ_t between two adjacent atomic layers are viewed as the addition of the inelastic displacements and the elastic shear displacements over the spacing of the adjacent atomic layers, i.e.

$$\delta_r = \Delta_r - h\tau(\Delta_r, \Delta_\theta)/\mu, \tag{4a}$$

$$\delta_\theta = \Delta_\theta - h\sigma(\Delta_r, \Delta_\theta)/c, \tag{4b}$$

where $c = \lambda + 2\mu$ is the uniaxial strain elastic modulus. λ and μ are the Lame constant and shear modulus, respectively.

We should point out that the classic formulation of the Peierls–Nabarro dislocation model does not distinguish the total displacement and the inelastic displacement between two adjacent atomic layers. This is not a rigorous mechanics formulation since the continuous distribution of infinitesimal dislocations only models displacement discontinuities defined over thickless surfaces but rather those between two atomic layers with a finite distance. The above Rice modification provides a rigorous mechanics formulation of the Peierls–Nabarro dislocation model. However, this modification also further localizes the nonlinear deformation on the thickless slip plane, making it difficult to conjecture whether this modification provides more accurate results. If the stress τ or σ is plotted against δ_r or δ_θ, the curve has an infinite slope at the origin, which

requires additional care in the numerical analysis. For some reasons, the classic formulation of the Peierls–Nabarro dislocation model is still widely used in the literature. The computation of the activation energy for homogeneous nucleation of dislocation loop indicates that the Rice modified model gives larger activation energy than the classic Peierls–Nabarro dislocation model (Xu and Argon, 2000). Calculation of the Peierls stress based on the Rice modified model is about several orders lower than that obtained based on the classic Peierls–Nabarro model (Xu, 2001).

By combining the sinusoidal type relation in simple shear and the Rose–Ferrante–Smith universal binding relation (Rose et al., 1981) in simple tension, the potential energy Φ and its related quantity Ψ, which are defined such that $\mathrm{d}\Phi = \tau\,\mathrm{d}\delta_r + \sigma\,\mathrm{d}\delta_\theta$ and $\mathrm{d}\Psi = \tau\,\mathrm{d}\Delta_r + \sigma\,\mathrm{d}\Delta_\theta$, are given by

$$\Phi(\delta_r, \delta_\theta) = \Psi(\Delta_r, \Delta_\theta) - \frac{h}{2\mu}\,\tau^2(\Delta_r, \Delta_\theta) - \frac{h}{2c}\,\sigma^2(\Delta_r, \Delta_\theta) \tag{5}$$

and

$$\Psi(\Delta_r, \Delta_\theta) = 2\gamma_s \left\{ 1 - \left[1 + \left(\frac{\Delta_\theta}{L}\right)\right] \exp\left(-\frac{\Delta_\theta}{L}\right) + \left[\sin^2\left(\frac{\pi\Delta_r}{b}\right) + \frac{\beta - 1}{4}\sin^2\left(\frac{2\pi\Delta_r}{b}\right)\right] \left[q + \left(\frac{q-p}{1-p}\right)\left(\frac{\Delta_\theta}{L}\right)\right] \exp\left(-\frac{\Delta_\theta}{L}\right) \right\}, \tag{6}$$

where γ_s is the surface energy of the slip plane; L is the characteristic length of the decohesion process; β is a parameter that describes the skewness of shear resistance; and p and q are two parameters that jointly characterize coupling between tension and shear. This type of relation can also be generalized to include the effect of surface production caused by dislocation nucleation, which is another important feature of dislocation nucleation from the surface when the Burgers vector is not parallel to the surface. Details on modeling of this type of atomic interlayer potential energy are described in Xu et al. (1995).

We noted that the above characterization of the interlayer potential is based on the constrained path approximation. Although this hypothesis is a good approximation in many cases, it becomes invalid when sliding in other directions cannot be ignored. Typical examples include dislocation dissociation into a pair of partial dislocations connected by a ribbon of a stacking fault. One way to solve this problem is to derive the atomic interlayer potential directly from the atomistic calculation of the so-called γ-surface (Vitek, 1968). The γ-surface, also termed the generalized stacking fault energy, represents the energy changes as two blocks of crystals slide uniformly across the slip plane in an arbitrary direction. At present, the γ-surface can be reliably obtained from ab initio calculations using electron density functional theory with local density approximation (e.g. Kaxiras and Duesbery, 1993). Schoeck (1999, 2001) suggested modeling the general atomic shear potential using the following form:

$$\gamma(\mathbf{t}) = \sum_j c_j \mathbf{e}^{\mathrm{i}2\pi g_j \mathbf{t}}$$

where $\mathbf{t}$ is the shear displacement vector between two adjacent atomic layers; $\mathbf{g}_j$ are reciprocal lattice vectors and $\mathrm{i} = \sqrt{-1}$. The coefficients c_j are determined by a set of interplanar energies $\gamma(\mathbf{t}_k)$ at specific positions $\mathbf{t}_k$. It appears that it may also be feasible to combine this potential function with the universal bonding relation to model the coupled tension effect across the slip plane.

Finally, the work of the traction $\boldsymbol{\sigma}$ applied on the crack surface and the slip plane is

$$P[\boldsymbol{\delta}] = \int_S \boldsymbol{\sigma} \cdot \boldsymbol{\delta} \, \mathrm{d}S, \tag{8}$$

where $\boldsymbol{\sigma}$ can be related to the remote stress by invoking the principle of superposition.

The minimization of the potential energy Π with respect to displacement leads to the non-linear integral equations by virtue of the non-linear interlayer potential. The finite element method with six-node triangular elements is used to discretize the slip plane and the crack. The $1/R$ singularity in the kernel of the double integration is handled by an effective and accurate numerical scheme. The resulting discretized nonlinear equations are solved by the Newton–Raphson iteration. The saddle-point configurations of dislocations are solved by recourse to displacement control, which is, in essence, the characteristic of a system with equality constraints enforced by Lagrange multipliers. The details of these techniques are described by Xu and Ortiz (1993) and Xu et al. (1995).

To reduce the numerical computation on the finite domain, a periodic condition is enforced in the x_2-axis direction. This assumption leads to an underestimate of the activation energy owing to the interaction between half-dislocation loops. This effect, however, can be minimized by increasing the period of the domain in the x_2-axis direction. The numerical results indicate that the activation energy converges quickly as this period increases, as also shown in the previous analysis of dislocation nucleation from crack tips (Xu et al., 1995). This is understandable because the interaction energy between two dislocation loops is similar to two dipoles, dropping rapidly as a function of their separation.

3. Analysis of dislocation nucleation from the surface

Depending on the surface morphology, crystallographic orientation, and loading condition, dislocation nucleation may occur in a wide variety of configurations. The critical condition for dislocation nucleation from a highly stressed perfectly flat surface is of great interest from both the fundamental viewpoint of material science and the practical application such as growth of high quality of strained heteroepitaxial semiconductor layer structures for high speed microelectronic devices. Because of the broadness of the subject, we limit our attention to a few relatively simple but important nucleation configurations. By comparing the results with those obtained using continuum dislocation theory, we emphasize the physical mechanisms that warrant further investigation in this subject.

We consider dislocation nucleation in a general slip plane with a slip direction parallel to the surface, i.e. $\phi = 0^\circ$ in Fig. 1. The driving force for nucleation of a screw

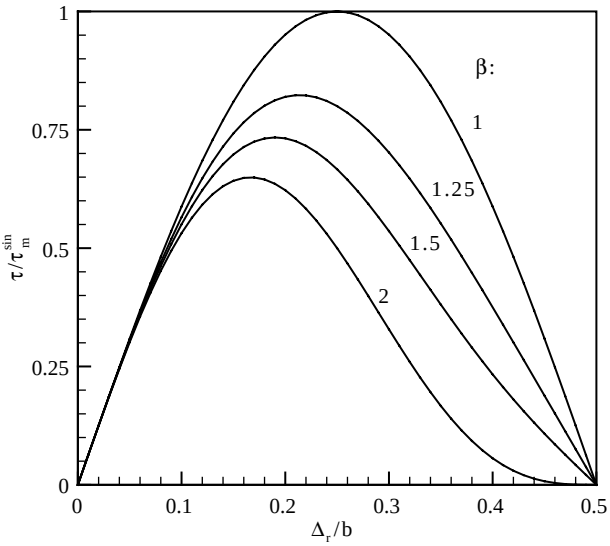

Fig. 4. The atomic interlayer shear resistance profiles for various values of parameter β.

dislocation is the simple shear stress acting parallel to the slip direction. We recognize that this configuration is somewhat uncommon as compared to the equal-biaxial stress state commonly found in strained heteroepitaxial thin films. We nevertheless select it for its simplicity and expect it to capture the essential features of dislocation nucleation in more realistic configurations. The same configuration was also used in an analysis of the effect of dislocation core spreading at the interfaces on strength of thin films (Baker et al., 2002). We note that no ledge formation is involved in this configuration, which further simplifies the analysis. The influence of ledge formation on dislocation nucleation from the surface has been considered in a previous analysis based on continuum elastic dislocation theory (Beltz and Freund, 1993). The crystal is assumed to be isotropic characterized by the shear modulus μ and Poisson's ratio $v = 0.3$. As a consequence of this assumption, only the displacement component along the slip direction is nonzero, assuming the moderate dilation effect caused by shearing can be ignored. The coupled tension and shear relation can be reduced to the simple shear relation as

$$\tau = \frac{\mu b}{2\pi h}\left[\sin\left(\frac{2\pi \Delta_r}{b}\right) + \frac{\beta - 1}{2}\sin\left(\frac{4\pi \Delta_r}{b}\right)\right], \tag{9a}$$

$$\delta_r = \Delta_r - \frac{b}{2\pi}\frac{1}{\beta}\left[\sin\left(\frac{2\pi \Delta_r}{b}\right) + \frac{\beta - 1}{2}\sin\left(\frac{4\pi \Delta_r}{b}\right)\right]. \tag{9b}$$

For the same shear modulus, the skewed profiles of shear resistance for various values of β are plotted in Fig. 4. The area under the shear resistance profile is defined by Rice (1992) as the unstable stacking energy γ_{us}, which is given by $\mu b^2/2\pi^2 h\beta$. The

ideal strength of the crystal is denoted by τ_m, and the ideal strength of the crystal of the sinusoidal shear resistance is denoted by $\tau_m^{\sin}$, where $\tau_m^{\sin} = \mu b/2\pi h$.

We shall note that the energetics of dislocation nucleation in a crystal is profoundly influenced by the profile of interlayer shear resistance. It appears that the shear modulus (the initial tangent of the curve), the ideal shear strength (the maximum stress of the curve), and the unstable stacking energy (the area under the curve) all together affect dislocation nucleation in the crystal. More realistic shear resistant profiles can be constructed based on ab initio calculations. In this paper, we use the above shear resistance model to explore the effects of various parameters on dislocation nucleation in from the crystal surface. We demonstrate that the analysis based on continuum elastic dislocation theory is inadequate for dislocation nucleation problems since only the elastic constants and the Burgers vector are relevant in the analysis.

As the shear stress increases from zero, the stress on the slip plane induces a stable slip until the shear stress reaches a critical value τ_c, which is equal to the ideal shear strength of the slip plane τ_m when the surface is perfectly flat. Because of the periodic interlayer potential, an embryonic dislocation can be formed and becomes unstable as the stress decreases from this critical point. Thus, there are two solutions associated with the same level of stress below this critical value, one is stable and the other is unstable. The energy difference between these two configurations is the activation energy E_{act} required for thermally assisted dislocation nucleation.

3.1. Nucleation of straight dislocations

We first consider nucleation of straight screw dislocations on general inclined slip planes that intersect with the perfectly flat surface. The goal is to illustrate the effects of the shear resistance profile and the angle of the slip plane on the energetics of dislocation nucleation in these simple two dimensional configurations. The study should also provide a valuable reference that can be compared to direct atomic simulation. Such comparison could be used to validate the presented approach and justify its application for the analysis of dislocation nucleation in more realistic three-dimensional configurations. One of the potential benefits of this study is to provide more reliable dislocation nucleation models that can be incorporated into discrete dislocation dynamics simulation, as advocated in multiscale mechanism-based modeling and simulation of mechanical behavior of crystalline materials.

Fig. 5 shows an example of successive saddle point configurations of an embryonic dislocation emitting on the slip plane that is perpendicular to the surface. The values of the corresponding levels of stress are also indicated in the figure. The sinusoidal shear resistance, i.e. $\beta = 1$, is assumed to hold along the slip direction on the slip plane. The coordinate r denotes the distance to the surface on the slip plane. It is noteworthy to point out that most embryonic dislocation configurations involve slip of less than a full atomic spacing and the size of the dislocation core is on the order of a few Burgers vectors. According to continuum elastic dislocation theory, the energy of a dislocation segment scales with μb^3. Therefore, the analysis of this problem based on continuum

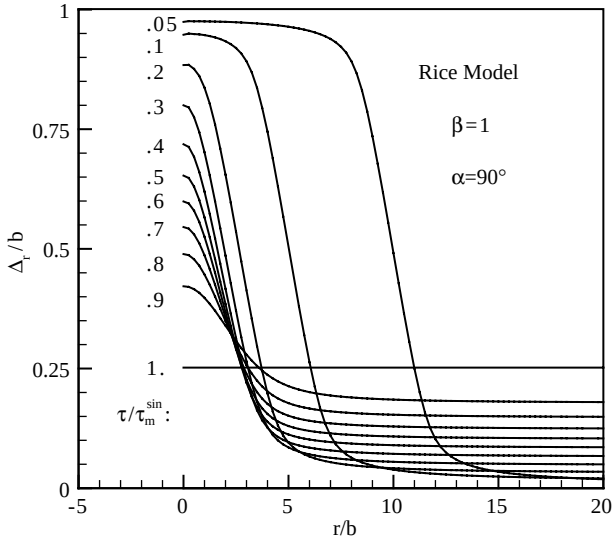

Fig. 5. The successive saddle point configurations of an embryonic dislocation corresponding to various stress levels. Δ_r represents the atomic interlayer shear displacement and r represents the distance to the surface on the slip plane. The Rice modification is implemented.

elastic dislocation theory which involves a full dislocation could considerably overestimate the activation energy required for nucleation of the dislocation from the surface. Indeed, a simple energy analysis similar to those used by Beltz and Freund (1993) indicates that the activation energy per unit length is infinite for any stress that is less than the critical stress.

Fig. 6a shows the activation energy per unit Burgers vector length for nucleation of a straight dislocation on slip planes of various orientations. The shear stress τ is normalized by the maximum shear stress $\tau_m^{\sin}$ of the sinusoidal shear resistance profile. The dashed lines correspond to the results when the Rice modification, i.e. Eq. (4), is incorporated. The solid lines correspond to the classic Peierls–Nabarro formulation, in which the inelastic displacement in the integral equation is replaced by the total displacement between two adjacent atomic layers. To distinguish the geometric effect on the energetics of dislocation nucleation, we have re-plotted the activation energy as a function of the critical resolved shear stress on the slip plane in Fig. 6b. It is evident that the inclined plane facilitates dislocation nucleation, which is expected since the free surface reduces the total energy of the dislocation.

Fig. 7a plots the activation energy per unit burger vector length for nucleation of a straight dislocation on the slip plane of $\alpha = 90^\circ$ for various values of parameter β. The remote shear stress τ is again normalized by the maximum shear stress of the sinusoidal shear resistance profile. In the analysis of dislocation nucleation from a crack tip, Rice (1992) concluded that the critical driving force for nucleation of a dislocation from the crack tip is scaled with the unstable stacking energy. Schoeck (1996) pointed out

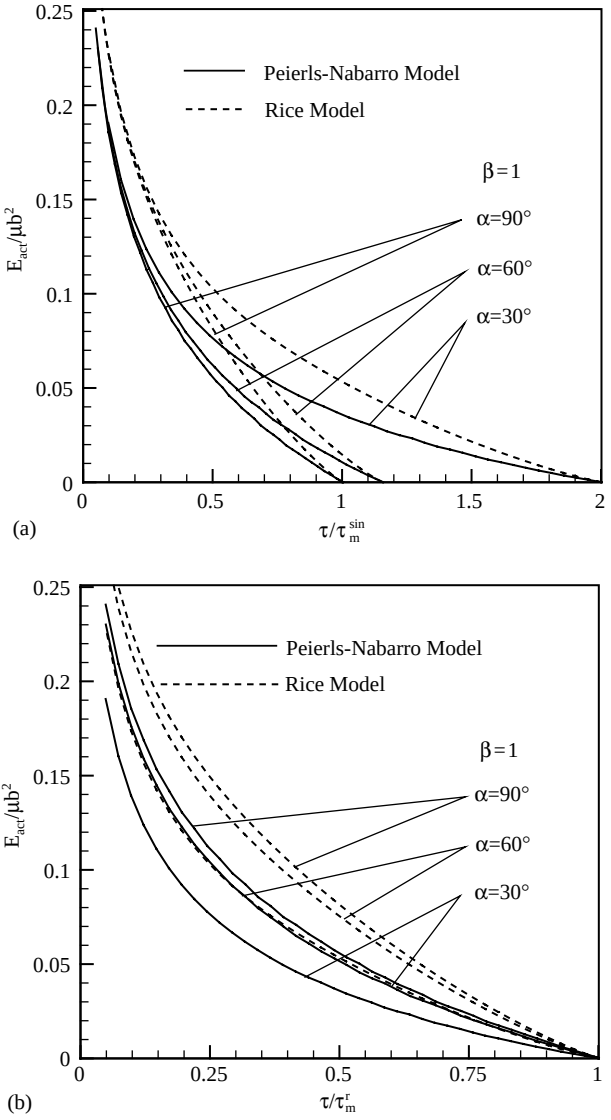

Fig. 6. Dependence of the activation energy on the shear stress for various angles of slip planes: (a) the shear stress is normalized by the maximum stress of the sinusoidal shear stress profile; (b) the shear stress is normalized by the critical resolved shear stress on the slip plane.

that the shape of the shear resistance also affects the critical condition for dislocation nucleation. Unlike dislocation nucleation from a crack tip, the critical driving force for instantaneous dislocation nucleation from the perfectly flat surface is completely determined by the maximum shear resistance between atomic layers. To distinguish the

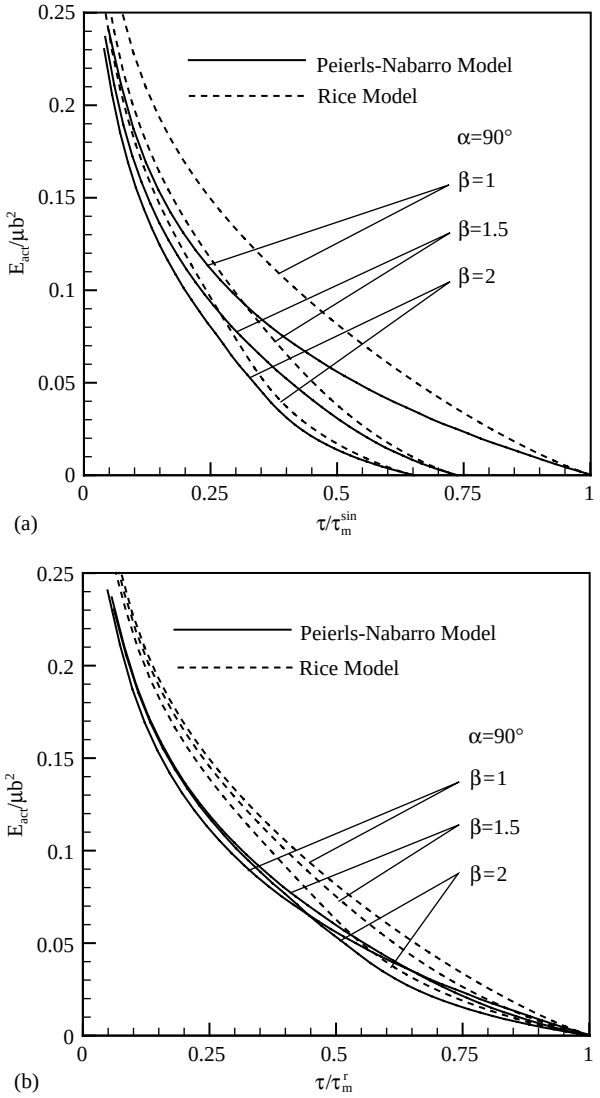

Fig. 7. Dependence of the activation energy on the shear stress for various values of parameter β: (a) the shear stress is normalized by the maximum shear stress of the sinusoidal shear resistance profile; (b) the shear stress is normalized by the maximum shear stress of the shear resistance profile.

shape effect on the activation energy for dislocation nucleation, we rescale the critical driving force with the maximum shear resistance of each individual shear resistance profile. Fig. 7b shows that the skewed shear resistance affects the activation energy, though the effects appear to be somewhat moderate for the shear resistance profiles adopted in this analysis.

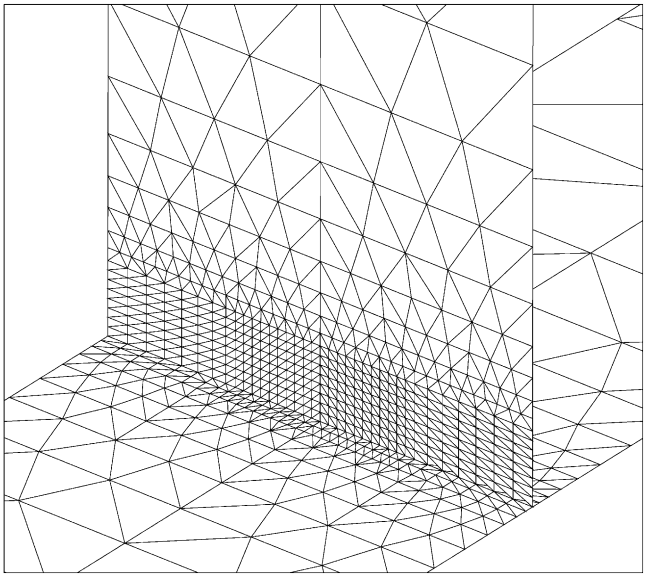

Fig. 8. Typical mesh used in the analysis. The period of the mesh is 50b. The surface is turned upside down for better visualization.

3.2. Nucleation of dislocation loops

Thermally assisted nucleation of a straight dislocation from the surface is theoretically impossible since the energy required for such an event to occur is infinite. The realistic scenario is the process of nucleation of a half-dislocation loop which can be viewed as a consequence of a localized outward protrusion of slip into an unstable saddle point configuration from the stable configuration of a straight embryonic dislocation. To obtain the bifurcation that leads to the saddle point configuration in computation, a tiny perturbation of the interlayer potential is introduced at the center of the surface so that the saddle point configuration of the dislocation loop can be activated when the stress approaches the critical value. A typical mesh used in the analysis is shown in Fig. 8. The period of the mesh is 50b. The surface is turned upside down for better visualization. The elements of optimal size are selected to ensure the results are accurate.

Fig. 9 shows the profiles of the saddle point configurations of an embryonic dislocation loop at various stress levels for slip planes of $\alpha = 90^\circ$ and 30°, respectively. The sinusoidal relation is assumed to hold in the slip direction on the slip plane. The contours represent the normalized shear displacement in the slip direction on the slip plane. The profiles of embryonic dislocations indicate that the activation process depends on the formation of Burgers vector as well as the geometry of the dislocation configuration. As the stress approaches the critical value for instantaneous nucleation of the dislocation loop, the analysis of this problem based on continuum elastic dislocation theory becomes increasingly inaccurate since the dimension of the embryonic

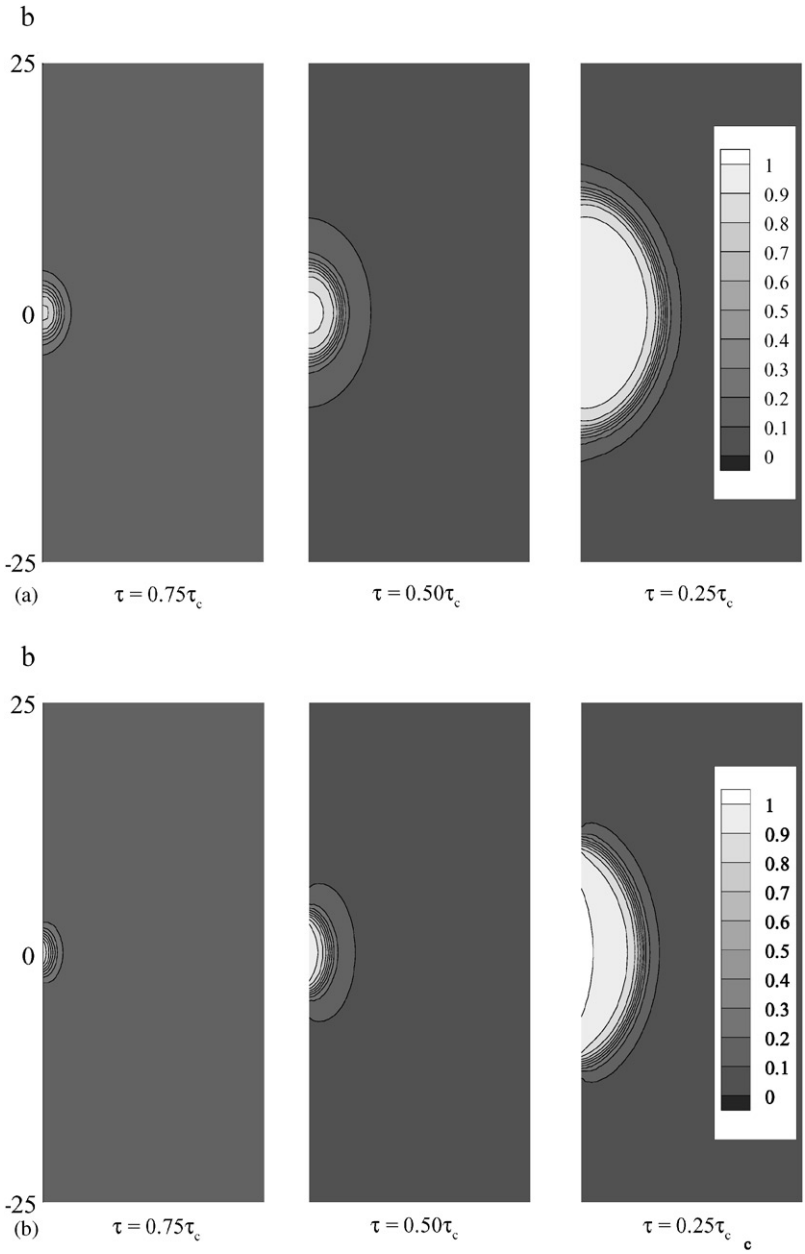

Fig. 9. The saddle point configurations of a half-dislocation loop at various stress levels. The contours represent the normalized shear displacement on the slip plane. The shear stress and slip direction are parallel to the free surface: (a) $\alpha = 90°$; (b) $\alpha = 30°$.

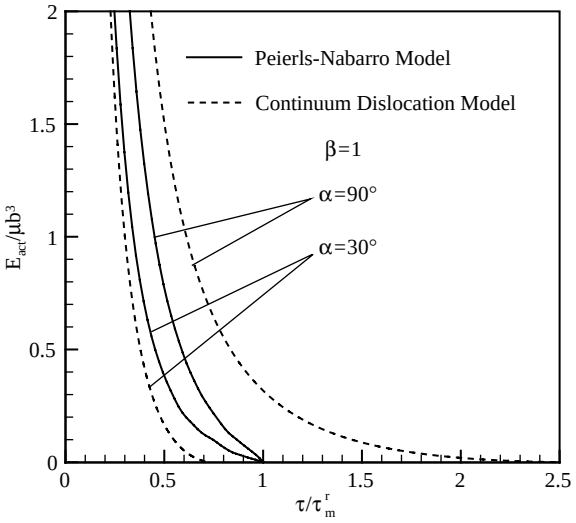

Fig. 10. Dependence of the activation energy for nucleation of half-dislocation loops on the shear stress for various inclined angles.

dislocation is comparable to the dislocation core size. Also, the dislocation loops appear to be elliptical in shape, as contrasted to the circular shape assumed in most previous analyses of this problem based on continuum elastic dislocation theory. Furthermore, the loop is more elliptical on the inclined slip plane ($\alpha = 30°$) than the vertical slip plane ($\alpha = 90°$), which can be attributed to the stronger effect of the image stress on the formation of the dislocation.

Fig. 10 shows the dependence of the activation energy on stress for nucleation of the dislocation loops for $\alpha = 30°$ and $90°$ slip planes, together with the results obtained in the appendix based on continuum elastic dislocation theory, in which the same core cutoff parameter $b/4$ is used as in the previous literature (Beltz and Freund, 1993). The significant effect of the core cutoff parameter is illustrated in Fig. 12 in the appendix, which plots the activation energy for various core cutoff parameters. A number of previous studies have estimated the activation energy required for nucleation of a dislocation based on the standard Arrhenius relation for the rate process (Fitzgerald et al., 1989; Kamat and Hirth, 1990; Rice and Beltz, 1994). Following Beltz and Freund (1993), we take activation energy to be $50kT$, where $k = 1.38 \times 10^{-23}$ J/K is Boltzmann constant and T is temperature in Kelvin. We estimate the normalized activation energy $E_{act}/\mu b^3$ at temperature $T = 300$ K for Au, Cu, Al, and Si to be 0.27, 0.23, 0.33, and 0.05, respectively. Here we take the shear modulus for Au, Cu, Al, and Si to be 31.0, 54.6, 26.5, and 68.1 GPa and the magnitude of the Burgers vector to be 2.88, 2.55, 2.86, and 3.84 Å, respectively. Not surprisingly, the result presented in Fig. 10 reaffirms previous conclusion (e.g. Kamat and Hirth, 1990) that thermal motion should be powerless in affecting nucleation of dislocation loops from the perfectly flat surface under a stress level considerably below the critical stress.

Compared with results based on continuum elastic dislocation theory, the activation energy presented here appears to rise somewhat more rapidly as the stress decreases from the critical stress, which implies the stress needs to be closer to the critical stress for thermally assisted dislocation nucleation. This result highlights, on the other hand, other alternative nucleation mechanisms, e.g., surface heterogeneities such as ledges, microcracks, and defects may significantly lower the critical stress, therefore facilitating dislocation nucleation (Xu, 2002).

4. Summary and conclusions

A previously developed variational boundary integral formulation of the Peierls–Nabarro dislocation model for three-dimensional dislocation configurations is further extended for the analysis of dislocation nucleation from a stressed crystal surface. Instead of using general elastic solutions of dislocations in a half-space, a rather straightforward approach is presented to rigorously account for the surface effect. In this approach, the surface is modeled as part of a very large crack embedded in an infinite solid and the problem is therefore solved in an equivalent system that is essentially composed of the slip plane and the crack embedded in the infinite solid. Since this approach does not require that the surface be perfectly flat, it is therefore far more advantageous in that it can be readily used to study dislocation nucleation from the surface of heterogeneities such as cracks, steps, and other quantum structures.

Depending on the surface morphology, crystallographic orientation, and loading condition, dislocation nucleation may occur in a wide variety of configurations. The basic feature of dislocation nucleation from a surface has been demonstrated through the studies of nucleation of straight screw dislocations and dislocation loops in a relatively simple geometry and loading condition. By solving the saddle point configurations of embryonic dislocations, we determined the stress-dependent activation energies required to activate dislocations from their stable to unstable saddle point configurations. Compared to previous analyses of this type of problem based on continuum elastic dislocation theory, we emphasize that the present analysis should provide more definitive solutions since it eliminates the uncertain core cutoff parameter by allowing for the existence of an extended dislocation core as the embryonic dislocation evolves. Moreover, the shape of the dislocation loop is solved by the variational principle instead of assumed to be semicircular as in previous analyses based on continuum elastic dislocation theory. The results indicate that the activation process depends on the formation of the Burgers vector as well as the geometry of the loop. As the stress approaches the critical value for instantaneous nucleation, the predictions of continuum elastic dislocation theory become increasingly unreliable. The results also further affirm that thermal motion plays no role in homogeneous dislocation nucleation from the surface under a normal stress level, which is in general markedly below the theoretical strength of materials. This highlights the importance of inhomogeneous dislocation nucleation mechanisms such as nucleation from surface heterogeneities where there are significant stress concentrations.

Finally, it is noteworthy to point out that the Peierls–Nabarro dislocation model provides an effective approach to incorporate atomistic information into a continuum approach to realistically handle the nonlinear effect associated with the extended dislocation core in relatively large systems. As a consequence, the method can reveal the effect of the interlayer shear resistance profile on nucleation processes of realistic dislocation nucleation configurations while in the analysis based on continuum dislocation theory only elastic constants and Burgers vector are relevant. This also justifies the use of more accurate atomic interlayer potentials such the general stacking fault energy surface obtained by density functional theory with local density approximation. Overall, the general methodology presented in this paper provides an effective approach to the study of fundamental dislocation mechanisms such as dislocation nucleation, mobility, intersection, cross slip in which dislocation core processes are important. The study of these mechanisms can complement conventional discrete dislocation dynamics simulations based on continuum elastic dislocation theory in which these mechanisms are implemented somewhat heuristically.

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Appendix A. Analysis of nucleation of half-dislocation loops from the surface based on continuum elastic dislocation theory

The energetics for nucleation of a half-circular dislocation loop on a inclined slip plane at a surface mentioned in the paper is analyzed based on the continuum elastic dislocation theory. Let R denote the radius of the dislocation loop, b the Burgers vector, R_0 the conventional dislocation core cut-off parameter, μ the shear modulus, and ν the Poisson's ratio. Following the previous work by Gao and Rice (1989) and Beltz and Freund (1993), the elastic strain energy of the dislocation loop may be expressed by

$$U^{\text{half}} = \frac{\mu b^2 R}{8}\frac{(2-\nu)}{(1-\nu)}\ln\left(\frac{8mR}{e^2 R_0}\right), \tag{A.1}$$

where m is a geometry-dependent energy correction factor, which, by definition, can be expressed by

$$\ln m = \frac{8}{\mu b^2 R}\frac{(1-\nu)}{(2-\nu)}\left(U^{\text{half}} - \frac{1}{2}U^{\text{full}}\right). \tag{A.2}$$

On the other hand, the elastic energy of a dislocation loop can be calculated by integrating work done in forming the dislocation loop. Hence,

$$\ln m = \frac{4}{\mu b R}\frac{(1-\nu)}{(2-\nu)}\int_{s_1}[\tau^{\text{half}} - \tau^{\text{full}}]\,\mathrm{d}A, \tag{A.3}$$

where τ^{half} is the shear stress on slip plane along the Burgers vector due to the half-loop at the surface, τ^{full} is the shear stress at the slip plane along the Burgers vector due to the full loop in the infinite solid, and s_1 is the area encircled by the half-dislocation loop.

Using the fundamental displacement field of an infinitesimal dislocation loop in the infinite medium

$$u_i(\mathbf{x}) = b_j c_{jkmn} U_{mi,n}(\mathbf{x} - \mathbf{x}') ds_k, \tag{A.4}$$

where c_{jkmn} are elastic constants, $U_{mi,n}$ are the Green's functions of a point force, and ds_k are the components of the surface encircled the dislocation loop, we can obtain the stress field of a full circular dislocation loop on the slip plane in the infinite medium as

$$\tau^{\text{full}} = -\frac{3\mu b}{4\pi(1-\nu)} \int_s \left[\frac{(1+\nu)}{3r^3} + \nu \frac{[(x_1 - x_1')\cos\alpha + (x_3 - x_3')\sin\alpha]^2}{r^5} \right] \mathrm{d}s', \tag{A.5}$$

where

$$r = \sqrt{(x_2 - x_2')^2 + [(x_1 - x_1')\cos\alpha + (x_3 - x_3')\sin\alpha]^2} \tag{A.6}$$

and s is the area encircled the full dislocation. The reference coordinates are selected so that the origin is on the surface at the center of the loop, x_2 axis is parallel to the Burgers vector, and x_3 axis is normal to the surface pointing into the medium.

The stress field due to a semicircular dislocation loop near the surface can be broken into three corresponding contributions (Bacon and Groves, 1970; Eshelby, 1979)

$$\tau^{\text{half}} = \tau^{\infty} + \tau^{I} + \tau^{s}, \tag{A.7}$$

where τ^{∞} is the stress due to the semicircular loop in the infinite elastic medium; τ^{I} is the stress due to the image semicircular loop in the infinite elastic medium; and $\tau^{s}$is the stress required to make the surface traction-free. Both τ^{∞} and τ^{I} can be conveniently obtained from Eq. (A.5) as

$$\tau^{\infty} = -\frac{3\mu b}{4\pi(1-\nu)} \int_{s_1} \left[\frac{(1+\nu)}{3r^3} + \nu \frac{[(x_1 - x_1')\cos\alpha + (x_3 - x_3')\sin\alpha]^2}{r^5} \right] \mathrm{d}s', \tag{A.8}$$

and

$$\tau^{I} = \frac{3\mu b}{4\pi(1-\nu)} \int_{s_1} \left[\frac{(1+\nu)}{3r_1^3} - \nu \frac{[(x_1 - x_1')\cos\alpha + (x_3 + x_3')\sin\alpha]^2}{r_1^5} \right] \mathrm{d}s', \tag{A.9}$$

where

$$r_1 = \sqrt{(x_2 - x_2')^2 + [(x_1 - x_1')\cos\alpha + (x_3 + x_3')\sin\alpha]^2}. \tag{A.10}$$

To obtain τ^s, we decompose the infinitesimal dislocation loop on the slip plane into two infinitesimal loops $b_1 = (0,1,0)b$, $ds_1 = (\sin\alpha, 0, 0)ds$; and $b_2 = (0,1,0)b$, $ds_2 = (0,0,\cos\alpha)ds$. Let du_i^s and dv_i^s, $i = 1,2,3$, denote the displacement components associated with these two infinitesimal dislocation loops. They are given by (Bacon and Groves, 1970; Eshelby, 1979)

$$\mathrm{d}u_1^s = k_1 \left\{ 2(1-v)\left[\left(\frac{1}{r_2}\right)_{,2} - r_{2,112}\right] - x_3'\left(\frac{x_3}{r_2}\right)_{,112} + 2(1-v)(1-2v)\left(\frac{x_1}{r_2 + x_3 + x_3'}\right)_{,12}\right\}, \tag{A.11}$$

$$\mathrm{d}u_2^s = k_1 \left\{ 2(1-v)\left[\left(\frac{1}{r_2}\right)_{,1} - r_{2,212}\right] - x_3'\left(\frac{x_3}{r_2}\right)_{,212} + 2(1-v)(1-2v)\left(\frac{x_1}{r_2 + x_3 + x_3'}\right)_{,22}\right\}, \tag{A.12}$$

$$\mathrm{d}u_3^s = k_1 \left\{ 2(1-v)\left[2x_3'\left(\frac{1}{r_2}\right)_{,12} - r_{2,312}\right] - x_3'\left(\frac{x_3}{r_2}\right)_{,312} - 2(1-v)(1-2v)\left(\frac{x_1}{r_2 + x_3 + x_3'}\right)_{,32}\right\}, \tag{A.13}$$

$$\mathrm{d}v_1^s = k_2 x_3' \left[-2v\left(\frac{1}{r_2}\right)_{,12} + \left(\frac{x_3}{r_2}\right)_{,123}\right], \tag{A.14}$$

$$\mathrm{d}v_2^s = k_2 x_3' \left[-2v\left(\frac{1}{r_2}\right)_{,22} + \left(\frac{x_3}{r_2}\right)_{,223}\right], \tag{A.15}$$

$$\mathrm{d}v_3^s = k_2 x_3' \left[(2v-4)\left(\frac{1}{r_2}\right)_{,32} + \left(\frac{x_3}{r_2}\right)_{,323}\right], \tag{A.16}$$

where

$$k_1 = \frac{b\sin\alpha \mathrm{d}s}{4\pi(1-v)}, \quad k_2 = \frac{b\cos\alpha \mathrm{d}s}{4\pi(1-v)}, \tag{A.17}$$

and

$$r_2 = \sqrt{(x_1 - x_1')^2 + (x_2 - x_2')^2 + (x_3 + x'^3)^2}. \tag{A.18}$$

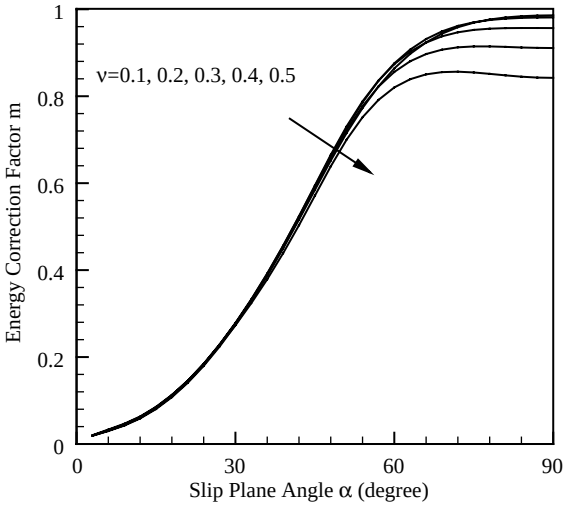

Fig. 11. Dependence of the energy correction factor on the angle of the slip plane.

The corresponding stress components can then be calculated from

$$\tau^s_{32} = \mu \int_{s_1} \frac{\partial(\mathrm{d}u^s_3 + \mathrm{d}v^s_3)}{\partial x_2} + \frac{\partial(\mathrm{d}u^s_2 + \mathrm{d}v^s_2)}{\partial x_3}\,\mathrm{d}s', \tag{A.19}$$

$$\tau^s_{12} = \mu \int_{s_1} \frac{\partial(\mathrm{d}u^s_1 + \mathrm{d}v^s_1)}{\partial x_2} + \frac{\partial(\mathrm{d}u^s_2 + \mathrm{d}v^s_2)}{\partial x_1}\,\mathrm{d}s' \tag{A.20}$$

and

$$\tau^s = -\tau^s_{32}\cos\alpha + \tau^s_{12}\sin\alpha. \tag{A.21}$$

The energy correction factor m can now be calculated from Eq. (A.3). The four-fold integrals were carried out numerically via 40-points Gauss–Kronrod rule. Fig. 11 plots the energy correction factor as a function of angle α for various Poisson's ratios.

It should be noted that the calculation of m requires appropriate treatment of the singularities involved in the integration. Normally the presence of the singularity of the inverse distance from the perimeter of the dislocation loop requires an elastic core cutoff of the dislocation so as the calculated energy of the dislocation loop is bounded. Here the choice of the core cutoff is avoided by calculating the bounded integral of the difference in stress $\tau^{\infty} - \tau^{\mathrm{full}}$. The singularities of certain integrants are eliminated in the integration based on the Anderson and Rice (1987) approach. By subtracting the null stress of uniformly displacement equal to the Burgers vector, the integration can be switched on the integrating area from s_1 to $\overline{s_1}$ with the change of the sign. Here $\overline{s_1}$ is the outside area of the semicircular loop.

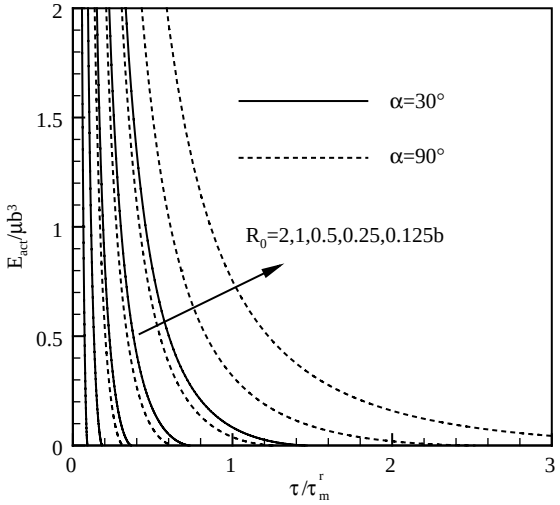

Fig. 12. The activation energy as a function of stress for various core cutoff parameters.

To obtain the critical condition for nucleation of a semicircular dislocation loop, we write the total energy

$$E = \frac{\mu b^2 R}{8}\frac{(2-\nu)}{(1-\nu)}\ln\left(\frac{8mR}{e^2 R_0}\right) - 0.5\pi R^2 \tau b \sin\alpha, \tag{A.22}$$

and render it stationary,

$$\frac{\partial E}{\partial R} = \frac{\mu b^2}{8}\frac{(2-\nu)}{(1-\nu)}\ln\left(\frac{8mR}{eR_0}\right) - \pi R\tau b \sin\alpha = 0, \tag{A.23}$$

$$\frac{\partial^2 E}{\partial R^2} = \frac{\mu b^2}{8R}\frac{(2-\nu)}{(1-\nu)} - \pi\tau b \sin\alpha = 0, \tag{A.24}$$

where the first condition is the equilibrium condition, and the second condition is a stability criterion. The critical stress and the critical radius at which dislocation nucleates instantaneously can be obtained by solving the above equations. For a given stress less than the critical value, Eq. (A.23) has two solutions of R, one solution corresponding to the local minimum of the total energy and the other solution corresponding to the local maximum of the energy. The energy difference between them is the activation energy required for thermally assisted nucleation of the semicircular dislocation loop. Fig. 12 plots the activation energy as a function of stress for various core cutoff parameters. It is evident that the result is sensitively dependent on the core cutoff parameter. This may be conveniently explained by plotting the equilibrium solution of R as a function of stress for a selected typical case in Fig. 13. It shows that the critical radius of the dislocation loop is on the order of the dislocation core size, therefore indicating that the obtained energetics of dislocation nucleation is unreliable because of the limitation of continuum elastic dislocation theory at the core region.

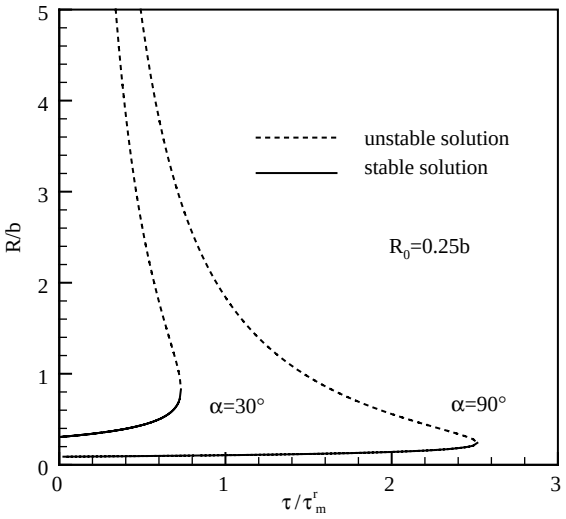

Fig. 13. The radius of the dislocation loop at equilibrium as a function of stress. The solid lines represent stable solutions. The dashed lines represent unstable solutions.

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