DISLOCATION EMISSION AT SURFACES

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ABSTRACT

An exact expression for the elastic energy associated with a semicircular shear dislocation loop emanating from a free surface, such as that of a stressed thin film, is derived (within continuum dislocation theory) and compared with earlier approximations. The energy required to activate a semicircular dislocation loop into its unstable "saddle-point" configuration is then re-calculated, based on the modified expression for the self-energy. It is found that the shear stress necessary to emit a loop, as a function of temperature, is almost 50% less than earlier estimates. The effects of ledges on the surface, as well as loop geometry, are discussed. The principal drawback to this type of calculation is pointed out, namely, that the critical radius of an incipient dislocation loop can be on the order of one atomic spacing, which is too small for a continuum theory to be valid.

INTRODUCTION

The behavior of dislocations in materials with electronic applications has been a topic of long-standing interest, because of the effect of dislocations on electrical properties. One example is the appearance of misfit dislocations in layers which have been epitaxially grown onto a substrate with a slightly different lattice parameter (see Figure 1). Invariably, this process involves materials which have been chosen primarily for their electronic properties, such as the band-gap width, the resistivity, and the type of charge carrier, and not for reasons related to their lattice parameters. The resulting strain that occurs is commonly relieved by the formation of misfit dislocations. If these dislocations are prevented from forming, the stress in the film is not necessarily detrimental -- the stress affects the electronic properties in a predictable manner and is often controlled by exploiting differences in lattice parameters, and subsequently changes in temperature, via a difference in thermal expansion coefficients.

The appearance of misfit dislocations during epitaxial growth has been observed experimentally to coincide with the attainment of a critical thickness, which in turn depends on the misfit strain, elastic constants, and the orientation of the various slip systems involved (e.g., Matthews [1], Hull *et al.* [2], and Houghton *et al.* [3]). Theoretical studies of this problem have established the validity of the critical thickness concept, starting with Frank and van der Merwe [4] and leading up to recent work by Freund *et al.* [5-7]. Most analyses to date, however, have concentrated on the stability of a single *pre-existing* threading dislocation, or a threading dislocation in the presence of an array of other dislocations. Another issue that must be addressed more carefully is the actual nucleation of dislocations. The prevention of dislocation formation at the source, rather that the reduction of already-formed dislocations, constitutes an alternative approach for defect minimization.

A possible location at which dislocations are actually generated during film growth is the film surface. The primary purpose of this paper is to re-examine the process of dislocation nucleation at a crystal surface, in light of recent developments with the theory of dislocation formation. First, an expression for the shear stress due to a general shear dislocation loop perpendicular to a free surface is presented, and immediately utilized to derive an accurate expression for the elastic self energy of a semicircular loop. Next, conditions for nucleation of the semicircular loop are worked out in the continuum framework described by Hirth [8] and subsequently by Fitzgerald *et al.* [9], but with the modified expression for the self energy of the loop. Finally, the potential utility of accurate expressions for stresses in connection with atomistic-type calculations is pointed out.

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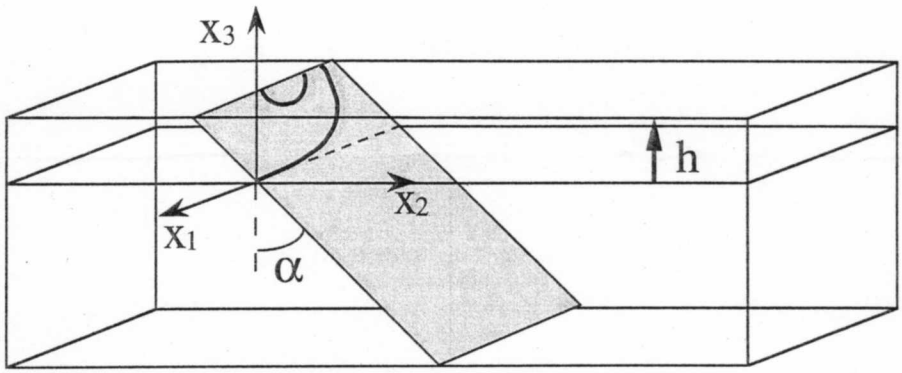

Figure 1. Schematic of an epitaxial substrate-layer system, with a slip plane (shaded) containing a threading dislocation segment joining an interfacial misfit with the surface, as well as an incipient loop.

THE ENERGY OF A SEMICIRCULAR DISLOCATION LOOP AT A FREE SURFACE

We present here a calculation of the self energy of a dislocation loop emerging perpendicularly from a free surface in an isotropic, elastic half-space. To understand the nature of the principal result of this section, recall that the elastic self energy for a full circular dislocation loop of radius r in an *infinite* elastic solid is given by [10]

$$U^{full} = \frac{\mu b^2 r}{4} \frac{(2-\nu)}{(1-\nu)} \ln\left(\frac{8r}{e^2 r_0}\right) \tag{1}$$

where μ is the shear modulus, b is the Burgers vector, ν is Poisson's ratio, r_0 is the core cut-off radius. In an analogous fashion to what Gao and Rice [11] have done for a general dislocation loop ahead of a crack, we will show here that the energy of the semicircular loop of radius r emerging from the free surface has the form

$$U^{half} = \frac{\mu b^2 r}{8} \frac{(2-\nu)}{(1-\nu)} \ln\left(\frac{8mr}{e^2 r_0}\right) \tag{2}$$

where m is a geometry-dependent correction factor. Early analyses of dislocation loop nucleation at cracks [12], as well as most analyses of nucleation at a free surface to date [8, 9, 13], begin with the assumption that m=1, i.e., by estimating U^{half} as half the energy of a full circular loop.

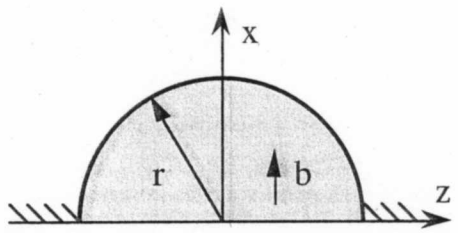

Figure 2. Geometry of an emergent semicircular shear dislocation loop at a free surface. The slip plane, as well as the Burgers vector, are perpendicular to the surface.

Simple physical arguments may be invoked to deduce that $0 < m < 1$. The former inequality is expected because the energy becomes unbounded as $m \to 0$. The latter inequality follows from considering the formation of a full circular dislocation loop in an infinite solid by bonding together two half-spaces, each containing a semicircular loop with the same radius (i.e., attaching the configuration in Figure 2 with its reflection about the z axis). The resultant energy must be the sum of the two energies of the half-space configurations, as well as the positive work that must be done on the free surfaces to make the two spaces match. I.e., the inequality $2U^{half} < U^{full}$ must hold, which is consistent with $m < 1$.

The calculation of m follows the procedure outlined by Gao and Rice [11] and Anderson and Rice [14] in that (1) and (2) may be combined and re-arranged to give the following expression for m:

$$\ln(m) = \frac{8}{\mu b^2 r}\frac{(1-\nu)}{(2-\nu)}\left(U^{half} - \frac{1}{2}U^{full}\right) \tag{3}$$

The difference in elastic energy between the dislocation emanating from the free surface and one half that of the corresponding full loop in an infinite body is calculated by integrating the corresponding difference in work done in forming the dislocations, $-(b/2)[\tau^{half}(x,0,z)-\tau^{full}(x,0,z)]$, over the entire area of the half-loop. The integral of the stress *difference* converges, even though the domain of integration extends up to and includes the dislocation line itself. Hence, an expression may be written for m that is independent of any core cutoff procedure:

$$\ln(m) = -\frac{4}{\mu br}\frac{(1-\nu)}{(2-\nu)}\int_A \left[\tau^{half}(x,0,z) - \tau^{full}(x,0,z)\right] dA \tag{4}$$

where τ^{half} and τ^{full} are, respectively, exact expressions (within continuum elastic dislocation theory) for the shear stress of the half-loop at the free surface and the full loop in an infinite solid. A common factor of r appears upon non-dimensionalization of the integral in (4). Hence, m depends only on ν for a given geometry.

Let a general Burgers displacement $\delta(x, z)$ (defined as $u_x^+(x,z) - u_x^-(x,z)$, where u_x^+ and u_x^- denote the displacement immediately above and below the slip plane) exist on a slip plane; eventually, $\delta(x, z)$ is replaced by b in a circular dislocated region when evaluating the integral in Equation (4). The shear stress difference associated with a dislocation loop in an infinite solid is [15]

$$\tau^{half} - \tau^{full} = -\frac{2\mu x}{4\pi(1-\nu)}\int_{-\infty}^{\infty}\frac{\delta(0^+,\tilde{z}) - \delta(0^+,z)}{[x^2+(z-\tilde{z})^2]^{3/2}}d\tilde{z} - \frac{2\mu}{4\pi(1-\nu)}\int_{-\infty}^{\infty}\int_{0^+}^{\infty} K^I(x,z;\tilde{x},\tilde{z})\,\delta(\tilde{x},\tilde{z})\,d\tilde{x}d\tilde{z}$$

$$+\frac{2\mu}{4\pi(1-\nu)}\int_{-\infty}^{\infty}\int_{0}^{\infty}\left[\frac{15\tilde{x}(\tilde{x}+x)^2}{R^7} - \frac{3\tilde{x}}{R^5}\right]\{\delta(\tilde{x},\tilde{z}) - \delta(0^+,z)\}\,d\tilde{x}d\tilde{z} \tag{5a}$$

where the operator $K^I(x, z; \tilde{x}, \tilde{z})$ is given by

$$K^I(x,z;\tilde{x},\tilde{z}) \equiv \frac{\tilde{x}+x}{R^3}\frac{\partial}{\partial\tilde{x}} + (1-\nu)\frac{\tilde{z}-z}{R^3}\frac{\partial}{\partial\tilde{z}} \tag{5b}$$

and $R \equiv \sqrt{(x+\tilde{x})^2+(z-\tilde{z})^2}$. The four-fold integral in (4) was carried out numerically via a 21-point Gauss-Kronrod rule with a relative error in the result of 10^{-4}. When $\nu = 0.3$, $m = 0.546$ and when $\nu = 0.218$, as appropriate for silicon, $m = 0.535$. In principle, analogous procedures to that presented here for the shear loop perpendicular to the free surface may be used to calculate m for general loop shapes, with arbitrary slip plane and Burgers vector orientations.

NUCLEATION OF A SEMICIRCULAR LOOP

The calculation presented in this section essentially follows that of Hirth [8], in which the energy associated with an incipient semicircular dislocation loop is determined, and then rendered stationary in order to find the critical radius of the loop, beyond which the loop will unstably enlarge. It is assumed that the dislocated plane, as well as the direction of slip, are perpendicular to the crystal surface (as in Figure 2). The loading is assumed to be a uniform, remotely applied shear stress τ. It is also assumed that the dislocation is not dissociated, i.e., that the stacking fault energy does not contribute in any fashion. The total energy of the loop then consists of three terms:

$$E = U^{\text{half}} + U^{\text{ledge}} - W^{\text{stress}}, \tag{6}$$

where U^{half} is as discussed in the previous section, U^{ledge} is the energy of the ledge that is created (or removed) at the surface due to the intersecting dislocated plane, and W^{stress} is the work done by the applied load

$$W^{\text{stress}} = \pi r^2 \tau b/2 \tag{7}$$

which is the product of the Peach-Koehler force τb and its work-conjugate displacement, the area that the dislocation has swept out.

The ledge energy is commonly written as

$$U^{\text{ledge}} = \pm 2\gamma b r, \tag{8}$$

where the positive value is used for ledge creation, the negative sign is taken for ledge removal, and γ is the surface energy. This is a questionable representation, since it is difficult to define a true thermodynamic surface energy for an area that is only one atomic spacing wide. It is perhaps best to interpret the single quantity γb as an effective energy per unit ledge-length. Following references [9] and [13], we estimate $\gamma = \mu b/8$. The conclusions noted later are relatively insensitive to the choice of this parameter.

At absolute zero, the condition for dislocation emission is given by rendering the total energy stationary,

$$\frac{\partial E}{\partial r} = \frac{\mu b^2}{8}\frac{(2-\nu)}{(1-\nu)}\ln\left(\frac{8mr}{er_0}\right) \pm 2\gamma b - \pi r \tau b = 0 \tag{9a}$$

$$\frac{\partial^2 E}{\partial r^2} = \frac{\mu b^2}{8r}\frac{(2-\nu)}{(1-\nu)} - \pi\tau b = 0 \tag{9b}$$

where the latter condition is a stability criterion, i.e., it insures that the energy *decreases* as the loop expands. Solving for the critical stress for which the loop would spontaneously enlarge gives $\tau^0_{\text{crit}} = 0.505\mu$, assuming ledge creation, or $\tau^0_{\text{crit}} = 0.0837\mu$, assuming ledge removal. If it is assumed that $m = 1$, then the critical stresses increase to 0.944μ and 0.163μ, respectively. Thus an accurate expression for the self-energy of a loop near the free surface leads to a decrease, by almost a factor of 2, of the critical stress necessary to homogeneously nucleate the loop. All the calculations presented here use $r_0 = b/4$ and $\nu = 0.218$.

The nucleation process, however, realistically occurs at temperatures well above absolute zero. The critical stress for emission may then be determined via an activation energy concept. Assume that the local shear stress is less than τ^0_{crit}. There will then exist *two* solutions to (9a) - one corresponding to a local minimum of the total energy ($r = r_1$), and the second corresponding to a local maximum of energy ($r = r_2$). In general, $r_2 > r_1$. The energy difference between these two states, $\Delta E \equiv E(r_2) - E(r_1)$, defines the activation energy. If energy from thermal vibrations is sufficient to overcome this activation energy, then the

dislocation loop is spontaneously emitted. The activation energy is plotted in Figure 3a for m = 0.535 as well as m = 1. Qualitatively, the behaviour is as expected: the energy barrier to dislocation emission decreases as the applied stress approaches its maximum value of τ^0_{crit}. The decrease in activation energy is relatively sharp for $\tau < \tau^0_{crit}$, but as the limiting stress is approached, the rate of decrease slows, suggesting that thermal vibrations may be sufficient to emit dislocations for a certain stress range below τ^0_{crit}. More importantly, note that using an appropriate value of m leads to significantly reduced activation energies -- for most loads there is more than a factor of 2 difference. Additionally, when it is assumed that the emitting dislocation is *removing* a ledge at the surface, that the energy barrier is significantly reduced.

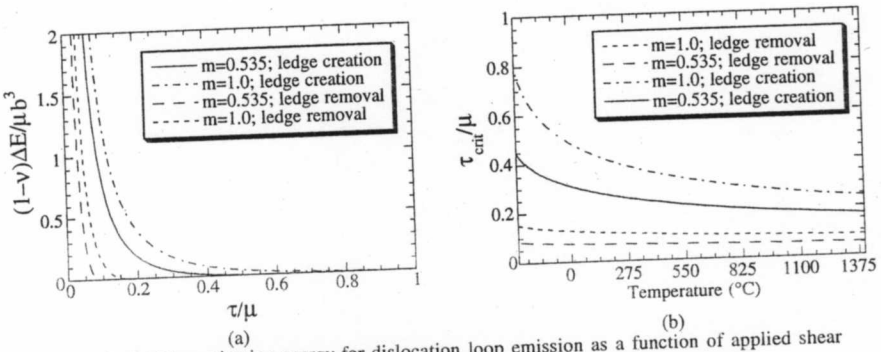

Figure 3. (a) The activation energy for dislocation loop emission as a function of applied shear stress. (b) Critical stress required to emit a dislocation loop as a function of temperature.

Now that the activation energy required for the emission of a dislocation from the surface is determined, we need some estimate of what energy is available for the process. An estimate by Rice and Beltz [17] is based on a standard Arrhenius-relation between the nucleation rate and $\Delta E/kT$ (k is Boltzmann's factor), and assumes that a "reasonable" nucleation rate is given by 1 dislocation per second per millimeter of crack front. This elementary calculation leads to an available energy of $43kT$. A similar argument by Hirth [8] gives $88kT$ of available energy. Given the uncertainty present in this type of calculation, we follow Fitzgerald *et al.* [9] and assume that the available energy is $50kT$. Based on the activation energies in Figure 3a, the stress necessary to emit a dislocation loop as a function of temperature is given in Figure 3b. As expected, a proper choice for m reduces the shear stress by a factor of about 2. Furthermore, the critical stress for a nucleation process associated with removal of a ledge at the surface is about 3 times less than the stress when the ledge is created.

VALIDITY OF THE CONTINUUM APPROACH

The largest source of uncertainty in the type of calculation presented in the previous section is the fact that a continuum-based description of a dislocation is used over length scales that are much too small. For example, the critical radius for dislocation emission at absolute zero, when a ledge is being removed, is $1.038b$, according to the theory outlined in the previous section. When a ledge is being created, the critical radius reduces to $0.505b$ (these numbers assume m= 0.535). In the latter case, the elastic energy predicted by (2) is *negative*. To realistically calculate the energy associated with a dislocation loop this small, an atomistic model is necessary to treat the core.

Furthermore, the expressions used in this communication assume that the dislocation is fully formed. One example of a situation where these considerations have been addressed more carefully is the problem of dislocation nucleation at crack tips, which up until recently has also relied on continuum energy expressions for dislocations. Recent analyses of dislocation

formation at cracks have suggested that the Burgers displacement (i.e., the function $\delta(x, z)$ discussed earlier), as well as the relative position of the dislocation core, should be regarded as configurational parameters when modeling dislocation nucleation and evaluating the activation energy. A reasonably exact treatment of this phenomenon has been given by Rice *et al.* [18] that makes use of the Peierls-Nabarro dislocation model [19]. In that treatment, the two-dimensional elasticity problem of a traction-free crack with a periodic, nonlinear stress versus displacement relation being satisfied as a boundary condition along a slip plane ahead of the crack tip is solved. Once this interfacial "constitutive" relation is specified (it could be as simple as the Frenkel sinusoidal law), and the elasticity problem solved, there is no need for the core-cutoff parameter. The advantage of this method is that it allows for the existence of an extended dislocation core during nucleation, and eliminates uncertainty involved when using expressions derived with the usual core cutoff procedures.

The same types of ideas may be applied to the problem of dislocation nucleation at a surface [20]. Although the problem may be quite straightforwardly worked out for the two dimensional case (yielding an activation energy per unit length of dislocation parallel to the surface), the three-dimensional case appears to be quite complex. The problem would essentially involve finding a saddle-point dislocation configuration at the surface, i.e., a function $\delta(x, z)$ that renders the total energy stationary. Numerical solutions to this problem within the Peierls-Nabarro framework would involve a suitable form of Equation (5).

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