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DISLOCATION THREADING THROUGH AN EPITAXIAL FILM: AN ANALYSIS BASED ON THE PEIERLS-NABARRO CONCEPT

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ABSTRACT

The Peierls-Nabarro theory of crystal dislocations is applied to estimate the critical thickness of a strained layer bonded to a substrate for a given mismatch strain. Previous analyses were based on the continuum theory of elastic dislocations, and hence depended on the artificial core cutoff parameter r_0. The Peierls-Nabarro theory makes use of an interplanar shear law, which leads to a more realistic description of the stresses and displacements in the vicinity of a dislocation core, thus eliminating the need for the core cutoff parameter. The dependence of the critical layer thickness on the mismatch strain in films with a diamond cubic lattice is found to be similar to that predicted by the continuum elastic dislocation theory, provided that a core cutoff radius equal to about one-tenth the Burgers displacement is used.

INTRODUCTION

The appearance of misfit dislocations in layers which have been epitaxially grown onto a substrate with a slightly different lattice parameter has been a topic of long-standing interest, due to the detrimental effect on the electrical properties of the materials involved. 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., work by Matthews [1], Hull *et al.* [2,3], and Houghton *et al.*, [4]). Theoretical studies of this problem have confirmed the validity the critical thickness concept, the earliest being due to Frank and van der Merwe [5]. Matthews [1], and more recently Freund [6], assumed the substrate to be a half-space, on which is deposited a layer having the same crystal structure and elastic properties as the substrate, but having a slightly different lattice parameter. The misfit dislocation was considered to form via the motion of a "threading" dislocation segment, shown schematically in Figure 1. Freund's analysis continues by observing that if the misfit dislocation were to form via this mechanism, then the curved threading dislocation segment shown in Figure 1 would translate in a self-similar manner. Thus, if the segment were to advance by a unit distance, the net result is the addition of a unit distance of material with a misfit dislocation far behind the threading segment, and the removal of a unit distance of un-dislocated material far ahead of the segment. In this manner, the problem may be analyzed in terms of the two-dimensional situations, far ahead and behind the threading segment. Two competing effects are taken into account when calculating the driving force on the dislocation segment: the work done by the layer stress (i.e., the Peach-Koehler force) in driving the segment forward, and the self energy of the resultant misfit dislocation near the free surface.

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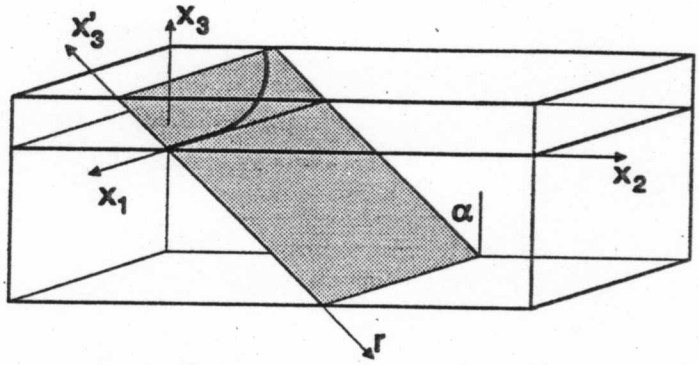

Figure 1. Configuration of the substrate-layer system, with a slip plane (shaded) containing a threading dislocation segment joining an interfacial misfit dislocation and the free surface.

The analyses mentioned thus far have made use of continuum dislocation theory, in which a dislocation is treated as a line singularity within a linear elastic solid (the so-called Volterra dislocation). An important input to the problem is the elastic energy of a dislocation parallel to a free surface, which has been calculated by Freund [6] as

$$W_{disl} = \frac{\mu b^2 \cos^2\phi}{4\pi(1-\nu)}\left\{\ln\left(\frac{2h}{r_0}\right) - \frac{1}{2}\cos 2\alpha - \frac{(1-2\nu)}{4(1-\nu)}\right\} + \frac{\mu b^2 \sin^2\phi}{4\pi}\ln\left(\frac{2h}{r_0}\right) \quad (1)$$

where μ is the shear modulus, ν is Poisson's ratio, ϕ is the orientation of the Burgers vector in the glide plane ($\phi = 0°$ corresponds to the misfit segment being of pure edge character while $\phi = 90°$ corresponds to the misfit segment being of pure screw character), α is the angle between the slip plane and the surface normal, h is the thickness of the strained layer (i.e., the distance of the dislocation from the surface), and r_0 is the core cutoff radius. Most dislocation problems do not depend heavily on the core cutoff radius; indeed, this is a rather intuitive statement because the elastic energy depends only logarithmically on r_0. In many applications, r_0 is approximated as b; however, more sophisticated schemes exist for estimating r_0 [7] which suggest that it should be regarded as low as $b/4$ in some cases. The critical thickness result obtained by Freund [6], which is essentially the same as Matthew's original result, depends strongly on r_0.

THE PEIERLS-NABARRO DISLOCATION MODEL

Assume the existence of a Peierls-type shear stress τ versus relative atomic displacement Δ relation, such as the sinusoidal representation in Figure 2; Δ denotes the translation of one atomic plane relative to another at the slip surface. The curve gives the shear stress needed to locally shear atoms with respect to one another on a given slip plane, and is the fundamental input to the Peierls-Nabarro dislocation model [8,9]. The initial slope of such a curve corresponds to an appropriate shear modulus. The parameter b is the length of a Burgers vector and represents the periodicity of the stress-displacement relation. The integral of such a curve from $\Delta = 0$ to the unstable equilibrium position at which the shear stress next vanishes (at $\Delta = b/2$ in simple cases) is known as the *unstable stacking energy*, denoted here by γ_{us} [10-12].

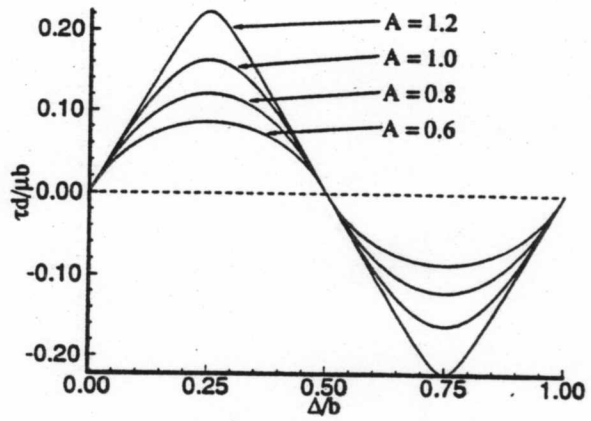

Figure 2. Forms used for the shear stress versus relative atomic displacement, based on Equation (2).

In this paper, we adopt the following form of τ versus Δ, valid for $0 \leq \Delta \leq b/2$:

$$\tau(\bar{\Delta}) = \frac{\mu b}{2\pi d} \begin{cases} \left(\sqrt{\omega} - \sqrt{\rho\bar{\Delta}^2 - \frac{1}{2}\rho\bar{\Delta} + \omega}\right) & \text{if } A > \pi^2/12, \\ \left(-\sqrt{\omega} + \sqrt{\rho\bar{\Delta}^2 - \frac{1}{2}\rho\bar{\Delta} + \omega}\right) & \text{if } A < \pi^2/12. \end{cases} \tag{2}$$

where $\bar{\Delta} \equiv \Delta/b$, $A \equiv 2\pi^2\gamma_{us}d/\mu b^2$, and ω and ρ are constants which satisfy the following pair of nonlinear algebraic equations:

$$A = \frac{2\pi^2 d}{\mu b}\int_0^{1/2} \tau(\bar{\Delta})d\bar{\Delta}, \qquad \frac{\rho}{\sqrt{\omega}} = \begin{cases} 8\pi & \text{if } A > \pi^2/12; \\ -8\pi & \text{if } A < \pi^2/12. \end{cases} \tag{3}$$

The former is required by the definition of A, and the latter enforces the fact that the initial slope of the function $\tau(\bar{\Delta})$ is $\mu b/d$. By symmetry, (2) is extended to obtain a function $\tau(\Delta)$ valid for *all* Δ.

With the exception of the slip plane, the material is taken as an isotropic, linear elastic solid with shear modulus μ and Poisson's ratio ν. Define δ as the displacement discontinuity on a mathematical cut coincident with the slip plane. We relate δ to the displacement Δ of the atomic planes at $y = \pm d/2$ by

$$\delta = u_x^{(+)} - u_x^{(-)} = \Delta - \frac{\tau d}{\mu} \tag{4}$$

where d is the interplanar spacing. This idealized cut represents the slip plane. By adding to the displacement discontinuity δ across the cut (in what is otherwise considered a linear elastic continuum) the additional "elastic" displacement $\tau d/\mu$, we simulate approximately the relative displacement $\Delta = \delta + \tau d/\mu$ between atomic planes a distance d apart. The next step is to enforce mechanical equilibrium along the slip plane, which is discussed in further detail in the next section for the case of a dislocation near a free surface.

The energy of the Peierls dislocation is calculated as the sum of two contributions: the elastic strain energy stored in the two half-crystals, which is analogous to the strain energy of the Volterra dislocation, and the "misfit" energy associated with the nonlinear

distortion of bonds across the slip plane. For a dislocation in an infinite crystal, the former is written as

$$W_{disl}^{el} = -\frac{1}{2}\int_{-\infty}^{\infty}[\tau(x) - \tau_0]\delta(x)dx \tag{5}$$

and the latter is written as

$$W_{disl}^{core} = \int_{-\infty}^{\infty}\Phi[\delta(x)]dx \tag{6}$$

where the energy quantity $\Phi(\delta)$, along with a related quantity $\Psi(\Delta)$, are defined such that $\tau d\delta = d\Phi$ and $\tau d\Delta = d\Psi$. Any pre-existing shear stress is given by τ_0. If the slip plane intersects a free surface, then the limits of integration must be appropriately modified.

SOLUTIONS FOR DISLOCATIONS NEAR FREE SURFACES

As with previous models of threading dislocations, it is assumed that there is a uniformly stressed thin layer bonded to an (initially) stress-free substrate. Consider the coordinate system shown in Figure 1. Since the crystal structures of the film and substrate are assumed to be identical, they share common slip planes. The slip plane to be analyzed is assumed to contain the x_1 axis and to lie at an angle α with respect to the x_3 axis. In the absence of any dislocations, the film (having shear modulus μ and Poisson's ratio ν) has a uniform isotropic extension, parallel to the plane of the interface. The extensional strain, denoted by ϵ_0, is set by the difference in lattice parameters of the substrate and the film, and gives rise to the stress components

$$\sigma_{11} = \sigma_{22} = \frac{2\mu(1+\nu)\epsilon_0}{(1-\nu)}, \qquad \sigma_{33} = 0 \tag{7}$$

The Peierls-Nabarro integral equation is based on the shear stress acting on the slip plane in the direction of the dislocation slip. Making the transformation leads to

$$\tau_0 = \frac{2\mu\epsilon_0(1+\nu)\sin\alpha\cos\alpha\cos\phi}{(1-\nu)} \tag{8}$$

The applied stress τ_0 is referred to a new coordinate system defined such that $r = -x_3'$. Thus, the film occupies $-h\sec\alpha \le r \le 0$ and the substrate occupies $r \ge 0$.

As discussed earlier, assume that a threading dislocation has passed and has laid down an interfacial misfit dislocation. Because of the discontinuity in τ_0 that occurs when r switches signs, a step function $U(r)$ is introduced such that $U = 1$ for $r < 0$ and $U = 0$ for $r \ge 0$. The Peierls-Nabarro integral equation is thus written as

$$\tau[\delta(r)] = \tau_0 U(r) - \frac{\mu}{2\pi(1-\nu)}\int_{-h\sec\alpha}^{\infty} T(r,s,\alpha,\phi)\frac{d\delta(s)}{ds}ds \tag{9}$$

where

$$T(r,s,\alpha,\phi) = T_{edge}\cos^2\phi + (1-\nu)T_{screw}\sin^2\phi \tag{10}$$

and $\mu b T_{edge}/2\pi(1-\nu)$ and $\mu b T_{screw}/2\pi$ give the shear stress at r due to a dislocation at s (defined identically to r). This stress distribution has been determined by Freund and Barnett [13]. Solutions to (9), as well as the numerical procedure for solving it, are discussed in further detail elsewhere [14].

CALCULATION OF THE CRITICAL THICKNESS

The critical thickness is said to be achieved when the total work associated with the unit advance of a threading dislocation is zero, namely,

$$W_{disl}^{el} + W_{disl}^{core} + W_{layer} = 0 \tag{11}$$

The first two terms comprise the energy of the misfit dislocation and the last term is the work per unit length done by the film stress during formation of the dislocation,

$$W_{layer} = -\int_0^{h \sec \alpha} \tau_0 \delta(x) dx = -\int_0^{h \sec \alpha} \frac{2\mu\epsilon_0(1+\nu)\sin\alpha\cos\alpha\cos\phi}{(1-\nu)}\delta(x)dx \tag{12}$$

The criterion assumes that the film/substrate system is infinite in the x_1-x_2 plane (in order to neglect edge-effects), and that the threading segment advances in a self-similar fashion. As mentioned earlier, the threading process may be likened to the removal of a segment of material of unit thickness from far ahead of the dislocation, and adding this segment far behind the threading segment. Consequently, only two-dimensional energy expressions are required in (11). Enforcing (11) leads to the following relation between the layer thickness and the mismatch strain:

$$\epsilon_0 = \frac{(1-\nu)[W_{disl}^{el}(\epsilon_0, h_c, A, \nu, \alpha, \phi) + W_{disl}^{core}(\epsilon_0, h_c, A, \nu, \alpha, \phi)]}{2\mu(1+\nu)\sin\alpha\cos\alpha\cos\phi\int_0^{h_c \sec\alpha}\delta(x)dx} \tag{13}$$

Unfortunately, the preceding equation cannot be solved explicitly for ϵ_0 or h_c. An iterative procedure is necessary. However, this presents no particular difficulties since the right hand side of (13) is weakly dependent upon ϵ_0.

In order to make a direct comparison of critical thickness results with those published in earlier work by Freund [6], we have taken $\alpha = \arcsin\sqrt{1/3} = 35.2644°$ with $\phi = 30°$. These values are appropriate for the case of a so-called 60° dislocation on a {111} plane in a cubic crystal oriented such that the [001] direction is normal to the interface. The interplanar spacing d/b is taken as $\sqrt{2/3}/4$, appropriate for a dislocation of the glide set in the diamond-cubic structure, and ν is taken as 0.3. The parameters of greatest interest here are A and d/b, which essentially replace the core cutoff radius. Based on estimates of the unstable stacking energy for fcc metals via the embedded atom method by Rice, Beltz, and Sun [12], A could range to values as low as 0.6. Calculations described in this paper are carried out for $A = 0.6, 0.8, 1.0$, and 1.2. The low end of the range is probably relevant for epitaxial metallic layers, while the high end is likely to be more relevant for silicon, its alloys, and other semiconducting materials that are thought to have dislocations with narrow core configurations [14].

The critical thicknesses predicted by (13) are shown in Figure 3 for the four values of A. In addition, Freund's result is plotted as a dashed line, using a core radius of $b/10$; this radius was chosen to best approximate the newer results here. The qualitative dependence of h_c on ϵ_0 is as expected. An important general conclusion is that the newer results predict a slightly larger critical thickness than theories based on continuum dislocation theory, markedly so in cases for which the dislocation core is narrower. Recent experimental results by Houghton *et al.*, [4], for $Si_{1-x}Ge_x$ films on Si(100), are included in Figure 3 as isolated points. The data are the most careful measurements to date, in that temperatures were large enough for equilibrium conditions to prevail, for extremely small dislocation densities. The numerical results slightly overestimate some of the experimental points. Nevertheless, using $r_0 = b/10$ appears to be a good approximation to the observed data.

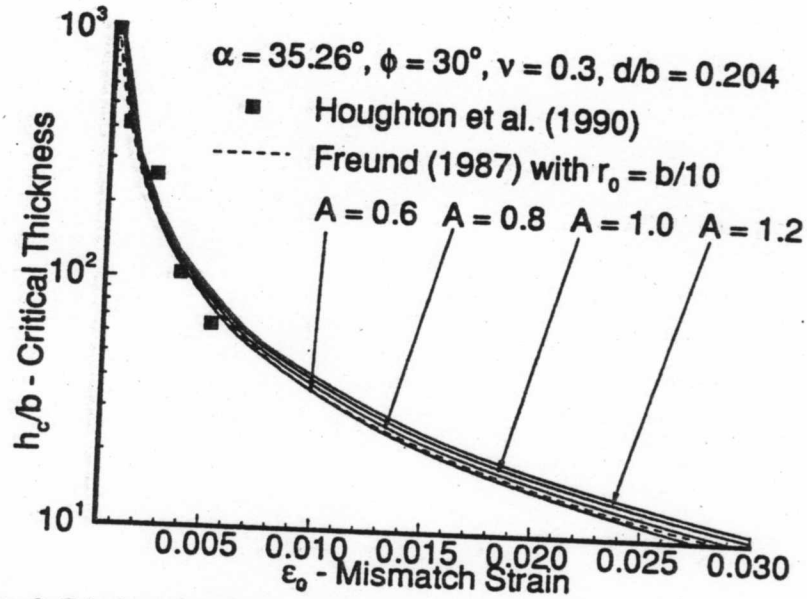

Figure 3. Calculated critical thickness versus mismatch strain for formation of an interfacial mismatch 60° dislocation, with $\nu = 0.3$, $\alpha = 35.2644°$, and $d/b = 0.2041$. The dashed curve is based on Freund's result [6], and experimental data due to Houghton *et al.* [4] are shown as isolated points.

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