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Critical epitaxial film thickness for forming interface dislocations

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Abstract

The system of an epitaxial film on a semi-infinite substrate of a different material is considered and the critical thickness of the film to form misfit interface dislocations is derived in the present study. The energy approach is used to predict the critical thickness and both the self-energy of the dislocation and the interaction energy between the dislocation and the mismatch strain are analyzed. The elastic stress field due to the interface dislocation is required in analyzing the energies and both the superposition principle and Fourier integral are adopted to derive this elastic stress field. The predicted stress fields in the system satisfy both the free surface condition at the film surface and the continuity condition at the interface. The predicted critical film thickness for forming interface dislocation decreases with the increase in the shear modulus ratio of the film to the substrate.

Keywords: Epitaxial film; Dislocation; Critical thickness; Modeling

1. Introduction

Many semiconductor devices and high temperature superconducting films require high quality of crystalline films grown epitaxially on substrates of different crystals. However, the film and the substrate generally have different lattice parameters. As a result, the lattice mismatch exists at the film/substrate interface and internal stresses are induced in the system. These internal stresses provide a driving force for the formation of interface dislocations [1–7] which, in turn, degrades the device performance. Hence, the study of the condition for the interface dislocation to form in the epitaxial film/substrate system is imperative in the materials design. The existence of a critical epitaxial film thickness for the interface dislocation to form was first proposed by Frank and van der Merwe [4]. When the film is sufficiently thin, the mismatch at the interface can be accommodated by the distortion of the lattice spacing of both the film and the substrate. As the film becomes thicker, there exists a critical thickness at which alignment between the film and the substrate can no longer be maintained and interface dislocations are formed. There have been many studies to analyze this critical film thickness [1–9]. However, due to the complexity of the problem, various simplifications in modeling have been adopted in order to obtain the solutions.

The purpose of the present study is to develop a better analytical model with a closed-form solution for the critical film thickness in forming the interface dislocation. First, the existing models are reviewed. Then, a new analytical model is presented in the present study. Finally, the critical film thickness for the interface dislocation to form is predicted and compared with existing solutions.

2. Summary of existing models

The major difficulty in analyzing the problem is the derivation of the elastic stress field due to the interface dislocation. This difficulty results from the following two factors. First, the dislocation is located at the interface of two different materials. Second, the stress field needs to satisfy the free surface condition at both the film surface and the substrate surface when both the film and the substrate have finite thickness. In order to simplify the problem, the early analyses made two assumptions: (1) the film and the substrate are isotropic elastic materials and have the same elastic constants and (2) the substrate is infinitely thick. With these assumptions, two approaches have been adopted to predict the critical film thickness for the interface dislocation to form. The first one is the force approach developed by Matthews and Blakeslee in which the force exerted by the misfit strain and the approximate tension in the dislocation line were considered [1]. The second one is the energy approach, in which the work of forming the dislocation due to the presence of internal stresses and the self-energy of

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the dislocation were analyzed. It has been noted that the predicted critical film thickness based on a thick substrate condition is too small to make it practical for device development. Recently, interest has been directed to thin (i.e. compliant) substrate to increase the critical film thickness. The system of a film deposited on a substrate with a finite thickness was first analyzed by Freund and Nix (FN) [2] using the energy approach; however, the film and the substrate are still assumed to have the same isotropic elastic properties. When the substrate is infinitely thick, there is only one free surface in the system and the 'image dislocation' technique can be used readily to derive the elastic stress field due to an interface dislocation. However, when the substrate has a finite thickness, there are two free surfaces in the system which, in turn, results in the complex interaction between the interface dislocation and free surfaces. A first order approximation was used by FN in analyzing the self-energy of the dislocation. As a result, the free-surface condition was not satisfied in the FN model. The FN model was recently improved by Zhang et al. [3] using the superposition principle and Fourier transformation to derive a complete analysis for the dislocation self-energy and to satisfy the free-surface condition.

The analyses described above assumed that the film and the substrate have the same elastic constants in order to simplify the analysis. When the difference in elastic constants between the film and the substrate is considered, the problem becomes much more complex. First, the equilibrium position is not at the interface but at some interatomic distances from the interface and inside the softer layer. This equilibrium position has been solved by Yu and Romanov [10] using the energy criterion. However, it is noted that the movement of the dislocation to its equilibrium position after its nucleation at the interface or at the harder phase depends on the temperature and the friction force. Second, considering an interface dislocation, the problem has been analyzed using Fourier transformation, however, the substrate was assumed to be infinitely thick in existing models. Also, other approximations were used in order to obtain the solutions for the critical film thickness. Willis et al. derived the stress field and energy arising from an array of dislocations [6] and dislocation dipoles [7] distributed uniformly on the perfectly bonded interface between an epitaxial film and a semi-infinite substrate of different isotropic elastic constants. Gosling and Willis [7] analyzed the energy of arrays of dislocations located periodically at the perfectly bonded interface between an epitaxial film and a semi-infinite substrate of the same anisotropic elastic constants. It is noted that the core energy was not included in the above analyses [6,7]. Using Fourier transformation and superposition proposed by Willis and co-workers [6,7], Zhang [8] studied the critical thickness of an epitaxial film on a semi-infinite substrate of different isotropic elastic constants. Following Stroh's approach of anisotropic elasticity, Zhang [9] also obtained the critical thickness of an epitaxial film on a semi-infinite substrate of different anisotropic elastic constants. However, it is noted that the displacement and the shear stress used in deriving the core energy in Zhang's analysis [8] did not satisfy the continuity condition at the interface.

3. The present model

Considering a film deposited epitaxially on a semi-infinite substrate with different isotropic elastic constants, the present analysis refines Zhang's analysis [8] to satisfy the continuity condition at the interface. The formulations of equations involved in deriving the present analytical solutions are formidable, only the essential analytical procedures are described here and the details will be published elsewhere [11]. A film of thickness h deposited epitaxially on a semi-infinite substrate as shown in Fig. 1, where μ and ν are shear modulus and Poisson's ratio and the subscripts f and s denote the film and the substrate, respectively. The Cartesian coordinates, x_1, x_2 and x_3 are used with the x_1-axis parallel to the in-plane interface, the x_2-axis perpendicular to the interface and the origin located at the interface. A dislocation with a Burgers vector $\boldsymbol{b} = [b_1, b_2, b_3]$ is located at the origin and the energies are calculated per unit length of the dislocation line or per unit depth of the film/substrate system in the present study. The formation energy E_f of the dislocation consists of two components: E_s the self-energy of the dislocation and E_{int} the interaction energy between the dislocation and mismatch strain. The energy components, E_s and E_{int} can be obtained by converting an area integral (with unit depth) to a line integral using a divergence theory. The analytical procedures in deriving E_s and E_{int} are described as follows.

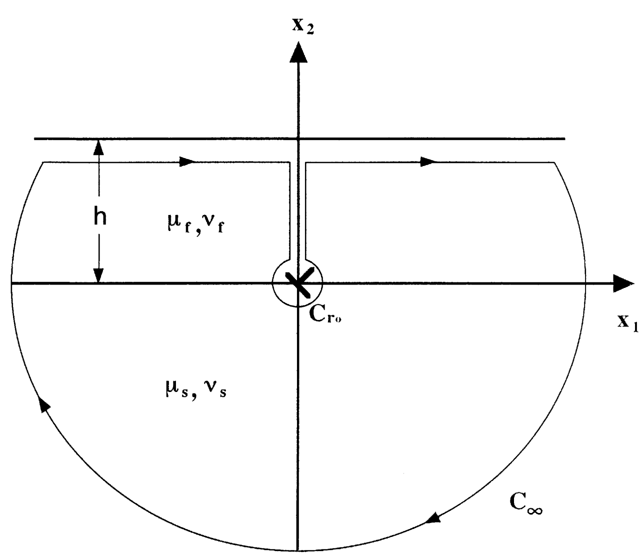

Fig. 1. A dislocation located at the perfectly bonded interface between an epitaxial layer of thickness h and a semi-infinite substrate.

3.1. The dislocation self-energy E_s

Since the elastic stress field induced by a dislocation is not valid in the core region, the integration path for E_s is selected as two contours C_{r_0} and C and an arbitrary cut (see Fig. 1) where r_0 is the core radius of the dislocation. Accordingly, the self-energy of the dislocation E_s can be decomposed into two components: E_c the integration along the core contour C_{r_0} (i.e. the dislocation core energy) and E_0, the difference between the self-energy and the core energy. It is noted that the solution of the self-energy is contingent upon the determination of the elastic stress field $\sigma_{a,ij}$ arising from the dislocation. However, due to the free surface condition at $x_2 = h$ and the difference in elastic constants between the film and the substrate, the derivation of the stress field $\sigma_{a,ij}$ is complex. Both the superposition principle [12] and Fourier integral [13] are adopted in the present study to derive the stress field $\sigma_{a,ij}$ resulting from an edge dislocation and a screw dislocation.

3.1.1. The stress field $\sigma_{a,ij}$ due to an edge dislocation at the interface

An edge dislocation of Burgers vector $[b_1, b_2, 0]$ located at the perfectly bonded interface between an epitaxial film and a semi-infinite substrate (Fig. 1) is considered. The stress field $\sigma_{a,ij}$ due to the interface dislocation can be derived by superposition of the following two stress components: (1) σ_{ij}^0, stress due to an interface dislocation assuming the film is also semi-infinite and (2) σ_{ij}^*, the stress due to prescribed tractions on the film surface which are the negative of those calculated from the first stress component at $x_2 = h$. Combination of the stress fields from the above two cases results in a traction-free surface at $x_2 = h$. While σ_{ij}^0 has been solved by Suo and Hutchinson [14], σ_{ij}^* can be obtained using the Fourier transform method [13], in which the stresses and the displacements can be related to two unknown potentials. These two potentials can be represented by Fourier integrals. By satisfying both the traction-free condition at the free surface (i.e. at $x_2 = h$) and the continuity conditions at the interface (i.e. at $x_2 = 0$), the unknown parameters in Fourier integrals can be determined which, in turn, yields the solution for σ_{ij}^*.

3.1.2. The stress field $\sigma_{a,ij}$ due to a screw dislocation at the interface

A screw dislocation of Burgers vector $[0, 0, b_3]$ located at the perfectly bounded interface of the film/substrate system is considered. The procedure for analyzing the elastic stress field is similar to that of an edge dislocation. That is, the solution is the superposition of the two cases described in Section 3.1.1. For a screw dislocation, σ_{ij}^0 has been solved by Weertman and Weertman [15]. The solution for σ_{ij}^* can be obtained following the same analytical procedures as those for an edge dislocation. However, only one potential, which is antisymmetric with respect to x_1, is required.

3.1.3. The core energy E_c and strain energy E_0

Because the core radius is much smaller than the film thickness, the stress and the displacement fields due to two semi-infinite medium can be used to calculate the core energy E_c. Using the polar coordinate system, the core energy is

$$E_c = \frac{1}{2}\oint \sigma_{ij}^0 n_j u_i^0 \,\mathrm{d}s = -\frac{1}{2}\int_{\theta_0}^{\theta_0+2\pi} (\sigma_{rr}^0 u_r^0 + \sigma_{r\theta}^0 u_\theta^0 + \sigma_{rz}^0 u_z^0) r_0 \,\mathrm{d}\theta \quad (1)$$

where θ_0 is the cutting angle, u_r^0, u_θ^0 and σ_{rr}^0, $\sigma_{r\theta}^0$ are due to the edge component and u_z^0 and σ_{rz}^0 are due to the screw component. Since σ_{rz} arising from the screw component is zero along the integration contour, only the edge component contributes to core energy. While the stress and displacement arising from an edge dislocation derived in Section 3.1.1 are expressed in the Cartesian coordinates, conversion to the polar coordinates is required before the integration of Eq. (1) can be performed. The stress and displacement remain continuous at the interface after the coordinate transformation; however, the displacement jumps at $\theta = \pi/2$ where the cut is made. It is noted that the coordinate conversion was not performed properly in Zhang's analysis and the continuity condition at the interface is not satisfied in Zhang's solution [8].

The strain energy E_0 can be obtained from the stress field obtained from Sections 3.1.1 and 3.1.2 using the following integral.

$$E_0 = -\frac{1}{2}\int_{r_0}^{L} \sigma_{a,ij} n_j b_i \,\mathrm{d}s \quad (2)$$

3.2. The interaction energy E_{int}

The derivation of the interaction energy E_{int} is straightforward. It can be obtained from the Burgers vector of the interface dislocation and the stresses in both the film and the substrate due to the lattice mismatch.

3.3. The criterion for forming interface dislocations

The dislocation could be generated if its formation energy is negative. The critical thickness h_0 of the film for the interface dislocation to form can be derived from zero formation energy. Letting the formation energy equal zero, the solution of h_0 can be obtained by solving the following equation.

$$\frac{(b_1^2 + b_2^2)(1+\alpha)}{\pi c_s(1-\beta^2)} \ln\left(\frac{h_0}{r_0}\right) + \frac{\mu_{\mathrm{eff}} b_3^2}{4\pi} \times \left[\ln\left(\frac{2h_0}{r_0}\right) + \sum_{n=1}^{\infty}\left(\frac{\mu_{\mathrm{f}} - \mu_{\mathrm{s}}}{\mu_{\mathrm{f}} + \mu_{\mathrm{s}}}\right)^n \ln\left(\frac{1+n}{n}\right)\right]$$

$$-\frac{1}{4\pi c_{\mathrm{f}}^2}\left\{2(b_1^2+b_2^2)\left[\frac{(1+\Lambda_1)^2}{\mu_{\mathrm{f}}}-\frac{(1+\Lambda_2)^2}{\mu_{\mathrm{s}}}\right]\right.$$
$$+(b_1^2-b_2^2)\left[\frac{(1+\Lambda_1)}{\mu_{\mathrm{f}}}\langle(k_{\mathrm{f}}-1)\Lambda_1+2\Lambda_2-3-3k_{\mathrm{f}}\rangle\right.$$
$$\left.\left.+\frac{(1+\Lambda_2)}{\mu_{\mathrm{s}}}\langle 2\Lambda_1+(k_{\mathrm{s}}-1)\Lambda_2+1+k_{\mathrm{s}}\rangle\right]\right\}$$
$$+E_{0,e_1}+E_{0,e_2}+E_{0,e_3}$$
$$=\frac{2\mu_{\mathrm{f}}(1+\nu_{\mathrm{f}})}{1-\nu_{\mathrm{f}}}|\varepsilon_{\mathrm{m}}^0 b_1|h_0 \quad (3)$$

where $\varepsilon_{\mathrm{m}}^0$ is the mismatch strain between the film and substrate, and

$$k_{\mathrm{f}}=3-4\nu_{\mathrm{f}},\quad k_{\mathrm{s}}=3-4\nu_{\mathrm{s}} \quad (4a)$$

$$\alpha=\frac{\mu_{\mathrm{f}}(k_{\mathrm{s}}+1)-\mu_{\mathrm{s}}(k_{\mathrm{f}}+1)}{\mu_{\mathrm{f}}(k_{\mathrm{s}}+1)+\mu_{\mathrm{s}}(k_{\mathrm{f}}+1)},$$
$$\beta=\frac{\mu_{\mathrm{f}}(k_{\mathrm{s}}-1)-\mu_{\mathrm{s}}(k_{\mathrm{f}}-1)}{\mu_{\mathrm{f}}(k_{\mathrm{s}}+1)+\mu_{\mathrm{s}}(k_{\mathrm{f}}+1)} \quad (4b)$$

$$\mu_{\mathrm{eff}}=\frac{2\mu_{\mathrm{s}}\mu_{\mathrm{f}}}{(\mu_{\mathrm{s}}+\mu_{\mathrm{f}})} \quad (4c)$$

$$c_{\mathrm{f}}=\frac{(k_{\mathrm{f}}+1)}{\mu_{\mathrm{f}}},\quad c_{\mathrm{s}}=\frac{(k_{\mathrm{s}}+1)}{\mu_{\mathrm{s}}} \quad (4d)$$

$$\Lambda_1=\frac{\mu_{\mathrm{s}}-\mu_{\mathrm{f}}}{\mu_{\mathrm{f}}+k_{\mathrm{f}}\mu_{\mathrm{s}}},\quad \Lambda_2=\frac{\mu_{\mathrm{s}}k_{\mathrm{f}}-\mu_{\mathrm{f}}k_{\mathrm{s}}}{\mu_{\mathrm{s}}+\mu_{\mathrm{f}}k_{\mathrm{s}}} \quad (4e)$$

E_{0,e_1}, E_{0,e_2} and E_{0,e_3} are complicated functions of b_1, b_2, α, β, c_{s}, c_{f}, μ_{f} and μ_{s} [11]. The first and second terms in Eq. (3) arise, respectively, from the stress field σ_{ij}^0 of the edge and the screw components of the dislocation. The third term in Eq. (3) corresponds to the stress field σ_{ij}^* of the screw component of dislocation calculated via the Fourier integral. The summation of next three terms containing curly braces is the core energy. The last three terms of left hand side in Eq. (3) are induced by the stress field σ_{ij}^0 of the edge component of dislocation calculated via the Fourier integral.

When the film and the substrate have the same elastic constants, Eq. (3) can be reduced to

$$\frac{\mu_{\mathrm{f}}}{4\pi(1-\nu_{\mathrm{f}})}[b_1^2+b_2^2+(1-\nu_{\mathrm{f}})b_3^2]\ln\left(\frac{2h_0}{r_0}\right)-\frac{\mu_{\mathrm{f}}b_2^2}{4\pi(1-\nu_{\mathrm{f}})}$$
$$=\frac{2\mu_{\mathrm{f}}(1+\nu_{\mathrm{f}})}{1-\nu_{\mathrm{f}}}|\varepsilon_{\mathrm{m}}^0 b_1|h_0 \quad (5)$$

and the core energy containing the curly braces in Eq. (3) is simplified as $E_{\mathrm{c}}=\mu_{\mathrm{f}}(b_1^2-b_2^2)/8\pi(1-\nu_{\mathrm{f}})$. If the core energy is ignored, Eq. (5) becomes the same as that obtained in the literature [3,6,7].

4. Results

The crystal structure of most semiconductor materials is diamond or zincblende. The principal types of dislocations in the strong Peierls potential of semiconductor crystals are the 60° dislocation and the screw dislocation lying in the ⟨1 1 0⟩ direction [16]. Because the screw dislocation does not contribute the mismatch stress, the pure screw dislocation is not considered in the present study. Instead, the 60° dislocation along the $[\bar{1}10]$ direction lying in the $[11\bar{1}]$ plane is analyzed, and a possible Burgers vector is $\boldsymbol{b}=b[0, 1/\sqrt{2}, 1/\sqrt{2}]$. Assume that an epitaxial layer of thickness h is grown on semi-infinite substrate. Formation of the dislocation at the interface is considered, the subsequent movement of the dislocation to its minimum energy position in the soft layer is not considered in the present study. A dislocation of Burgers vector $\boldsymbol{b}=b[1/2, \bar{1}/\sqrt{2}, 1/2]$ is located at the origin of interface as shown in Fig. 1 where x_1, x_2 and x_3-axes are in the [1 1 0], [0 0 1], and $[\bar{1}10]$ directions, respectively. Using Eq. (1), and $\nu_f=\nu_s=0.3$, the critical thickness of the film h_0 to form a dislocation as a function of the shear modulus ratio $\mu_{\mathrm{f}}/\mu_{\mathrm{s}}$ is plotted as the solid line in Fig. 2 at different magnitudes of mismatch strain $|\varepsilon_{\mathrm{m}}^0|$. It is found that the critical thickness decreases monotonically with increasing shear modulus ratio of the film to the substrate $\mu_{\mathrm{f}}/\mu_{\mathrm{s}}$ and mismatch strain. The results from Zhang's analysis are also shown in Fig. 2 by the dashed lines. Comparing to Zhang's results [17], the present results predict a smaller critical film thickness, however, the difference decreases with increasing shear modulus ratio $\mu_{\mathrm{f}}/\mu_{\mathrm{s}}$. The formation energy as a function of film thickness with different core radius and mismatch strain is plotted in Fig. 3 for $\mu_{\mathrm{f}}/\mu_{\mathrm{s}}=0.1$. It is found that the formation energy increases with decreasing core radius and increasing mismatch strain for given shear modulus ratio and film thickness. The formation energy increases to a maximum and then decreases with increasing film thickness. The critical thickness increases with decreasing core

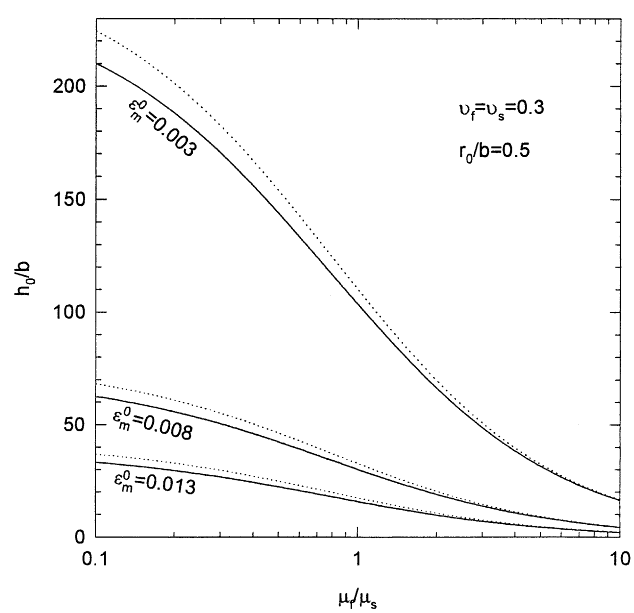

Fig. 2. The critical thickness as a function of shear modulus with mismatch strain $\varepsilon_{\mathrm{m}}^0$.

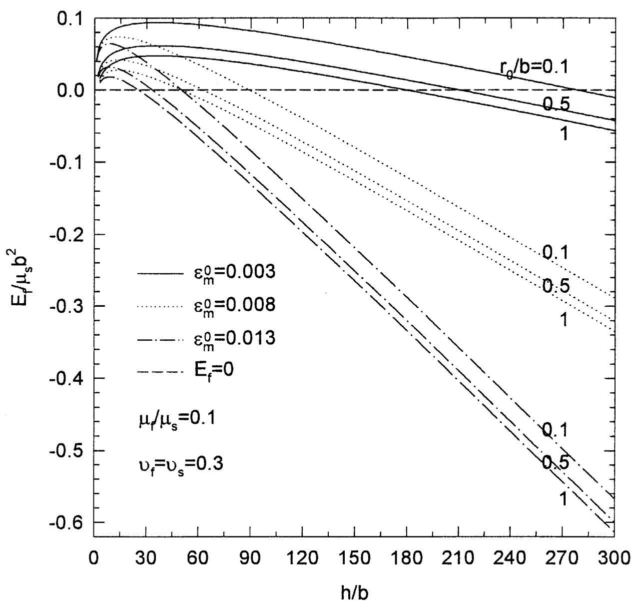

Fig. 3. The formation energy of interface dislocation as a function of film thickness with parameters of mismatch strain and core radius.

radius and mismatch strain. Note that the minimum root of formation energy is defined as the critical film thickness for the interface dislocation to form.

5. Conclusions

The critical epitaxial film thickness for forming interface dislocations is investigated. The energy approach is proposed to predict the critical thickness. The total energy consists of the self-energy of the dislocation and the interaction between dislocation and mismatch strain. In order to yield the strain energy, the stress field arising from the interface dislocation is required that can be derived based on the superposition principle and Fourier integral. The stress fields satisfy the free surface condition and continuity at the interface. The critical thickness decreases with increase of shear modulus ratio of the film to the substrate, magnitude of mismatch strain, and core radius.

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