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Equilibrium position of misfit dislocations in thin epitaxial films

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Abstract
The role of the free surface in determining the equilibrium position of misfit dislocations in thin epitaxial films is considered. When the film is elastically stiffer than the substrate, the core of the dislocation is predicted to lie at some distance from the interface in the softer substrate. On the other hand, when the film is softer than the substrate, the core of the dislocation is always predicted to lie close to the interface.

1. Introduction

With the advent of high resolution transmission electron microscopy (HRTEM) techniques, there have been a number of experimental observations of misfit dislocations that demonstrate that the core of the dislocation is often not precisely located at the interface, but is displaced some distance into the elastically softer phase [1, 2]. Theoretical predictions of the magnitude of the displacement from the interface location have been given by Mader and Knauss [3] using a force balance argument, and by Gutkin *et al* [4] using an energy approach. The problem was treated using two elastically isotropic, semi-infinite solids with different elastic constants, having a uniaxial misfit in the interface plane. Both authors adopted the approach of Mura [5] to solve the elasticity problem, although Mura's solution in turn was implicit in the earlier work of Head [6, 7].

Semiconductor thin films are usually grown on substrates from the same class of material e.g. $Si_{1-x}Ge_x$/Si (or Ge), $In_{1-x}Ga_xAs_yP_{1-y}$/InP (or GaAs) systems. The ratio of the shear modulus between the semiconductor film and substrate (μ_f/μ_s or μ_s/μ_f, the subscripts s and f denote substrate and film, respectively) is then less than 1.5. With such a small difference in shear moduli between the film and substrate, it is expected [3, 4] that the misfit dislocations should be very close to the interface either in the film or substrate, i.e. within a distance of the order of the dislocation core dimensions (a few Å). However, our experimental observations suggest otherwise [8]: in a 2% tensile strained, 100 nm thick $In_{0.25}Ga_{0.75}As$ film grown on a (100) InP substrate, the 90° leading partial dislocations bounded by stacking faults are frequently observed to locate below the interface and inside the InP substrate over a range of a few hundred angstroms. The ratio of the shear moduli of the $In_{0.25}Ga_{0.75}As$ film and the InP substrate (μ_f/μ_s) is 1.3. Another example is shown in figure 1. This is a $[0\bar{1}1]$ cross-section TEM image ($\mathbf{g}$ = 200) of a 100 nm thick, 2% tensile strained $In_{0.72}Ga_{0.28}P$ film grown on (100) InP substrate. Clearly, twins often penetrate some distance into the substrate as well ($\mu_f/\mu_s = 1.22$). Similar observations can be seen in the paper of Wegscheider *et al* [9] although they did not address the phenomenon. Wegscheider *et al* [9] studied the strain relaxation mechanism in 200 nm thick, 1% tensile strained Si_3Ge_9 superlattices grown on (001) Ge substrate. Figures 2 and 3 of their paper show that 90° partial dislocations are often not terminated at the interface between the Si_3Ge_9 superlattices and Ge substrate. Instead, they locate inside the Ge substrate and are a few hundred angstroms away from the SiGe/Ge interface. Since $\mu_{Si} > \mu_{Ge}$, the film (SiGe) is again elastically harder than the substrate (Ge) ($\mu_f > \mu_s$). Oktyabrsky *et al* [10] investigated misfit dislocations in epitaxial growth of Ge films on (001) Si substrates. In this case, the film (Ge) is elastically softer than the substrate (Si) ($\mu_f < \mu_s$). Their HRTEM observations show that many misfit dislocation cores are located above the Ge/Si interface (in the Ge film) but very close to the interface. They estimated the equilibrium position of misfit dislocations using two isotropic semi-infinite solids, the method used by Mader and Knauss [3], and Gutkin *et al* [4].

We have studied the forces acting on twinning dislocations due to the interface and free surface [8]. In this paper,

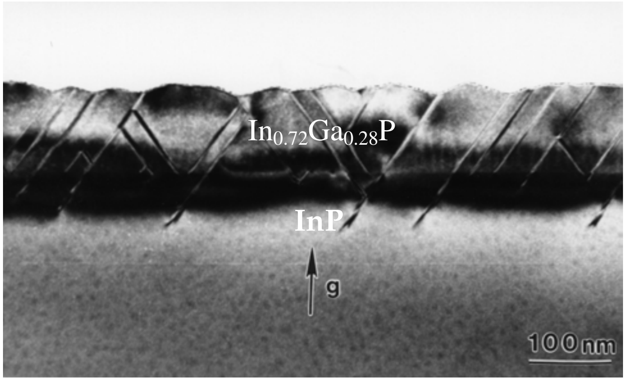


Figure 1. $[0\bar{1}1]$ cross-section TEM image ($\mathbf{g} = 200$) of 100 nm thick, 2% tensile strained $In_{0.72}Ga_{0.28}P$ film on InP substrate. The 90° partial dislocations bounded by stacking faults penetrate some distance into the substrate.

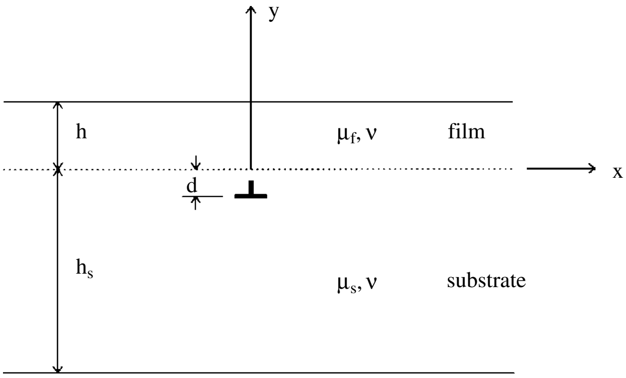


Figure 2. Schematic illustration of film–substrate combination.

we present the studies on the equilibrium position of misfit dislocations in epitaxially grown systems where typically the thickness of the epitaxial film (h) is orders of magnitude smaller than the thickness of the substrate (h_s). Under these conditions, the presence of the free surface is extremely important and destroys the symmetry found with the two semi-infinite crystal geometry. The magnitude of the displacement of the core of the dislocation from the interface now depends on whether the film is elastically stiffer or softer than the substrate.

2. Forces acting on dislocations

The geometry of the isotropic film–substrate combination is shown in figure 2 for the condition where the substrate is elastically softer and has a larger lattice parameter than the film. The film is then under bi-axial tension, while the substrate is under bi-axial compression. The stresses in the film and substrate are given by

$$\sigma_{xx}^f = 2\mu_f \frac{(1+\nu)}{(1-\nu)}\varepsilon_{xx}^f \qquad \sigma_{xx}^s = 2\mu_s \frac{(1+\nu)}{(1-\nu)}\varepsilon_{xx}^s \tag{1}$$

with

$$\varepsilon_{xx}^f - \varepsilon_{xx}^s = f \tag{2}$$

where μ_f and μ_s are the shear moduli of the film and substrate, ν is Poission's ratio (assumed to be the same in both the film and substrate), ε_{xx}^f and ε_{xx}^s are the strain in the film and substrate and f is the misfit between the lattice parameters of the bounding phases. In equation (1), we have ignored wafer bending effect, which is a valid approximation here as the substrate thickness (h_s) is much greater than the film thickness (h).

Mechanical equilibrium of the system requires that

$$\int_0^h \sigma_{xx}^f + \int_{-h_s}^0 \sigma_{xx}^s = 0 \qquad \text{i.e.} \quad \sigma_{xx}^f h + \sigma_{xx}^s h_s = 0 \tag{3}$$

where h and h_s are the thicknesses of the film and substrate.

Solving the equations (1)–(3), the following expressions for the stresses in the film and substrate are obtained:

$$\begin{aligned}\sigma_{xx}^f &= \frac{2h_s\mu_f\mu_s(1+\nu)f}{(h_s\mu_s + h\mu_f)(1-\nu)} \\ \sigma_{xx}^s &= -\frac{2h\mu_f\mu_s(1+\nu)f}{(h_s\mu_s + h\mu_f)(1-\nu)}.\end{aligned} \tag{4}$$

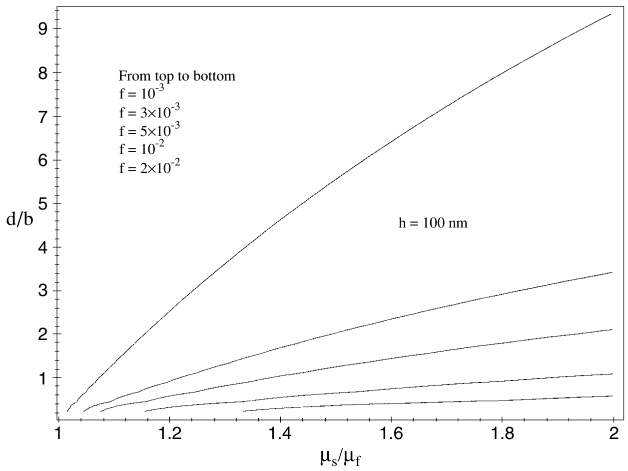
A single edge dislocation $\mathbf{b} = (b, 0, 0)$ is introduced into the softer phase, lying at the point $(0, -d)$ from the interface and at a distance $(h + d)$ from the free surface. The total climb force (F) acting on this dislocation arises from three factors: (i) the interaction between the dislocation and the stress in the substrate, (ii) the interaction between the dislocation and the free surface and (iii) the interaction between the dislocation and the interface. The solution to (i), the Peach–Koehler force, is well known and equals $-\sigma_{xx}^s b$. The solutions to (ii) and (iii) can be obtained following Head [7] and Mura's [5] analysis. Head provided an exact solution for the case of a screw dislocation. In Head's analysis, he introduced the concept of image dislocations to account for the presence of both a free surface and an interface where there is a discontinuity in the elastic properties [7]. Using Head's approach and Mura's analysis, we solved the problem for an edge dislocation, and presented the results in our previous paper [8]. The solution given by Head is exact for the screw dislocation case, and is an excellent approximation for the edge dislocation provided that the ratio of μ_f/μ_s or μ_s/μ_f is less than 1.5. The exact analysis for the edge dislocation given by Weeks *et al* is extremely complex [11], but for μ_f/μ_s or μ_s/μ_f less than 1.5, Weeks *et al* showed that the image method gives the same result as the exact solution. The force acting on the dislocation due to the interface and free surface is $-\frac{\mu_s b^2}{4\pi(1-\nu)d}\left[m - (1-m^2)\sum_{i=1}^{\infty}\frac{d}{d+\mathrm{i}h}m^{i-1}\right]$ [8]. m, which can be thought of as the strength of the first image dislocation, located at $(0, +d)$, is given by $-\frac{1}{2}(A+B)$, where $A = \frac{1-\Gamma}{1+\kappa\Gamma}$, $B = \frac{\kappa(1-\Gamma)}{\kappa+\Gamma}$, $\kappa = 3 - 4\nu$ and $\Gamma = \frac{\mu_f}{\mu_s}$.

Thus the total force acting on the dislocation is given by

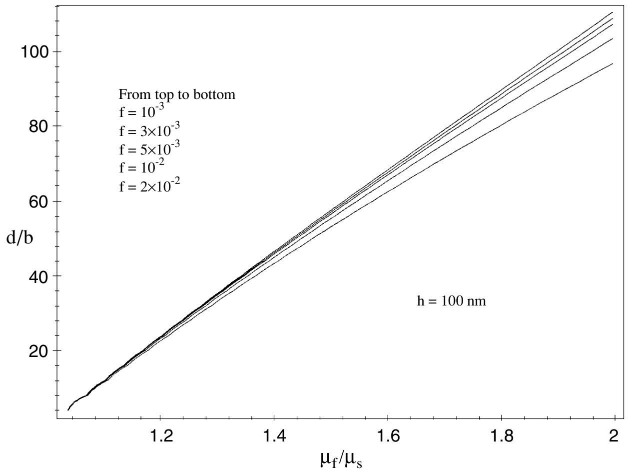
$$F_y = \frac{2h\mu_f\mu_s(1+\nu)fb}{(h_s\mu_s + h\mu_f)(1-\nu)} - \frac{\mu_s b^2}{4\pi(1-\nu)d} \times \left[m - (1-m^2)\sum_{i=1}^{\infty}\frac{d}{d+\mathrm{i}h}m^{i-1}\right]. \tag{5}$$

The situation where the film is softer than the substrate follows the same reasoning, but now the dislocation core is located in the film. In this case the force F_y is given by

$$F_y = -\frac{2h_s\mu_f\mu_s(1+\nu)fb}{(h_s\mu_s + h\mu_f)(1-\nu)} + \frac{\mu_f b^2}{4\pi(1-\nu)d} \times \left[n - (1-n^2)\sum_{i=1}^{\infty}\frac{d}{\mathrm{i}h-d}n^{i-1}\right] \tag{6}$$



(a)



(b)

Figure 3. The dependence of dislocation equilibrium position on the ratio of shear modulus at various misfit values ($h_s = 375\ \mu$m, $h = 100$ nm, $\nu = 0.3$ and $b = 4$ Å). (*a*) d/b versus μ_s/μ_f for the isolated dislocation located in the film. (*b*) d/b versus μ_f/μ_s for the isolated dislocation located in the substrate.

where $n = -\frac{1}{2}(A' + B')$, with $A' = \frac{1-\Gamma'}{1+\kappa\Gamma'}$, $B' = \frac{\kappa(1-\Gamma')}{\kappa+\Gamma'}$, $\kappa = 3 - 4\nu$ and $\Gamma' = \frac{\mu_s}{\mu_f}$.

If $h_s \gg h$, equation (5) becomes

$$F_y = -\frac{\mu_s b^2}{4\pi(1-\nu)d}\left[m - (1-m^2)\sum_{i=1}^{\infty}\frac{d}{d+\mathrm{i}h}m^{i-1}\right]. \qquad (7)$$

This is the equation for the dislocation in the unstrained substrate because $\sigma_{ij}^s \approx 0$ when $h_s \gg h$.

Some well-known results can be recovered from equation (7) in the following limiting cases:

(1) $\Gamma = 0$ (i.e. $\mu_f = 0, A = B = 1, m = -1$):

$$F_y = \frac{\mu_s b^2}{4\pi(1-\nu)d}. \qquad (8)$$

This is the force acting on an edge dislocation, a distance d from a free surface in a semi-infinite solid

(2) $\Gamma = 1$ (i.e. $\mu_f = \mu_s, A = B = 0, m = 0$):

$$F_y = \frac{\mu_s b^2}{4\pi(1-\nu)(d+h)}. \qquad (9)$$

This is the force acting on an edge dislocation, a distance $(d + h)$ from a free surface in a semi-infinite solid.

(3) $\Gamma = \infty$ $\left(A = -1/\kappa, B = -\kappa, m = \frac{\kappa^2+1}{2\kappa}\right)$:

$$F_y = -\frac{\mu_s b^2}{4\pi(1-\nu)}\frac{\kappa^2+1}{2\kappa}. \qquad (10)$$

This is the result of having a rigid boundary at $y = 0$. Since $F_y < 0$, the dislocation would always be repelled from the interface in this case

(4) $h = \infty$:

$$F_y = -\frac{\mu_s b^2}{4\pi(1-\nu)}m. \qquad (11)$$

This is the result for the two semi-infinite crystals case given by Mader and Knauss [3].

3. Equilibrium position of dislocations

For a dislocation to be at equilibrium, the total force acting on the dislocation must vanish. Therefore, the equilibrium position can be determined by solving $F_y = 0$. The equilibrium position is given by

$$\frac{2h\mu_f\mu_s(1+\nu)fb}{(h_s\mu_s + h\mu_f)(1-\nu)} - \frac{\mu_s b^2}{4\pi(1-\nu)d}\left[m - (1-m^2)\times\sum_{i=1}^{\infty}\frac{d}{d+\mathrm{i}h}m^{i-1}\right] = 0 \qquad \text{if} \quad \mu_f > \mu_s \qquad (12)$$

for the dislocation core located in the substrate, and

$$-\frac{2h_s\mu_f\mu_s(1+\nu)fb}{(h_s\mu_s + h\mu_f)(1-\nu)} + \frac{\mu_f b^2}{4\pi(1-\nu)d}\left[n - (1-n^2)\times\sum_{i=1}^{\infty}\frac{d}{\mathrm{i}h-d}n^{i-1}\right] = 0 \qquad \text{if} \quad \mu_f < \mu_s \qquad (13)$$

for the dislocation core located in the film.

If $h_s = h \gg d$, equations (12) and (13) become

$$\frac{d}{b} = \frac{(1+\Gamma)m}{8\pi(1+\nu)\Gamma f} \qquad (14)$$

and

$$\frac{d}{b} = \frac{(1+\Gamma')n}{8\pi(1+\nu)\Gamma' f}. \qquad (15)$$

Equations (14) and (15) are identical to Mader and Knauss's [3] solution for the equilibrium position of the dislocation for the case of two semi-infinite crystals. (Mader and Knauss considered a uniaxial misfit; taking their expression for σ_{xx}^s leads to $\frac{d}{b} = \frac{(1+\Gamma)m}{8\pi\Gamma f}$ and $\frac{d}{b} = \frac{(1+\Gamma')n}{8\pi\Gamma' f}$ in our terminology.)

If $\mu_f = \mu_s$, then $m = n = 0$, and both equations (14) and (15) give $d/b = 0$, i.e. the dislocation is located at the interface as expected.

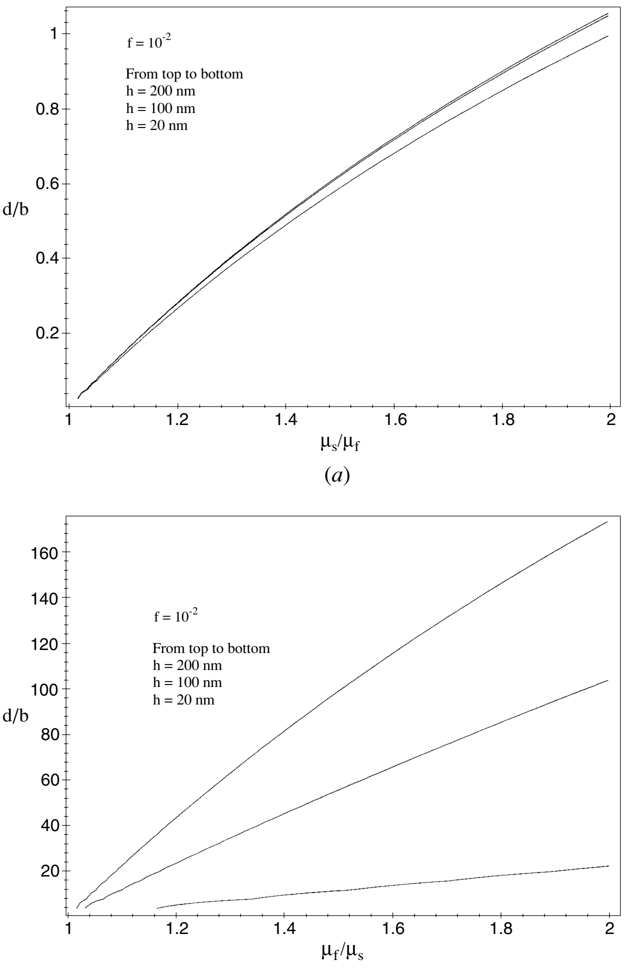
If $h_s \gg h$, equations (12) and (13) become

$$-m + (1-m^2)\sum_{i=1}^{\infty}\frac{d}{d+\mathrm{i}h}m^{i-1} = 0 \qquad \text{if} \quad \mu_f > \mu_s \quad (16)$$

for the dislocation core located in the substrate, and

$$-8\pi(1+\nu)f\frac{d}{b} + n - (1-n^2)\sum_{i=1}^{\infty}\frac{d}{\mathrm{i}h-d}n^{i-1} = 0 \qquad \text{if} \quad \mu_f < \mu_s \qquad (17)$$

for the dislocation core located in the film.



(*a*)

(*b*)

Figure 4. The dependence of dislocation equilibrium position on the ratio of shear modulus at various film thicknesses ($h_s = 375\ \mu$m, $f = 10^{-2}$, $\nu = 0.3$ and $b = 4$ Å). (*a*) d/b versus μ_s/μ_f for the isolated dislocation located in the film. (*b*) d/b versus μ_f/μ_s for the isolated dislocation located in the substrate.

Equations (16) and (17) clearly demonstrate the asymmetry in the behaviour anticipated in the introduction. If the dislocation lies in the substrate, the climb force due to the misfit f (driving it back to the interface) is essentially zero $\left(\left|\sigma_{xx}^{f}\right| \gg \left|\sigma_{xx}^{s}\right|\right)$, and the equilibrium position is given by Head's original analysis [7]. On the other hand if the dislocation lies in the film, there is a substantial climb force (due to σ_{xx}^{f}) driving the dislocation towards the interface. At large values of f, this term dominates the behaviour, and the equilibrium position of the dislocation is very close to the interface.

Figures 3 and 4 compare the predictions of the equilibrium position of the isolated edge dislocation given by the two expressions, equations (12) and (13), assuming $\nu = 0.3$, (i.e. $\kappa = 1.8$), $b = 4$ Å and $h_s = 375\ \mu$m. In figure 3, the equilibrium position (d/b) is compared for a film thickness $h = 100$ nm over a range of μ_f/μ_s (μ_s/μ_f) values from 1 to 2 for values of misfit f from 1×10^{-3} to 2×10^{-2}. If the dislocation lies in the film ($\mu_f < \mu_s$) (figure 3(*a*)), the equilibrium position is closer to the interface by at least an order of magnitude in comparison to the situation where $\mu_f > \mu_s$ (with the dislocation in the substrate) (figure 3(*b*)), over the whole range of misfit values considered. For example, at $f = 10^{-3}$, d/b is 4.6 for $\mu_s/\mu_f = 1.4$ with the dislocation in the film, while d/b is 48 for $\mu_f/\mu_s = 1.4$ with the dislocation in the substrate.

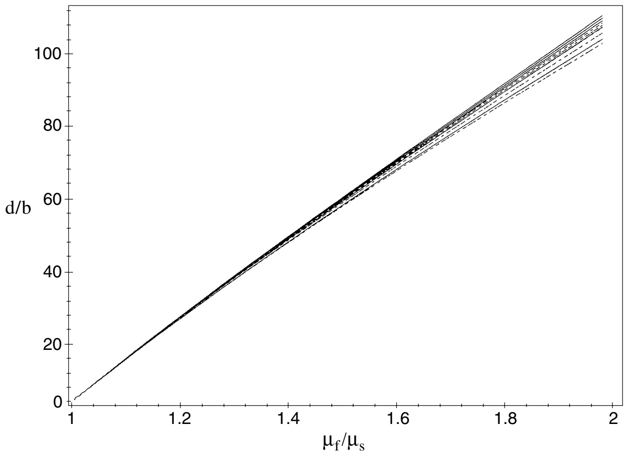


Figure 5. Comparison of the dependence of the equilibrium position (d/b) on the ratio of shear modulus (μ_f/μ_s) at various misfit values (see figure 3(*b*)) for the isolated dislocation located in the substrate. The dashed line: edge dislocation; the solid line: 60° dislocation ($h_s = 375\ \mu$m, $h = 100$ nm, $\nu = 0.3$ and $b = 4$ Å).

Figure 4 shows the influence of the film thickness h in the range 20 to 200 nm at a misfit of $f = 10^{-2}$ for the two situations. There is little variation of the equilibrium position with h when the dislocation lies in the film (figure 4(*a*)), but a strong dependence of the equilibrium position on h when the dislocation lies in the substrate (figure 4(*b*)).

The analysis is readily extended to mixed dislocations. The total force acting on a mixed dislocation at (0, $-d$) is given by

$$F_y = \frac{2h\mu_f\mu_s(1+\nu)fb}{(h_s\mu_s + h\mu_f)(1-\nu)}\sin\beta\cos\varphi\cos 2\varphi - \frac{\mu_s b^2\sin^2\beta}{4\pi(1-\nu)d}\left[m - (1-m^2)\sum_{i=1}^{\infty}\frac{d}{d+\mathrm{i}h}m^{i-1}\right]\cos 2\varphi - \frac{\mu_s b^2\cos^2\beta}{4\pi d}\left[p - (1-p^2)\sum_{i=1}^{\infty}\frac{d}{d+\mathrm{i}h}p^{i-1}\right] \qquad (18)$$

where β is the angle between the Burgers vector of the dislocation and the dislocation line, φ is the angle between the slip plane and the free surface (interface) and $p = \frac{\Gamma-1}{\Gamma+1}$ with $\Gamma = \frac{\mu_f}{\mu_s}$.

In the growth of semi-conducting (group IV or III–V) epitaxial layers, on $\langle 001\rangle$ oriented substrates, strain relief often occurs by the formation of 60° $(a/2)\langle 110\rangle$ dislocations gliding on $\{111\}$ planes, i.e. $\beta = 60°$ and $\varphi = 54.74°$. Figure 5 compares the predictions of the equilibrium position d/b for the edge dislocation and the 60° dislocation (from equations (12) and (18)) for a film thickness $h = 100$ nm and a substrate thickness $h_s = 375\ \mu$m over the same range of μ_f/μ_s and misfit (f) values shown in figure 3(*b*). The offset of the edge and 60° dislocations from the interface are very similar.

4. Conclusions

In conclusion, we studied the equilibrium position of misfit dislocations in thin epitaxial films where the thickness of the epitaxial film is orders of magnitude smaller than the thickness of the substrate. When the film is elastically stiffer than the substrate, the core of the dislocation is predicted to lie at some distance from the interface in the softer substrate. On the other hand when the film is softer than the substrate, the core of the dislocation is always predicted to lie close to the interface. There is a strong dependence of the equilibrium position on the film thickness when the dislocation lies in the substrate, but little variation when the dislocation lies in the film. The equilibrium position behaviour of the edge and 60° dislocations are very similar.

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