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The first stage of stress relaxation in tensile strained $\text{In}_{1-x}\text{Ga}_x\text{As}_{1-y}\text{P}_y$ films

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ABSTRACT

The first stages of stress relaxation have been studied in a series of 2% tensile strained $(\text{In}, \text{Ga})(\text{As}, \text{P})$ films of various compositions by transmission electron microscopy. Ternary $\text{In}_{1-x}\text{Ga}_x\text{As}$ and $\text{In}_{1-x}\text{Ga}_x\text{P}$ films relaxed by a combination of twinning and cracking, while the quaternary $\text{In}_{1-x}\text{Ga}_x\text{As}_{1-y}\text{P}_y$ film relaxed only by twinning. The differences between the behaviours of the ternary and quaternary systems were correlated with the surface topography of the films. The surface nucleation of 90° partial dislocations was shown to be feasible at the growth temperature of the films (480°C) in the presence of surface roughness but, in the absence of a critical roughness, cracking was the preferred mechanism for coherency loss. The critical film thicknesses observed for stress relaxation by either twinning or cracking were shown to be in good agreement with the calculated values. The twins themselves often terminated inside the substrate (InP) rather than at the substrate–film interface. This behaviour was related to the elastic mismatch that exists between the harder film and softer substrate.

§1. INTRODUCTION

The growth of semiconductor films by techniques such as molecular-beam epitaxy has been a fruitful area of research to probe the nucleation and growth of defects such as dislocations and cracks, as well as surface roughening, all of which play an important role in stress relaxation of strained epitaxial films. The pioneering work of Matthews and Blakeslee (1974, 1975, 1976) first demonstrated the concept of a critical thickness; films below the critical thickness are fully coherent, while above the critical thickness a driving force exists for the relaxation of the coherency stresses. At the time of the studies by Matthews and Blakeslee, the principal stress relaxation mechanism was thought to be plastic flow, but later studies have shown that surface roughening (Srolovitz 1989, Grilhe 1993) and cracking (Murray *et al.* 1996, Dieguez *et al.* 1997) are also important factors in the loss of coherency. The misfit f between the film and substrate is the key microstructural parameter that determines which mechanisms are likely to evolve as film growth proceeds. For example in low-misfit systems ($|f| < 0.01$) the driving force is insufficient to support the homogeneous nucleation of dislocations; so strain relaxation must involve either the propagation of threading dislocations or the operation of heterogeneous nucleation sites. In higher-misfit systems ($|f| > 0.02$) the driving force can support the

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homogeneous nucleation of dislocations, particularly from free surfaces (Freund 1990, Hirth 2000). Similar trends can be noted in studies of cracking, although the literature base is much less extensive. Cracking is usually only observed in high-misfit systems, where the stress in the film lies above a critical threshold value for cracking.

In this paper we present the results of a study of the first stage of stress relaxation in a series of $\text{In}_{1-x}\text{Ga}_x\text{As}_{1-y}\text{P}_y$ films grown by molecular-beam epitaxy on InP (100) substrates. The compositions of the films ($\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$, $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}_{0.5}\text{P}_{0.5}$ and $\text{In}_{0.72}\text{Ga}_{0.28}\text{P}$) were chosen so that $f = 0.02$. Marked differences were found between the two ternary alloy films on the one hand and the quaternary film on the other hand; the ternary films relaxed by a combination of twinning and cracking in the first stages of growth while the quaternary alloy film relaxed only by twinning. The emphasis is placed on the twinning behaviour and the relationship between the surface morphology of the film and twinning. The critical factors that determine whether the film relaxes by twinning or cracking are discussed. Complete accounts of the cracking behaviour in the two ternary films have been presented elsewhere (Wu and Weatherly 1999, 2000).

§ 2. EXPERIMENTAL PROCEDURE

A variety of lattice-mismatched films ($\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$, $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}_{0.5}\text{P}_{0.5}$ and $\text{In}_{0.72}\text{Ga}_{0.28}\text{P}$) with $f = 0.02$ were grown on n-type InP(100) substrates at 480°C using gas-source molecular-beam epitaxy (Okada *et al.* 1997). The films were usually grown as single uncapped layers, but for some runs the samples were grown in a multilayer stack of increasing alloy layer thickness, separated by InP spacer layers. [011] and $[0\bar{1}1]$ cross-section samples were prepared for cross-sectional transmission electron microscopy (XTEM) following standard procedures and examined in a Philips CM12 at 120 kV and a JEOL 2010F at 200 kV. Scanning probe microscopy (SPM) studies were performed in air using a Digital Instruments Nanoscope IIA system.

§ 3. OBSERVATIONS

Both the $\text{In}_{1-x}\text{Ga}_x\text{As}$ and $\text{In}_{1-x}\text{Ga}_x\text{P}$ films showed the same behaviour in the first stages of growth. In $[0\bar{1}1]$ XTEM observations the initial stage of stress relaxation was found to have occurred by twinning, while in the $[011]$ sections stress relief occurred by cracking (figure 1). The critical thickness for twinning (about 10 nm) was slightly less than that for cracking (about 20 nm). The surfaces of the films 10 and 20 nm thick were already rough, but the roughening was much more marked along the $[011]$ than the $[0\bar{1}1]$ direction. In thicker films this anisotropy becomes very pronounced, with the surface evolving into (411) and $(\bar{4}11)$ facets. This anisotropy is illustrated as a function of film thickness in the SPM images of figure 2. The twins often appeared to have nucleated at the re-entrant parts of the roughened surface, where the stress concentration effects would aid nucleation (figure 3). High-resolution transmission electron microscopy (HRTEM) was used to determine the nature of the leading partial associated with twinning. An example is shown in figure 4, where a Burgers circuit has been constructed around the leading partial in the Fourier filtered image from a film 20 nm thick (figure 4(b)). The leading partial is a 90° edge type, in agreement with earlier studies of tensile strained films (Maree *et al.* 1987, Zou and Cockayne 1993). Figure 4(c) shows the complete determination of the dislocations associated with twins 1 and 2 in figure 4(a). Twin 1 is associated with a single partial dislocation at the interface, with a second partial dislocation located

Figure 1. XTEM observations of the first stage of coherency loss in $\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$ films: (a) [011] cross-section of a film 10 nm thick, showing isolated twins, $\mathbf{g} = 200$, (b) [011] cross-section of a film 20 nm thick, showing isolated cracks, $\mathbf{g} = 022$.

roughly at the midpoint between the free surface and the interface. Twin 2 is three (111) planes thick, with all three partial dislocations lying at the interface. There was a small but detectable increase in the average twin thickness in thicker films. Figure 5 shows a twin consisting of five (111) planes in a 200 nm $\text{In}_{1-x}\text{Ga}_x\text{As}$ film. This observation is also in excellent agreement with recent calculations of the variation in twin thickness with film thickness in those systems where twinning is the dominant stress relief mechanism (Dyna and Marty 1998).

In the first stages of the loss of coherency, the 90° twinning dislocations lay at the film-substrate interface (figure 4), but in thicker films, as the density of twins increased, the twins were often observed to penetrate some distance into the substrate (figure 6). Once the twinning dislocations penetrate the interface, they enter a region (the substrate) that is essentially unstressed, so that the forces acting on the dislocation depend on the presence of the free surface, the stacking-fault or twin energy, and any elastic mismatch between the substrate and the film.

The first stages of stress relaxation in the $\text{In}_{1-x}\text{Ga}_x\text{As}_{1-y}\text{P}_y$ film displayed a different pattern of behaviour. Twinning was again the dominant mode of relaxation in the films, but in this case both the [011] and the $[0\bar{1}1]$ XTEM sections showed twinning (figures 7(a) and (b)). The critical thickness for twinning was again approximately 10 nm (see figure 7(c)). The surface roughness in these films was equally pronounced in both the [011] and the $[0\bar{1}1]$ directions, and there was no tendency for the film to develop (411) and $(\bar{4}11)$ facets as growth proceeded (compare figure 8 for $\text{In}_{1-x}\text{Ga}_x\text{As}_{1-y}\text{P}_y$ with figure 2 for the $\text{In}_{1-x}\text{Ga}_x\text{As}$ film). This observation is used in the next section to argue that the nucleation of a 90° partial dislocation has to be aided by the stress concentrations associated with a roughened surface. In the absence of pronounced roughening, film cracking becomes a compe-

Figure 2. SPM observations showing the development of surface roughness in $\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$ films: (a) film 20 nm thick; (b) film 500 nm thick. Note the development of pronounced (411) and $(\bar{4}11)$ facets in the thicker film.

Figure 3. Nucleation of twins at re-entrant parts of an $\text{In}_{0.72}\text{Ga}_{0.28}\text{P}$ film 100 nm thick.

(a)

Figure 4. HRTEM observations of twins in an $\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$ film 20 nm thick: (a) HRTEM image, (b) inverse fast Fourier Transform image of area surrounded by box at termination of twin 1, where the Burgers circuit shows that the dislocation is a 90° partial dislocation; (c) schematic illustration of arrangement of partial dislocations at twins 1 and 2.

(b)

(c)

Figure 4. (continued)

titive or preferred process to plastic relaxation at the stress levels developed in these films in the $[011]$ cross-section.

§ 4. DISCUSSION

The discussion is divided into three sections. In § 4.1 the nucleation of half-loops of perfect or partial dislocations at the free surface of a roughened film is considered. In § 4.2 the critical thickness for dislocation and cracking mechanisms are compared with the experimental observations. In § 4.3 the forces acting on twinning dislocations that penetrate the film–substrate interface are calculated.

Figure 5. HRTEM observation of a twin, five $\{111\}$ planes in thickness, in an $\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$ film 200 nm thick.

4.1. Dislocation nucleation

The nucleation of half-loops of faulted or perfect dislocations (assisted by thermal fluctuations) at a free surface of a tensile strained film has been considered by a number of workers (Maree *et al.* 1987, Kamat and Hirth 1990, Zou and Cockayne 1993). If the surface of the growing film is flat, the change in energy of the system on the introduction of a circular half-loop of radius r is

$$\Delta E = \frac{\mu b^2 r (1 - \nu/2)}{4(1 - \nu)} \ln \left(\frac{\alpha r}{b} \right) \pm 2rb\gamma_s \sin \theta \pm \frac{1}{2}\pi r^2 \gamma_{\text{SF}} - \frac{1}{2}\pi r^2 \tau b, \quad (1)$$

Figure 6. Penetration of twins into the InP substrate in an $\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$ film 100 nm thick ($g = 022$).

where μ is the shear modulus, ν is Poisson's ratio, α is a parameter that is related to the dimensions of the dislocation core, b is the Burgers vector, γ is the surface energy, θ is the angle between the dislocation Burgers vector and the line of intersection of the slip plane and the free surface, γ_{SF} is the stacking-fault energy and τ is the shear stress on the plane of the dislocation loop. τ is related to the biaxial tensile stress σ by the Schmid factor $\tau = \sigma \cos \phi \cos \lambda$, where ϕ is the angle between σ and the slip plane normal, and λ is the angle between σ and the slip direction. σ is given by $[2\mu(1 + \nu)f]/(1 - \nu)$, where f is the misfit.

The first term on the right-hand side of equation (1) is the self-energy of a half loop, taking into account the effects of the free surface, while the fourth term is the work done by the shear stress. The second and third terms represent the energies associated with the formation (annihilation) of surface steps, and the formation (annihilation) of a stacking fault. In the analysis that follows, a surface step is assumed to be annihilated; so the negative sign is used in this case for the second term. The third term does not apply when a perfect (60°) dislocation is nucleated, while it gives a positive contribution if a partial dislocation is formed. If the surface of the film is rough, the effects of the surface roughness have be considered. If the shape of the undulated surface is described by a sinusoidal function of wavelength λ and amplitude e , that is $y = e \sin(2\pi x/\lambda)$, the stress in the film is given by

$$\sigma = \frac{2\mu(1 + \nu)f}{1 - \nu} [1 - ek(ky - 2) \exp(-ky) \sin(kx)], \quad (2)$$

where $k = 2\pi/\lambda$. The maximum stress concentration factor occurs when $\sin(kx) = 1$, and the work done (E_τ) now becomes

Figure 7. XTEM observations of the first stage of coherency loss in $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}_{0.5}\text{P}_{0.5}$ films: (a) [011] cross-section, showing twinning, $g = 200$; (b) [011] cross-section, showing twinning, $g = 200$; (c) progressive development of twinning in a multilayer stack of $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}_{0.5}\text{P}_{0.5}$ films of various thicknesses separated by InP spacer layers, $g = 200$. Note that the 2 and 5 nm films are twin free, while the 10 and 20 nm films show twinning.

Figure 8. SPM observations showing the development of surface roughness in $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}_{0.5}\text{P}_{0.5}$ films: (a) film 20 nm thick; (b) film 500 nm thick. Note the development of islands without the formation of pronounced (411) or $(\bar{4}11)$ facets, as seen for example in figure 2.

Table 1. Properties of $\text{In}_{1-x}\text{Ga}_x\text{As}_{1-y}\text{P}_y$ compounds

Parameter (units)	Value for following compounds				Reference
	$\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$	$\text{In}_{0.5}\text{Ga}_{0.5}\text{As}_{0.5}\text{P}_{0.5}$	$\text{In}_{0.72}\text{Ga}_{0.28}\text{P}$	InP	
μ (GPa)	29.1	28.3	27.1	22.3	Adachi (1982)
ν	0.322	0.333	0.345	0.360	Adachi (1982)
b (60° perfect) (Å)	4.069	4.071	4.0672	4.1499	Adachi (1982)
b (90° partial) (Å)	2.349	2.35	2.35	2.396	Adachi (1982)
α	4	4	4	4	Hirth and Lothe (1982)
γ (J m^{-2}) {011}	0.79	0.83	0.86	0.75	Wu and Weatherly (1999)
γ^{SF} (mJ m^{-2})	49	36	24	18	Gottschalk <i>et al.</i> (1978)
r_f ($= 2\gamma$) (J m^{-2})	1.58	1.66	1.72	1.50	

$$E_{\tau} = \int \tau b \pi y \, dy = \frac{\mu(1 + \nu)}{1 - \nu} f b \pi r^2 \cos \phi \cos \lambda [1 + 2ek \exp(-kr) \sin(kx)]. \quad (3)$$

Equation (1) in combination with equation (3) can be used to calculate how ΔE varies with the loop radius r for smooth and rough films. The parameters used for the $\text{In}_{1-x}\text{Ga}_x\text{As}$ films in the calculations are listed in table 1. For a smooth film the critical value of the activation energy is approximately 16 eV for a 90° leading partial, and 80 eV for a 60° perfect dislocation (figure 9(a)). Both of these values are well above the available free energy of $50kT$ from thermal fluctuations (Hirth and Lothe 1982), which at the growth temperature of 480°C is 3.3 eV. For the rough film the values of e and λ can be estimated from figure 3 to be 2.5 and 20 nm respectively. Substituting these values into equation (3) leads to critical activation energies of 3.4 eV for the 90° partial dislocation, and 47 eV for the perfect dislocation (figure 9(b)). The critical loop radius for the 90° partial is less than 2 nm; so the validity of a continuum elasticity model to describe the nucleation process is questionable. Nevertheless it probably provides a reasonable estimate of the critical energy for nucleation and thus for the roughened film thermal fluctuations could provide sufficient energy to nucleate a half-loop, in agreement with the observations.

The calculations were made for $\text{In}_{0.25}\text{As}_{0.75}\text{As}$ films, but very similar results can be obtained for the other two films. We believe that the different modes of relaxation observed between the two ternary films and the quaternary film must be related to the surface topography of the films. The quaternary film is equally rough in the [011] and $[0\bar{1}1]$ directions, and the local stress concentrations associated with the roughened surface are sufficient to promote the nucleation of 90° partial edge dislocations, leading to four sets of {111} twins, two of which are seen in each of the (011) XTEM images. On the other hand, the two ternary films are much rougher along [011] than $[0\bar{1}1]$; so the critical activation energy to nucleate twins is reached in only one of the two directions.

4.2. Critical thickness considerations

When a defect (dislocation or crack) is formed in a strained film of thickness h , the change in elastic energy of the system is given by

$$\Delta E = E_e + E_{\text{def}}, \quad (4)$$

Figure 9. The variation in ΔE with half-loop radius r for 2% strained $\text{In}_{1-x}\text{Ga}_x\text{As}$ films: (a) for a smooth film; (b) for a rough film taking values of $e = 2.5 \text{ nm}$ and $\lambda = 20 \text{ nm}$ from the HRTEM image in figure 3.

where E_e is the elastic energy relieved by the defect and E_{def} is the energy associated with the defect. The critical thickness for the formation of the defect can be obtained by solving

$$\Delta E = 0. \quad (5)$$

For the formation of a crack, E_{def} is the energy associated with the newly formed crack surfaces. The critical thickness h_c for the formation of a crack is given by (Wu and Weatherly 1999)

$$h_c = \frac{\Gamma_f(1-\nu)^2}{3.96(1+\nu)\mu f^2}, \quad (6)$$

where Γ_f is the fracture resistance of the film.

For the introduction of either a 60° perfect dislocation or a 90° partial dislocation, the elastic energy per unit length relieved by the dislocation is given by

$$E_e = -\frac{2\mu(1+\nu)|f|hb\sin\beta\cos\varphi}{1-\nu}, \quad (7)$$

where β is angle between the Burgers vector of the dislocation and dislocation line, and φ is the angle between the slip plane and the free surface (or interface). The elastic energy per unit length associated with the dislocation is given by

$$E_{\text{def}} = \frac{\mu b^2(1-\nu\cos^2\beta)}{4\pi(1-\nu)}\ln\left(\frac{2h}{r_0}\right) + \frac{\mu b^2\sin^2\beta}{8\pi(1-\nu)}\left(\cos^2\varphi - \sin^2\varphi - \frac{1-2\nu}{2(1-\nu)}\right) \quad (8)$$

for a 60° perfect dislocation, and

$$\begin{aligned} E_{\text{def}} &= E_{\text{disl}} + E_{\text{SF}} \\ &= \frac{\mu b^2(1-\nu\cos^2\beta)}{4\pi(1-\nu)}\ln\left(\frac{2h}{r_0}\right) + \frac{\mu b^2\sin^2\beta}{8\pi(1-\nu)}\left(\cos^2\varphi - \sin^2\varphi - \frac{1-2\nu}{2(1-\nu)}\right) \\ &\quad + U_{\text{core}} + \frac{\gamma_{\text{SF}}h}{\sin\varphi} \end{aligned} \quad (9)$$

for a 90° partial dislocation. r_0 is the dislocation core radius and U_{core} is the energy per unit length of the dislocation core.

Combining equations (4)–(9) leads to two equations defining the critical thickness for the formation of dislocations as follows:

$$\frac{b}{16\pi}\left[(4-\nu)\ln\left(\frac{2h_c}{r_0}\right) - \frac{1}{2} + \frac{29+6\nu}{4(1-\nu)}\right] = (1+\nu)fh_c \quad (10)$$

for a 60° perfect dislocation, and

$$\frac{\mu b^2}{4\pi(1-\nu)}\left[\ln\left(\frac{2h_c}{r_0}\right) - \frac{1}{6} + \frac{7+2\nu}{4(1-\nu)}\right] + \frac{3^{1/2}\gamma_{\text{SF}}h_c}{2^{1/2}} = \frac{2\mu(1+\nu)fh_cb}{3^{1/2}(1-\nu)} \quad (11)$$

for a 90° partial dislocation. Cottrell's (1953) approximation $U_{\text{core}} = (\mu b^2)/[2\pi(1-\nu)^2]$ has been substituted for the dislocation core energy in deriving the results of equations (10) and (11).

A plot of critical thickness h_c versus misfit f for the 60° perfect dislocation, 90° partial dislocation and crack (equation 6) in an $\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$ film is shown in figure 10. The data used for this plot are given in table 1. When $f = 0.02$, h_c for a 90°

Figure 10. The critical thicknesses h_c for the 60° perfect dislocation, the 90° partial dislocation and a crack as functions of the misfit f between the film and substrate.

partial dislocation is approximately 5 nm, while for a crack (assuming that the fracture resistance of the film is 2γ , i.e. the fracture process is purely elastic (Wu and Weatherly 1999)), the corresponding value is 12 nm. If there is no barrier to the surface nucleation of the 90° partial dislocation, stress relief by twinning should be the preferred mode of stress relaxation. On the other hand, if surface nucleation of the 90° partial dislocation is not possible, cracking becomes favoured at a film thickness approximately twice that at which twinning would be predicted. These predictions agree with the trends shown by the $\text{In}_{1-x}\text{Ga}_x\text{As}$ and $\text{In}_{1-x}\text{Ga}_x\text{P}$ films in this study.

4.3. Forces acting on twinning dislocations

In this section we consider first the forces acting on a single twinning dislocation once it has penetrated the film–substrate interface (see figure (6)) and attempt to explain the observation that the twin terminates at some distance from the interface. The analysis is then extended to thicker twins, terminated by several 90° partial dislocations. There are three forces acting on the 90° partial dislocation; a force due to the stacking fault, a force due to the presence of the free surface, and a force due to the elastic mismatch between the film and substrate. Since the film is elastically harder than the substrate (see table 1), the mismatch force would drive the dislocation away from the interface towards the softer substrate, while the other two forces would act to drive the dislocation towards the free surface. The solution to this problem, using Head's (1953) approach with an infinite series of image dislocations, is described in appendix A. Head's method gives an exact solution to the problem if the dislocations are pure screw in character, but it is only an approximate

solution for the edge dislocation. The exact analysis for the edge dislocation is extremely complex (Weeks *et al.* 1968) but, for values of the anisotropy factor $\Gamma \leq 1.5$ ($\Gamma = \mu_f/\mu_s$, where the subscripts f and s stand for the film and substrate respectively), Weeks *et al.* (1968) showed that the image method gives the same result as the exact solution. Since Γ is in the range 1.22–1.3 for the films and substrate used in this study, Head's approach, using image dislocations, should be valid.

The total glide force acting on the 90° partial dislocation is given by equation (A 5) in appendix A. The result is

$$F_g^{\text{total}} = -\frac{\mu_s b^2}{4\pi(1-\nu)d} \left(m - (1-m^2) \sum_{i=1}^{\infty} \frac{d}{d+ih} m^{i-1} \right) \sin \varphi + \gamma_{\text{SF}}. \quad (\text{A } 5)$$

Using this expression with $h = 100$ nm, the force F_g^{total} can be found as a function of the distance d separating the partial from the interface. (Note that in the image shown in figure 6, d lies in the approximate range 5–25 nm.) The equilibrium position of the single partial dislocation ($F_g^{\text{total}} = 0$) is given when $d \approx 5$ nm (figure 11). The maximum value of the force acting to restore the dislocation to this equilibrium position is about 0.024 J m^{-2} (note that this is only slightly greater than γ_{SF} for InP), corresponding to a shear stress of about 100 MPa. For thicker twins, the analysis is simply extended by replacing b by nb , where n is the number of 90° edge dislocations terminating the twin. The force due to the twin will still be given by γ_{SF} , since to a first approximation the twin energy γ_{T} is given by $\gamma_{\text{T}} = \gamma_{\text{SF}}/2$, and the force due to the two surfaces of the twin will be γ_{SF} . From the form of equation (A 5), the first term on the right-hand side of the equation will quickly dominate the

Figure 11. Plots of equation (A 5) in appendix A, for the case of a 90° partial dislocation, with (---) or without (—) consideration of the force due to the stacking fault (twin).

second term as n increases, and the equilibrium position will be given by the solution inside the large parentheses. This is just the original expression due to Head (1953). The equilibrium position (ignoring γ_{SF} in equation (A 5)) is given by $d \approx 15$ nm (see figure 11). The predicted range (5–15 nm) is in reasonable accord with the experimental observations (5–25 nm) for films 100 nm thick. Note also that equation (A 5) would predict that the equilibrium position d of the dislocation increases as the film thickness increases. This agrees with the trends that we observed.

§ 5. CONCLUSIONS

- (1) 2% strained $\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$ and $\text{In}_{0.72}\text{Ga}_{0.28}\text{P}$ films grown on $\text{InP}(100)$ substrates initially relax by twinning (as seen in $[0\bar{1}1]$ cross-sections) and by cracking (as seen in $[011]$ cross-sections).
- (2) Homogeneous nucleation of 90° partial dislocations at the free surface is possible at the growth temperature of 480°C , provided that a critical degree of surface roughness is present to aid the nucleation process by locally enhancing the stress. In the absence of pronounced surface roughening (as seen in $[011]$ cross-sections), the preferred stress relaxation mechanism is cracking.
- (3) 2% strained $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}_{0.5}\text{P}_{0.5}$ films initially relax by twinning in both the $[0\bar{1}1]$ and the $[011]$ cross-sections. This was associated with a three-dimensional surface roughening, in contrast with the two-dimensional roughening of the ternary films, which permitted surface nucleation of twins on all four possible twin systems.
- (4) The critical thickness at which either twinning or cracking was observed correlated well with calculations based on criteria first introduced by Matthews and Klokholm (1972) and Matthews and Blakeslee (1974).
- (5) The observation that the twins often penetrated the interface, with the 90° partial dislocations lying in the InP substrate, can be explained by considering the equilibrium between forces associated with the elastic mismatch between the film and substrate, the free surface and the stacking-fault or twin energy.

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APPENDIX A

FORCES ACTING ON TWINNING DISLOCATIONS

For a 90° partial dislocation bounded by a stacking fault shown in figure 6 (note that the 90° partial dislocation is located in the InP substrate), the total force acting on this dislocation arises from three factors. Assuming that all the misfit strain is confined in the film (i.e. there is no misfit strain in the substrate, which is valid when the film thickness is much less than that of the substrate), these are

- (a) the force due to the stacking fault,
- (b) the interaction between the dislocation and the free surface and
- (c) the interaction between the dislocation and the interface.

The solution to (a) is simply the stacking-fault γ_{SF} energy of InP. The solutions to (b) and (c) can be obtained as follows.

Consider first an infinite isotropic elastic solid of shear modulus μ_f for $y > 0$, and μ_s for $y < 0$, having the same Poisson's ratios. An edge dislocation with Burgers vector $b = (b \cos \varphi, b \sin \varphi, 0)$ (φ is the angle between the slip plane and the interface) is located at $(0, -d)$. Then the stress field for $y < 0$ is given by the superposition of the original dislocation stress field and an image dislocation at $(0, d)$ with the following stress field (Mura 1968):

$$\begin{aligned}\sigma_{xx} &= \frac{\mu_s b \cos \varphi}{2\pi(1-\nu)} \frac{1}{2d} \left[-\frac{1}{2}(A+B) \right], \\ \sigma_{yy} &= \frac{\mu_s b \cos \varphi}{2\pi(1-\nu)} \frac{1}{2d} \left[+\frac{1}{2}(A+B) \right], \\ \sigma_{xy} &= \frac{\mu_s b \sin \varphi}{2\pi(1-\nu)} \frac{1}{2d} \left[-\frac{1}{2}(A+B) \right],\end{aligned}\quad (\text{A } 1)$$

where $A = (1 - \Gamma)/(1 + \kappa\Gamma)$, $B = \kappa(1 - \Gamma)/(\kappa + \Gamma)$, $\kappa = 3 - 4\nu$ and $\Gamma = \mu_f/\mu_s$.

This can be extended to the case of a semi-infinite isotropic solid of modulus μ_s for $y < 0$, and μ_f for $0 < y < h$, with a free surface at $y = h$, and an edge dislocation with Burgers vector $b = (b, 0, 0)$ ($\varphi = 0^\circ$) situated at $(0, -d)$. In this case, the force acting on the dislocation due to the interface and free surface arises from the climb force of σ_{xx} and can be described by an infinite set of image dislocations located at $(0, y)$ with strengths as in table A 1 (Head 1953). The total force acting on the dislocation due to the free surface and interface is given by

$$-\sum_{i=1}^{\infty} \sigma_i b = -\frac{\mu_s b^2}{4\pi(1-\nu)d} \left(m - (1 - m^2) \sum_{i=1}^{\infty} \frac{d}{d + ih} m^{i-1} \right). \quad (\text{A } 2)$$

Table A 1. Strengths of an infinite set of image dislocations at $(0, y)$, where $m = -\frac{1}{2}(A+B)$ is the strength of the first image dislocation, located at $(0, +d)$.

Position of image: value of y	Strength of image	σ_{xx}
d	m	$\frac{\mu_s b}{2\pi(1+\nu)} \frac{1}{d+d} m$
$d + 2h$	$-(1 - m^2)$	$\frac{\mu_s b}{2\pi(1+\nu)} \frac{1}{d+d+2h} [-(1 - m^2)]$
$d + 4h$	$-(1 - m^2)m$	$\frac{\mu_s b}{2\pi(1+\nu)} \frac{1}{d+d+4h} [-(1 - m^2)m]$
$d + 6h$	$-(1 - m^2)m^2$	$\frac{\mu_s b}{2\pi(1+\nu)} \frac{1}{d+d+6h} [-(1 - m^2)m^2]$
$d + 8h$	$-(1 - m^2)m^3$	$\frac{\mu_s b}{2\pi(1+\nu)} \frac{1}{d+d+8h} [-(1 - m^2)m^3]$
$\vdots$	$\vdots$	$\vdots$

For an edge dislocation with Burgers vector $b = (b \cos \varphi, b \sin \varphi, 0)$, it can be shown that the total climb force (acting perpendicular to the slip plane) due to the free surface and interface is given by

$$F_c = -\frac{\mu_s b^2}{4\pi(1-\nu)d} \left(m - (1-m^2) \sum_{i=1}^{\infty} \frac{d}{d+ih} m^{i-1} \right) \cos \varphi, \quad (\text{A } 3)$$

while the total glide force (acting along b) is

$$F_g = -\frac{\mu_s b^2}{4\pi(1-\nu)d} \left(m - (1-m^2) \sum_{i=1}^{\infty} \frac{d}{d+ih} m^{i-1} \right) \sin \varphi. \quad (\text{A } 4)$$

Therefore the total glide force acting on the 90° dislocation is given by

$$F_g^{\text{total}} = -\frac{\mu_s b^2}{4\pi(1-\nu)d} \left(m - (1-m^2) \sum_{i=1}^{\infty} \frac{d}{d+ih} m^{i-1} \right) \sin \varphi + \gamma_{\text{SF}}, \quad (\text{A } 5)$$

with $\varphi = 54.74^\circ$.

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