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The surface topography of cracks in strained $In_{0.72}Ga_{0.28}P$ films

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ABSTRACT

Cracks in a 2% tensile strained $In_{0.72}Ga_{0.28}P$ film grown on an InP substrate by molecular-beam epitaxy have been studied by cross-section transmission electron microscopy and scanning probe microscopy. A dislocation analogue (i.e. replacing the crack by an array of equivalent infinitesimal edge dislocations) is employed to account for the ratio of the crack-opening displacement to the normal surface displacement associated with the crack.

§ 1. INTRODUCTION

Highly strained epitaxial films can relax by surface roughening, by plastic deformation or by cracking (if the film is under tension). The latter mechanism is also commonly found in films where the strains are associated with a thermal mismatch between the film and substrate (Hutchinson and Suo 1991). Cracking of strained compound semiconductor films has been reported by Murray *et al*. (1996) and Wu and Weatherly (1999). Murray *et al*. (1996) noted that the cracking process was associated with a normal displacement of the free surface of the film in the vicinity of the crack, and used this observation to estimate the amount of stress (strain) relaxation associated with film cracking.

In this letter we report a combined transmission electron microscopy (TEM) and scanning probe microscopy (SPM) investigation of cracks in a 2% tensile-strained $In_{0.72}Ga_{0.28}P$ film 100 nm thick grown on an InP(100) substrate. We demonstrate that both the crack-opening displacement and the normal displacement of the free surfaces in the crack vicinity can be understood by considering the equivalent dislocation analogue of the surface crack.

§ 2. EXPERIMENTAL DETAILS

A lattice-mismatched $In_{0.72}Ga_{0.28}P$ film 100 nm thick with a 2% tensile strain was grown on an n-type InP (100) substrate at 480°C using gas-source molecular beam epitaxy (Okada *et al*. 1997). [011] and $[01\bar{1}]$ cross-section samples were prepared for TEM following standard procedures and examined in a Philips CM12 operating at 120 kV. SPM studies were performed in air using a Digital Instruments Nanoscope III system.

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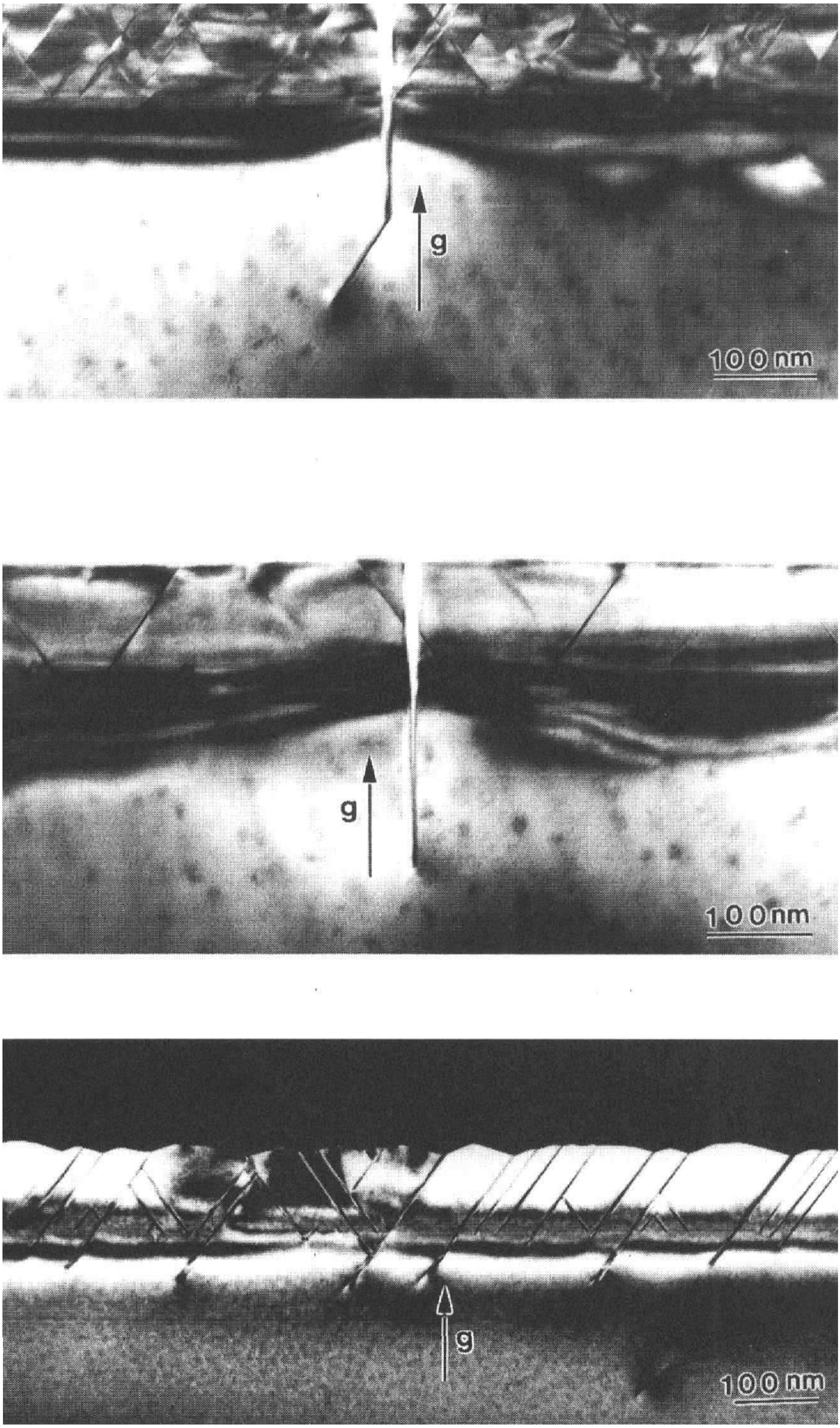


(*a*)

(*b*)

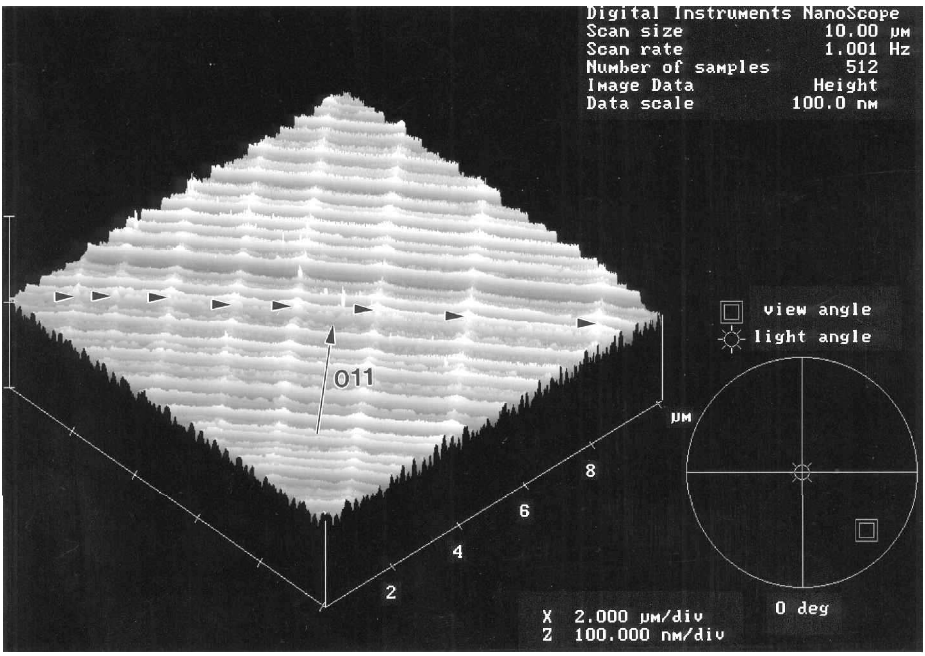
(*c*)

Figure 1. $\mathbf{g} = 400$ cross-section TEM images. (*a*) The crack arrests on the $(1\bar{1}1)$ plane after penetrating into the substrate along (011) in the $[011]$ cross-section. (*b*) The crack arrests on the $(0\bar{1}1)$ plane after penetrating into the substrate along in $(0\bar{1}1)$ in the $[011]$ cross-section. (*c*) Planar defects and surface undulation in the $[0\bar{1}1]$ cross-section.

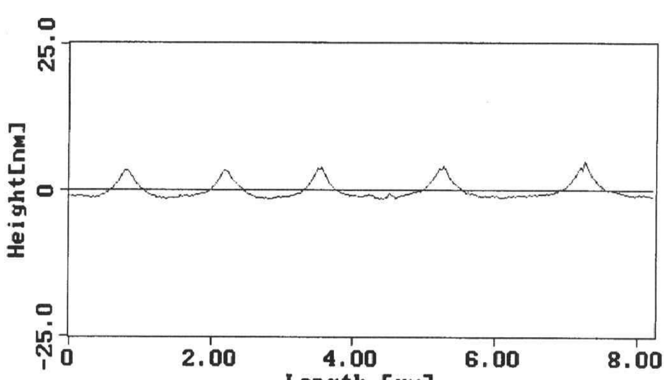
§ 3. Observations

A variety of crack morphologies were found in the films, as shown by the [011] cross-section TEM observations in figure 1. The majority of the cracks penetrated some distance into the substrate along the $(0\bar{1}1)$ plane, before deviating and arresting on the $(1\bar{1}1)$ or $(\bar{1}\bar{1}1)$ planes (figure 1 (*a*)). However, on occasion, cracks were observed to arrest after penetrating into the substrate only along the $(0\bar{1}1)$ plane (figure 1 (*b*)). The stress relaxation mechanisms observed in the orthogonal $[0\bar{1}1]$ section were a combination of surface roughening and twinning (figure 1 (*c*)). The reasons for this behaviour have been discussed by Wu and Weatherly (1999).

The SPM observations from the same set of cracks are summarized in figures 2 and 3. If a relatively large area (10 μm × 10 μm) was scanned, the normal surface



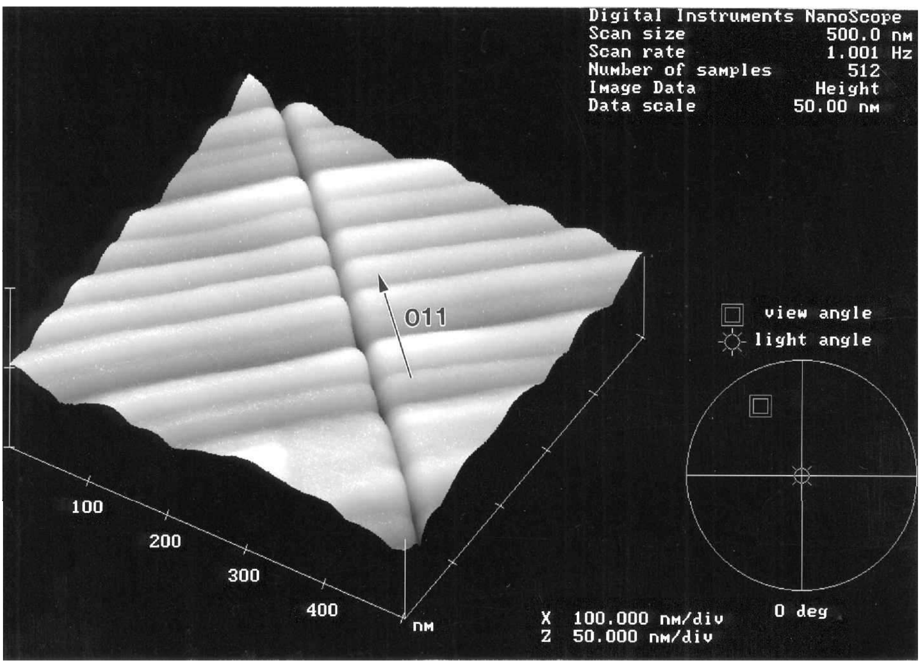
(*a*)



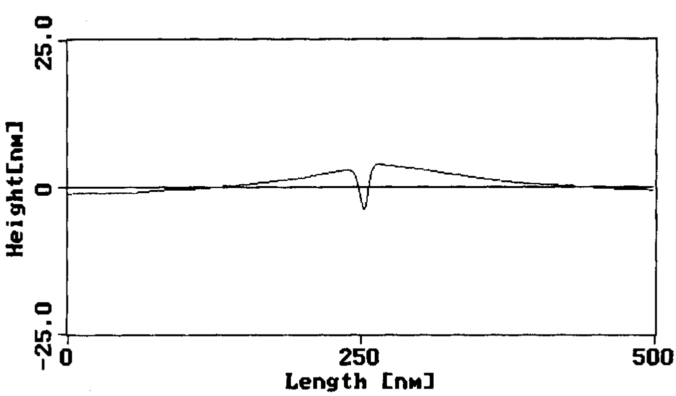
(*b*)

Figure 2. SPM image and surface profile. (*a*) Eight cracks (indicated by arrowheads) running along the [011] direction. The normal surface displacement associated with the cracks is visible. (*b*) Surface profile along the direction perpendicular to the [011] direction.

displacement associated with the cracks was readily detected, but the cracks themselves (and the crack-opening displacement) were not seen. The positions of the cracks are indicated by arrowheads in figure 2 (*a*), and the corresponding surface topography, as measured in a direction normal to the plane of the crack, are shown in figure 2 (*b*). The assessment of the overall surface morphology in these films is complicated by the roughening associated with surface faceting on (411) and $(4\bar{1}\bar{1})$ planes (Okada *et al.* 1997). This phenomenon is clearly seen in the image in figure 3 (*a*). However, measurements of the surface displacement associated with cracking were obtained from line traces where there was no interference from the surface roughening. SPM images taken at a higher magnification showed both the crack-opening displacement and the normal displacement (figures 3(*a*) and (*b*)).



(*a*)



(*b*)

Figure 3. SPM image and surface profile. (*a*) A crack running along [011] direction. The crack opening displacement is visible. (*b*) Surface profile along the direction perpendicular to the [011] direction.

Table 1. Summary of SPM observations on an $In_{0.72}Ga_{0.28}P$ film 100 nm thick.

δ_0 (nm)	l (nm)
18.5	5.2
19.5	5.2
20.5	6.0
20.5	6.3
19.5	7.1
19.7	7.5
	6.0
	7.1
	5.2
	6.0
19.7 ± 0.7	6.2 ± 0.8

Table 1 summarizes measurements of the crack-opening displacement δ_0 and maximum normal surface displacement (l) obtained from a number of SPM images of cracks in the $In_{0.72}Ga_{0.28}P$ film 100 nm thick. The average value of δ_0/l is approximately three.

§ 4. Discussion

We start the discussion by first considering the use of a dislocation analogue for a surface crack in a thin epitaxial film, within the framework of isotropic elasticity. The geometry of the crack is shown in figure 4 (*a*), with the dislocation analogue in figure 4 (*b*). This analogy has been used in a recent theoretical study of grain-boundary 'diffusion wedges' by Gao *et al.* (1999), although they concentrated on time-dependent stress relaxation phenomena rather than cracking *per se*. These workers used Head's (1953) approach to describe the stress field of an array of infinitesimal

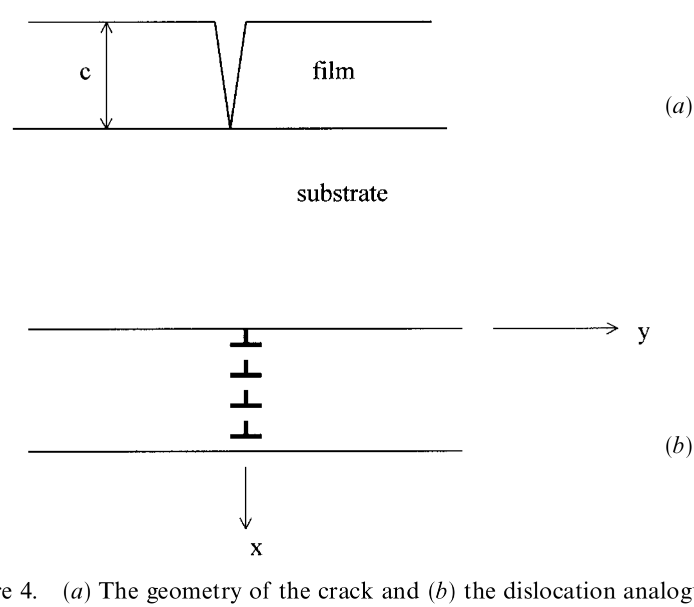


Figure 4. (*a*) The geometry of the crack and (*b*) the dislocation analogue.

edge dislocations, $b(x')\,\mathrm{d}x'$, extending from the free surface ($x = 0$) to the tip of the diffusion wedge (or crack) at $x = c$. For a dislocation at a distance h from the free surface, Head's solutions for σ_{xx} and σ_{yy} are

$$\sigma_{xx} = \frac{\mu b(x')\,\mathrm{d}x'}{2\pi(1-\nu)}\left(\frac{(x-h)[(x-h)^2-y^2]}{[(x-h)^2+y^2]^2} - \frac{(x-h)[(x-h)^2-y^2]}{[(x+h)^2+y^2]^2} + 2h\,\frac{(3x+h)(x+h)^3-6x(x+h)y^2-y^4}{[(x+h)^2+y^2]^3}\right) \qquad (1\,a)$$

$$\sigma_{yy} = \frac{\mu b(x')\,\mathrm{d}x'}{2\pi(1-\nu)}\left(\frac{(x-h)[(x-h)^2+3y^2]}{[(x-h)^2+y^2]^2} - \frac{(x-h)[(x-h)^2+3y^2]}{[(x+h)^2+y^2]^2} - 2h\,\frac{(x-h)(x+h)^3-6x(x+h)y^2+y^4}{[(x+h)^2+y^2]^3}\right) \qquad (1\,b)$$

where μ and ν are the shear modulus and Poisson's ratio respectively.

When $y = 0$, these two expressions reduce to

$$\sigma_{xx} = \frac{\mu b(x')\,\mathrm{d}x'}{2\pi(1-\nu)}\left(\frac{1}{x-h} - \frac{1}{x+h} + 2h\,\frac{3x+h}{(x+h)^3}\right) \qquad (2\,a)$$

$$\sigma_{yy} = \frac{\mu b(x')\,\mathrm{d}x'}{2\pi(1-\nu)}\left(\frac{1}{x-h} - \frac{1}{x+h} - 2h\,\frac{x-h}{(x+h)^3}\right) \qquad (2\,b)$$

The dislocation array will be equivalent to the crack if the stress σ remote from the crack annuls the stress associated with the dislocation array at $y = 0$, that is

$$\sigma = \frac{\mu}{2\pi(1-\nu)}\int_0^c b(x')\left(\frac{1}{x-x'} - \frac{1}{x+x'} - 2x'\,\frac{x-x'}{(x+x')^3}\right)\mathrm{d}x'. \qquad (3)$$

Gao *et al.* (1999) have given the solution to equation (3). They showed that the crack-opening displacement $\int_0^c b(x')\,\mathrm{d}x'$ at the free surface, is approximately $5.8\sigma c/E$, where E is Young's modulus. This result, as expected, is identical with the classical fracture mechanics result for δ_0 for a surface crack given by Tada *et al.* (1985).

The dislocation analogy can also be used to estimate the surface displacements, u_x and u_y. Using Head's equations (1 *a*) and (1 *b*), we can show that at the free surface ($x = 0$) the normal displacement u_x is given by

$$u_x = -\frac{b(x')\,\mathrm{d}x'}{\pi}\,\frac{h^2}{h^2+y^2}. \qquad (4)$$

(The negative sign indicates that the surface relaxation corresponds to a local bulging of the surface, as observed.)

The total displacement at $y = 0$ is obtained by superposition, leading to the final result that

$$u = -\frac{1}{\pi}\int_0^c b(x')\,\mathrm{d}x'. \qquad (5)$$

$|u|$ is identically equal to the experimental measurement l; so this simple analogy suggests that $|\delta_0/l| = \pi$. This is in excellent agreement with the average δ_0/l ratio of 3.2 found experimentally (see table 1).

The analysis leading to the conclusion $\delta_0/l = \pi$ will still hold for cracks that penetrate into the substrate without deviating (figure 1(*b*)), but an asymmetry in the surface profile would be expected for cracks that deviate on to $\{111\}$ planes before arresting. Indeed we have often observed a small asymmetry in the surface profiles (see for example figure 3 (*b*)) but, as most of the contribution to l comes from the $b(x')\,dx'$ components nearest to the surface, this will have little overall effect on the magnitude of l or on the ratio δ_0/l.

Finally, it should be noted that the surface relaxation associated with the cracks is entirely consistent with the state of strain in the film prior to cracking. The film is in a state of biaxial tension prior to stress relief, so that the through-thickness strain (in the x direction) is given by $-[\nu/(1-\nu)](\varepsilon_{zz} + \varepsilon_{yy})$, where ν is Poisson's ratio. It is the local relaxation of this strain in the neighbourhood of the crack that leads to the surface profiles found by SPM. The elastic strain energy released by cracking must be evaluated from the integral $-\frac{1}{2}\int_{\delta_b}^{\delta_0} \sigma\delta(x)\,dx$, where δ_b and δ_0 are the crack opening displacements at the film–substrate interface and free surface respectively (Hutchinson and Suo 1991, Ye *et al.* 1992, Wu and Weatherly 1999).

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