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DISLOCATION NUCLEATION AND PROPAGATION IN SEMICONDUCTOR HETEROSTRUCTURES

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Abstract

This paper considers misfit dislocation nucleation and propagation in dilute magnetic semiconductor heterostructures in the CdTe-ZnTe-MnTe system. It is shown that, where the deposit is in tension, $1/2\langle 110\rangle$ dislocations with inclined Burgers vectors propagate by glide along interfacial $\langle 110\rangle$ directions and may dissociate giving intrinsic stacking faults. In cases where the deposit is in compression, $1/2\langle 110\rangle$ dislocations show no evidence of dissociation and propagate by extensive cross-slip to give networks of dislocations close to interfacial $\langle 100\rangle$ directions.

Evidence for dislocation sources in ZnTe/GaSb films is presented. ZnTe films contained stacking fault pyramids, single Frank faults and a new type of "diamond defect" are present at densities up to about 10^7 cm^{-2} . Analysis showed that the diamond defects, which were four-sided defects on $\{111\}$ planes with $\langle 110\rangle$ edges, were of vacancy type with $1/3\langle 111\rangle$ Frank Burgers vectors and intrinsic stacking faults. Although faulted defects showed no tendency to grow by climb, evidence is given for an unfaulted reaction in which a glissile $1/2\langle 110\rangle$ dislocation is generated. This new model for dislocation nucleation is discussed.

Key Words: Misfit dislocations, stacking fault pyramids, nucleation of dislocations, CdTe/CdMnTe, ZnTe/GaSb, diamond defects, transmission electron microscopy.

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Introduction

The introduction of misfit dislocations during the epitaxial growth of (001) semiconductor heterostructures has been widely studied. In this paper, we consider misfit dislocation nucleation and growth in a comparatively new dilute magnetic semiconductor system CdTe-ZnTe-MnTe. The samples were grown by molecular beam epitaxy in a Varian V80H system at the University of Hull, U.K. Growth was carried out using InSb or GaSb substrates, with substrate temperatures in the range 240-290°C and at growth rates of 1-2 Å seconds⁻¹.

In the paper, we concentrate on the role of the sign of the misfit stress on dislocation propagation, the propagation mechanism (glide or climb) and on the question of misfit dislocation nucleation.

Dislocation Propagation

Background

It is generally agreed that the presence of $1/2\langle 110\rangle$ dislocations with inclined Burgers vectors in (001) heterostructures is due to glide on inclined $\{111\}$ planes. There is good evidence that the propagation mechanism depends on the sign of the misfit strain. For example, Marée *et al.* (1987) compared misfit dislocations found in Si/GaP, where the deposit was in tension, with those in $\text{In}_{0.07}\text{Ga}_{0.93}\text{As}/\text{GaAs}$ where the deposit was in compression. In both systems, dislocations were of $1/2\langle 110\rangle$ type with Burgers vectors inclined to the (001) plane. However, whereas in Si/GaP dislocations tended to lie accurately along interfacial $\langle 110\rangle$ directions and were often dissociated, those in $\text{In}_{0.07}\text{Ga}_{0.93}\text{As}/\text{GaAs}$ were undissociated and often deviated from the interfacial $\langle 110\rangle$ directions. The reasons for different behaviour in the tension and compression cases have been discussed by Cherns (1987). The basic point is that the dissociation of 60° dislocations on inclined $\{111\}$ planes into 90° and 30° partials is such that the leading partial is of 90° type when the deposit is in tension and of 30° type when the deposit is in compression (Fig. 1).

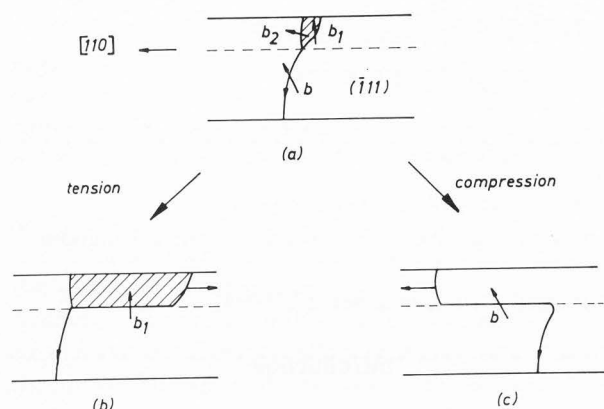


Figure 1. (a) Dissociation of a threading dislocation with Burgers vector b in a bicrystal into a 90° partial b_1 , and a 30° partial b_2 . With the greater misfit force acting on the 90° partial, dislocations should tend to dissociate when the top layer is under tension (b) and remain undissociated when the top layer is compressed (c).

Since the greater force due to the misfit stress is on the 90° partial, dislocations in layers under tension should tend to dissociate. Conversely, in cases where the deposit is under compression, we might expect partial separations to be less than their equilibrium values or for dislocations to exist in undissociated form. In the latter case, it is easy to envisage that misfit dislocations propagating on one $\{111\}$ plane might undergo glide or climb on a second plane such that misfit dislocations deviate from the interfacial $\langle 110 \rangle$ directions. Bonar *et al.* (1992) observed dislocations at InGaAs/GaAs interfaces close to $\langle 100 \rangle$ interfacial directions and concluded that glide on $\langle 110 \rangle$ planes was involved. In preliminary work (Cherns *et al.*, 1993), we have shown that $\langle 100 \rangle$ segments of misfit dislocation in CdMnTe/CdTe and CdMnTe/ZnTe layers probably arise through cross-slip on $\{111\}$ planes. We consider this further below for the CdMnTe/CdTe system.

Observations on CdMnTe/CdTe interfaces

In order to examine the influence of misfit strain on misfit dislocation propagation in CdMnTe/CdTe layers, we have examined pairs of equivalent structures in which CdMnTe layers were deposited on thick relaxed CdTe epilayers or vice versa. Such structures enable us to examine the effect of reversing the sign of the misfit strain.

Figure 2a shows misfit dislocations in a 1200 \AA $\text{Cd}_{0.845}\text{Mn}_{0.155}\text{Te}/2.4 \mu\text{m CdTe}/(001)\text{InSb}$ sample. The misfit dislocations, located at the CdMnTe/CdTe interface, lie predominantly along interfacial $\langle 110 \rangle$ directions. Some dislocations were dissociated giving intrinsic

stacking faults which often extended several micrometers along the interface. Figure 2a contains several such faults, possibly lying on the same $\{111\}$ slip plane. Figure 2b shows misfit dislocations in a 1100 \AA CdTe/ $2.3 \mu\text{m Cd}_{0.831}\text{Mn}_{0.169}\text{Te}/230 \text{ \AA CdTe}/(001)\text{InSb}$ sample. In this case, dislocations, located at the top CdTe/CdMnTe interface, lie predominantly along interfacial $\langle 100 \rangle$ directions. A close inspection shows that $\langle 100 \rangle$ segments zig-zag on a fine scale between the $[110]$ and $[\bar{1}\bar{1}0]$ directions.

The sample illustrated in Figure 2a was such that the CdMnTe top layer grew on a predominantly relaxed CdTe epilayer, and thus, initially (when pseudomorphic) had a tensile strain of about 0.3% in the (001) plane. The sample in Figure 2b was such that the CdMnTe should be relaxed, thus, putting the CdTe top layer into a compressive strain of about 0.3%. The results in Figure 2 are, thus, in agreement with the idea that dislocations in layers under tension tend to move in dissociated form, and thus, remain confined to a single $\{111\}$ slip plane. The $\langle 100 \rangle$ segments in Figure 2b imply that misfit dislocations in the compressed CdTe layer become undissociated. The zigzagged configuration strongly suggests cross-slip, which can be easily envisaged if the threading segment adopts screw orientation, i.e., along the $\langle 110 \rangle$ direction common to two intersecting $\{111\}$ slip planes.

Experimentally, it was found that the threading segments of $\langle 100 \rangle$ misfit dislocations deviated significantly from screw orientation, particularly near the top surface, tending to be close to $\langle 112 \rangle$ directions in one of the two $\{111\}$ slip planes. If the process is indeed cross-slip, this means that the threading segment has either changed orientation following cessation of slip or that movement of jogged segments is involved. In the latter case, emission or absorption of point defects at the jogs, i.e., climb, must also take place (e.g., see Hirth and Lothe, 1968). There is no evidence for $\{110\}$ slip (Bonar *et al.*, 1992) since we would expect threading segments to lie wholly within the vertical $\{110\}$ slip plane in this case (perhaps stabilized by dissociation within this plane). The interfacial segments of misfit dislocation would also lie accurately along $\langle 100 \rangle$ directions, the line of intersection of the (001) and $\{110\}$ planes, which is not observed.

Climb versus glide

The possibility of climb during cross-slip has been raised in the previous section. We should therefore consider whether there is further evidence for climb in these foils. First, it should be noted that, in addition to $1/2 \langle 110 \rangle$ interfacial dislocations, all of the samples considered in this paper contained stacking fault pyramids and single stacking faults which emanated from the

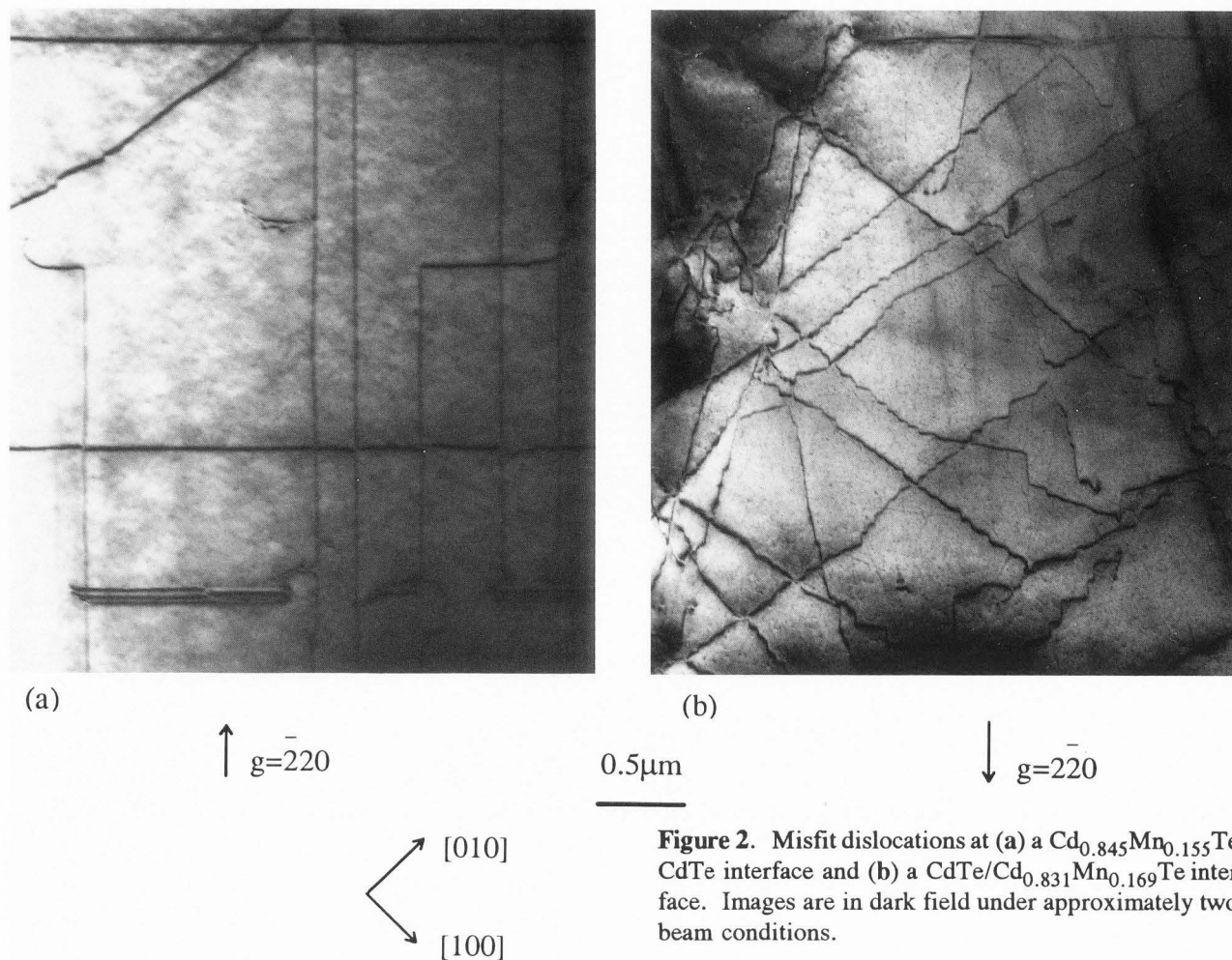


Figure 2. Misfit dislocations at (a) a $\text{Cd}_{0.845}\text{Mn}_{0.155}\text{Te}/\text{CdTe}$ interface and (b) a $\text{CdTe}/\text{Cd}_{0.831}\text{Mn}_{0.169}\text{Te}$ interface. Images are in dark field under approximately two-beam conditions.

epilayer/substrate interface (e.g., see later, Figs. 5 and 6). It is generally expected that such faults result from heterogeneous nucleation indicative of impurities at the substrate surface prior to growth. Analysis showed that the majority of single faults were of Frank type with $1/3 \langle 111 \rangle$ Burgers vectors. Since the Burgers vectors are perpendicular to the fault plane, these Frank dislocations can only extend in the interface by climb. The fact that none of these faults was observed to be extended in the interfacial plane suggests that dislocation climb was, in general, insignificant.

Diamond Defects

Observations on ZnTe/GaSb films showed the presence of small faulted loops which lay on $\{111\}$ planes and had edges along $\langle 110 \rangle$ directions. Figure 3 shows an area from a $0.22 \mu\text{m}$ ZnTe/GaSb sample containing several such loops, which divide the two $\{111\}$ planes whose normals project along the direction of g . By analogy with similarly shaped loops found in Si/SiGe foils (Eaglesham *et al.*, 1989; see Humphreys *et al.*,

1989 for a review), we shall call these "diamond defects." In addition to diamond defects, Figure 3 shows a low density of $1/2 \langle 110 \rangle$ interfacial dislocations as expected from the low natural mismatch in ZnTe/GaSb (0.07%).

Observations showed that the diamond defects in ZnTe/GaSb lay on only one of the two sets of $\{111\}$ planes. Analyses were carried out to determine the defect type. Some of the salient points are illustrated in Figure 4 which shows a pair of diamond defects lying on oppositely inclined $\{111\}$ planes imaged under two-beam conditions in various reflections. In Figures 4a and 4b, taken in $g = 220$ and $g = \bar{2}20$, respectively, the defects show inside/outside contrast with the defect A being in outside contrast in Figure 4a and inside contrast in Figure 4b while defect B shows the opposite behaviour.

Both diamond defects in Figure 4 appear in residual contrast in $g = \bar{2}20$ (Fig. 4c) implying $g \cdot b = 0$ (and $g \cdot R = 0$ for the fault). The image in $g = 02\bar{2}$ (Fig. 4f), taken with the defect B nearly normal to the electron beam, also shows defect A in residual contrast. Together, these observations suggest a Burgers vector parallel

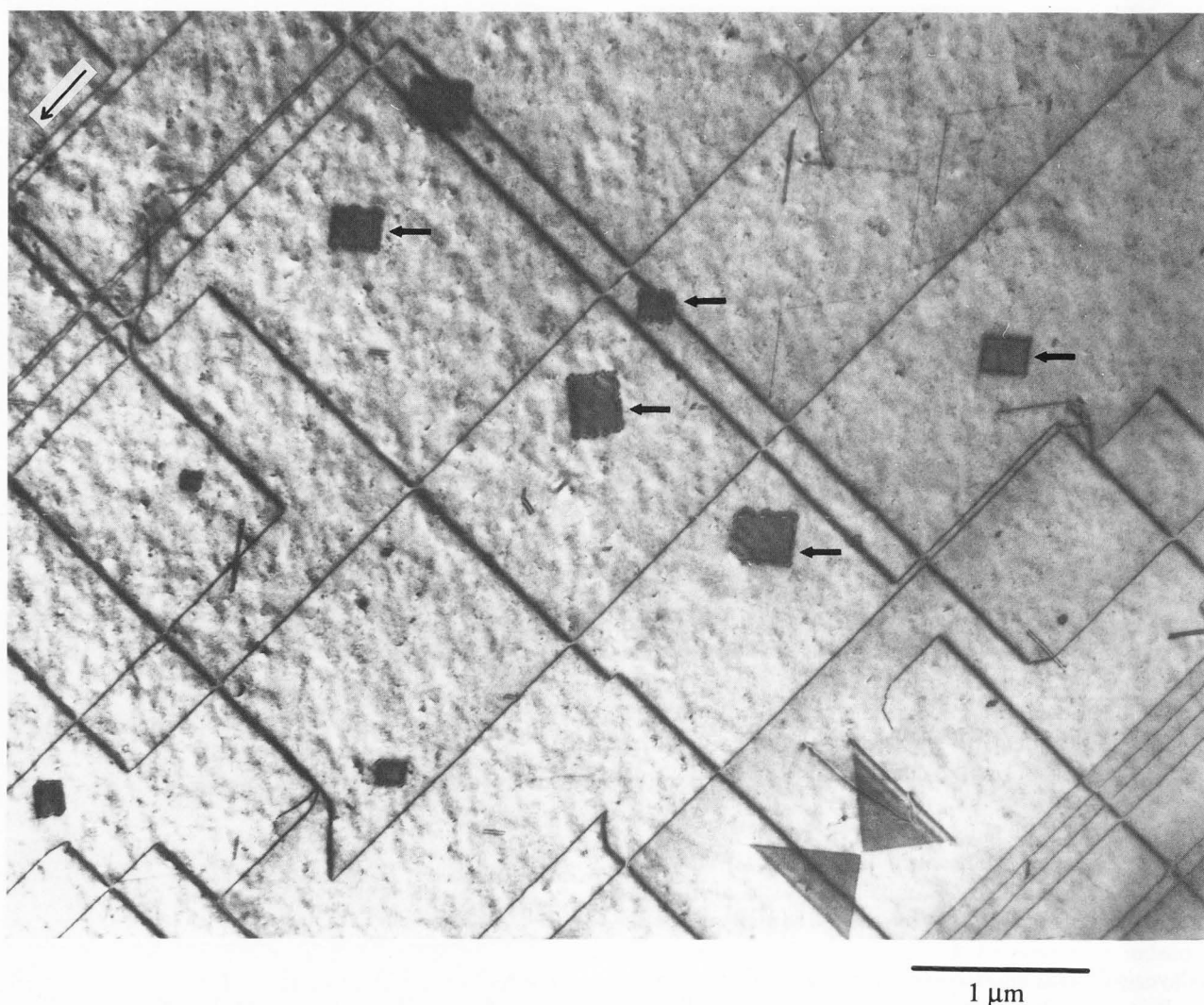


Figure 3. Diamond defects in a $0.22\mu\text{m}$ ZnTe/GaSb bicrystal. The diamond defects (some are arrowed) lie on either of the inclined $\{111\}$ planes whose traces run bottom right to top left (c.f., the partially visible stacking fault pyramid, bottom right).

to the $\langle 111 \rangle$ fault normal implying a $1/3\langle 111 \rangle$ Frank dislocation. The sense of the inside/outside contrast in Figures 4a and 4b implies that the Frank is of vacancy type.

The defect A in addition extends through the foil and emerges from the bottom surface of the foil (the ZnTe surface) where the dark field fringe contrast is strongest (Fig. 4d). The sense of the terminating fringe (light) implies that the fault is of intrinsic type (Gevers *et al.*, 1963), as expected for a vacancy-type Frank defect.

The analysis in Figure 4 has been repeated for other diamond defects which all appear to be of the same type. The diamond defects in ZnTe/GaSb thus differ from those in Si/SiGe which were found to be interstitial in

character with $1/6\langle 114 \rangle$ Burgers vectors (Eaglesham *et al.*, 1989).

Dislocation Nucleation

Experimental results

As the diamond defects in Si/SiGe have been proposed as nucleation sources for glide dislocations {see Humphreys *et al.* (1989) for a correct model}, we have considered whether the Frank defects in ZnTe/GaSb can act as dislocation sources. First, it should be noted that intrinsic Frank faults are present either as diamond defects, as part of incomplete stacking fault pyramids, or as single triangular faults whose geometry is equivalent to one face of a pyramid.

Dislocation nucleation and propagation

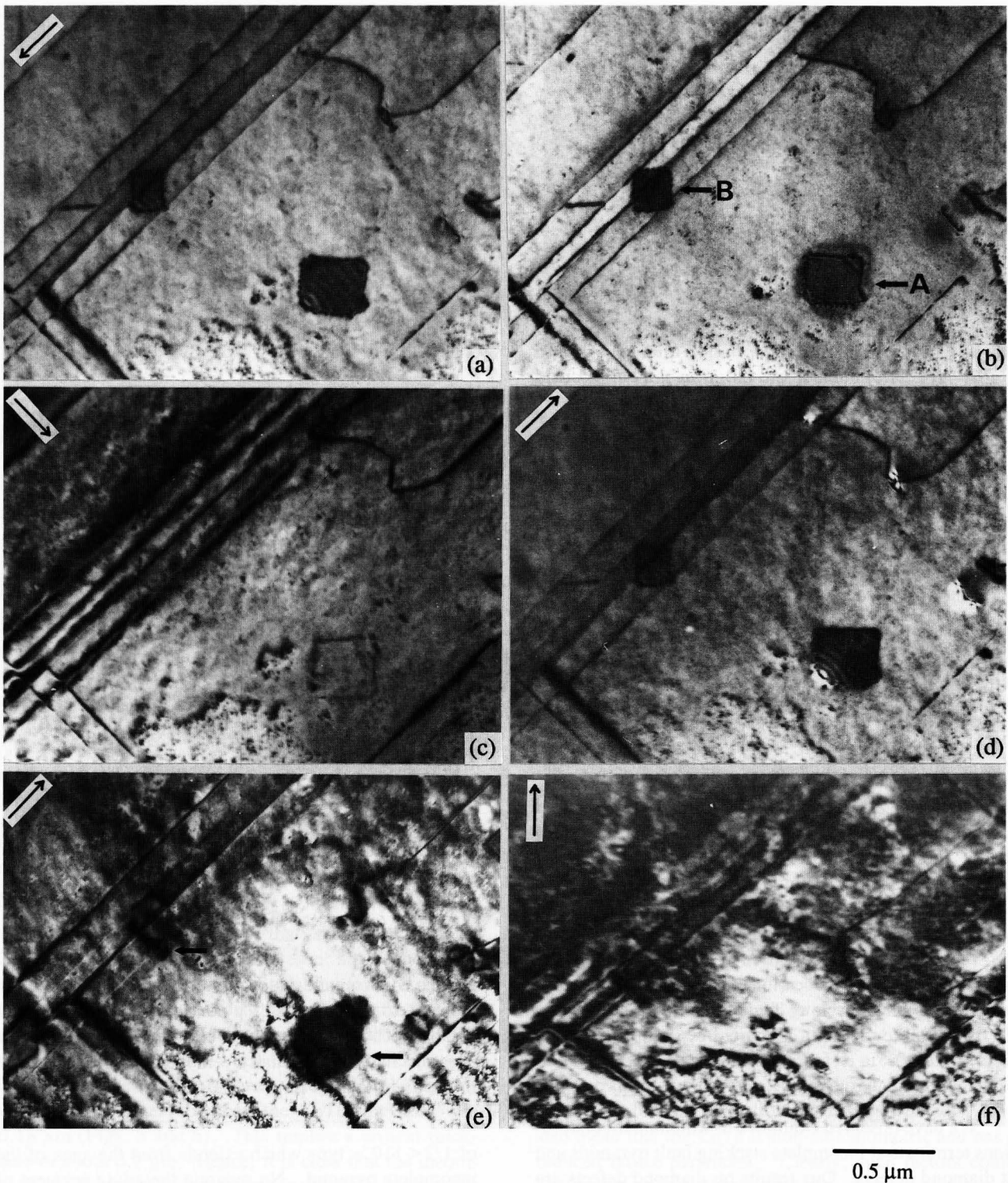
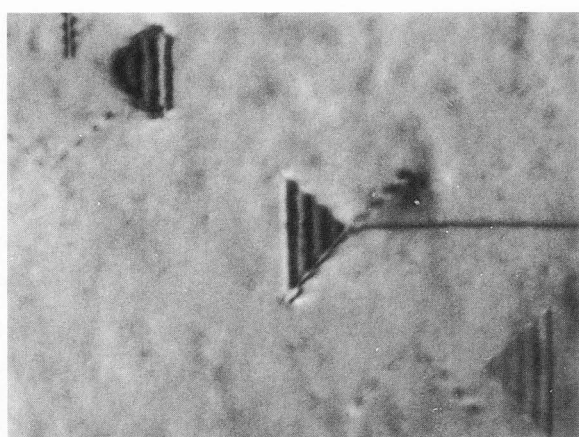
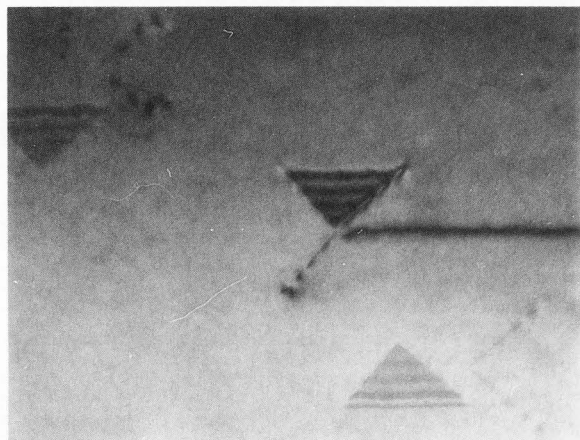


Figure 4. A sequence illustrating the analysis of two oppositely inclined diamond defects A and B. Images are all bright field except for (d), in approximately two beam conditions with g indicated in the top left of each micrograph (a) $g = 220$, (b) $g = \bar{2}\bar{2}0$, (c) $g = \bar{2}20$, (d) $g = \bar{2}\bar{2}0$ (dark field), (e) $g = \bar{1}\bar{1}1$, and (f) $g = 02\bar{2}$. In (e), arrows show B edge on and A nearly horizontal.



(a)

0.5μm \overline{g}

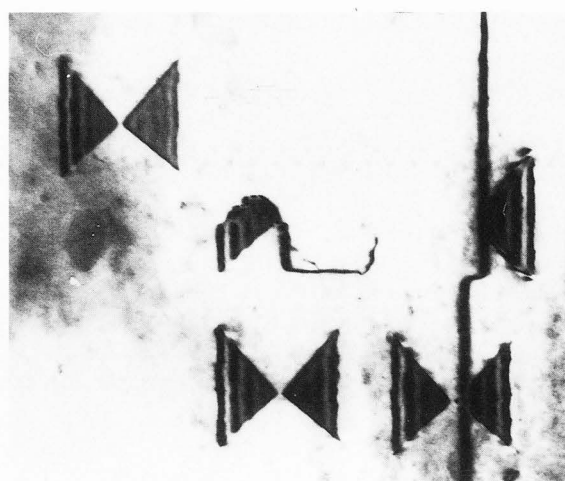


(b)

\overline{g}

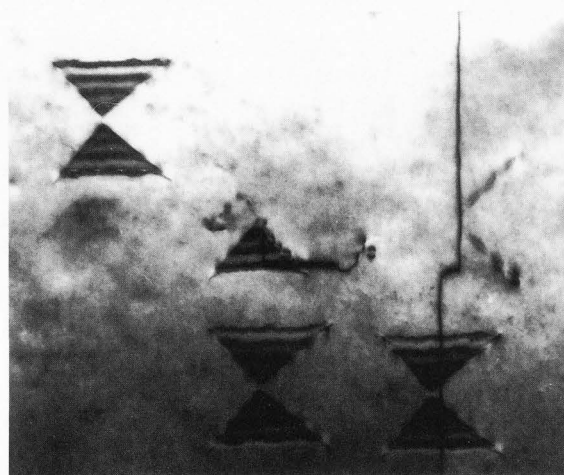
Figure 5. A misfit dislocation emanating from the apex of an incomplete stacking fault pyramid in a $0.18 \mu\text{m}$ ZnTe/GaSb bicrystal (a) dark field $g = 220$, (b) bright field $g = 2\bar{2}0$.

We have observed examples in which misfit dislocations terminate at incomplete stacking fault pyramids and at diamond defects. Our results on diamond defects are preliminary and will be reported at a later date (Mylonas *et al.*, in preparation). In this paper, we consider nucleation at stacking fault pyramids. Figure 5 shows an example from an $0.18 \mu\text{m}$ ZnTe/GaSb sample. The area shows an incomplete stacking fault pyramid consisting of two adjoining faults. Several single Frank faults are also visible. The figure shows an interfacial dislocation



(a)

0.5μm \overline{g}



(b)

\overline{g}

Figure 6. A misfit dislocation joined to the apex of an incomplete stacking fault pyramid in $0.18 \mu\text{m}$ ZnTe/GaSb which has undergone cross-slip. One face of the pyramid has been partially removed. (a) and (b) are bright field images in $g = 220, 2\bar{2}0$.

of $1/2 \langle 110 \rangle$ type which extends from the apex of the incomplete pyramid. No separate threading segment of perfect dislocation is visible, implying that the bounding dislocations of the pyramid comprise the necessary threading segments. Figure 6 shows a second example in which a stacking fault pyramid with two faces is attached to an interfacial dislocation. In this case, one triangular fault of the pyramid, determined to be of intrinsic type, has been partially removed. The interfacial

Dislocation nucleation and propagation

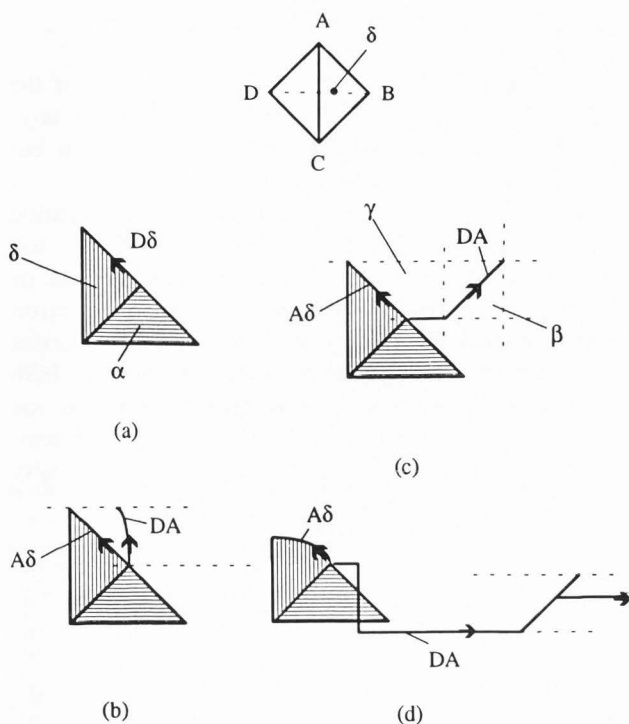


Figure 7. Proposed model for nucleation of interfacial dislocations from an intrinsic Frank dislocation in an incomplete stacking fault pyramid, c.f., Figure 6. (a) and (b). Frank dislocation $D\delta$ dissociates into Shockley $A\delta$ and perfect dislocation DA . (c) and (d) glide of DA on first γ then β , and glide of $A\delta$ on δ produce the observed configuration.

dislocation has suffered cross-slip before threading through to the ZnTe growth surface.

Nucleation mechanisms

It is reasonable to suppose that, at an early stage of ZnTe growth, the only defects present are diamond defects, complete and incomplete stacking fault tetrahedra and that interfacial misfit dislocations are introduced at a later stage. Experimentally, the interfacial dislocation spacing was about $1 \mu\text{m}$ when the ZnTe thickness was $0.22 \mu\text{m}$ (Figs. 3 and 4) whereas interfacial dislocations were seldom observed when the ZnTe thickness was $0.18 \mu\text{m}$ (Figs. 5 and 6). This implies a critical thickness of about $0.2 \mu\text{m}$. Hence, it is clear that the incomplete pyramids in Figures 5 and 6 precede the generation of the associated interfacial dislocations and that we should consider stacking fault pyramids as a possible source for misfit dislocation nucleation.

Figure 7 suggests a possible nucleation mechanism based on the observed geometry in Figure 6. In Figure 7a, it is assumed that the fault on δ was an intrinsic Frank dislocation, $D\delta$ in Thompson notation. Dissocia-

tion of the segment $D\delta$, which was assumed to lie originally along the inclined $\langle 110 \rangle$ direction at the intersection of slip planes δ and β (i.e., the direction AB), can thus take place by the reaction



This produces a perfect dislocation DA which can glide on slip plane γ and a Shockley dislocation $A\delta$ which is glissile on δ . Glide of DA on γ and then cross-slip on β is then needed to produce the observed interfacial dislocation (Fig. 7c). Finally glide of $A\delta$ on δ can take place to partially remove the stacking fault as observed. A similar mechanism can be envisaged for the source in Figure 5 by slip of the perfect dislocation on one slip plane following an initial dissociation (c.f., Fig. 7b).

Discussion

Since the mechanism in Figure 7 requires an intrinsic Frank loop initially, it is clear that a similar unfauling mechanism should apply to diamond defects as well as incomplete stacking fault pyramids. The mechanism in Figure 7 can also produce interfacial dislocations of either sign, depending on whether slip proceeds to the right or left (Figs. 7b and 7c). In our case, to fit experimental results, the dislocation DA is interstitial, i.e., with its extra half plane in the ZnTe. This is somewhat surprising since the equilibrium lattice parameters of ZnTe and GaSb, $a = 6.1037 \text{ \AA}$ and $a = 6.09593 \text{ \AA}$ respectively, imply that we need dislocations of opposite sign. The reason for this unexpected result, confirmed by transmission electron microscopy on individual dislocations, and in agreement with preliminary X-ray diffraction results (Hogg, private communication), is unclear at present. Detailed studies of the ZnTe/GaSb interface by high resolution electron microscopy show an interfacial reaction in which a Ga_2Te_3 phase is generated (Chou *et al.*, 1993). The lattice parameter of Ga_2Te_3 , which has an ordered vacancy structure, based on a sphalerite unit cell, is some 3% smaller than GaSb, consistent with the generation of interstitial misfit dislocations to relieve the misfit strain. The presence of a high concentration of vacancies, as required for the Ga_2Te_3 phase and for the formation of diamond defects, may also mean that the ZnTe is non-stoichiometric and has a reduced lattice parameter. Clearly, such factors could be significant given the small mismatch in this system (0.07%).

Conclusions

The main results of this work are as follows:

- (1). The propagation mechanism for $1/2 \langle 110 \rangle$ misfit dislocations is different for layers grown under

tension and compression, but can be understood by considering the order of dissociation into partial dislocations and the forces acting on the partials.

(2). New diamond defects have been observed in ZnTe/GaSb films. Analysis has shown that these defects are intrinsic Frank loops and are thus different from the diamond defects observed in Si/SiGe (Eaglesham *et al.*, 1989).

(3). A new mechanism of nucleation of interfacial dislocations has been proposed, starting with an intrinsic Frank dislocation present either in incomplete stacking fault pyramids (Figs. 5 and 6) or as diamond defects.

Acknowledgments

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Discussion with Reviewers

D.D. Perovic: What is the dislocation density of the InSb and GaSb used in this work? What effect, if any, does the substrate quality have on the nucleation behaviour observed in this study?

Authors: The InSb and GaSb substrates had dislocation densities of 10^2cm^{-2} and $2 \times 10^4\text{cm}^{-2}$ respectively, too low to explain the nucleation of diamond defects or stacking fault pyramids. Reflection high energy electron diffraction (RHEED) was used to confirm that substrates were atomically smooth and clean prior to growth. InSb substrates were cleaned by repeated cycles of Ar ion bombardment followed by annealing at the growth temperature, whereas GaSb substrates were thermally cleaned at 490°C to remove surface oxygen.

C.J. Humphreys: Are diamond defects nucleated at the epilayer/substrate interface, or are they nucleated within the epilayer? Is there any evidence of impurity atoms associated with the diamond defects?

D.D. Perovic: Have the authors considered what may be the initial source of the stacking faults? For example, de Coteau *et al.* [*Solid State Phenomena*, **19-20**, 27 (1991)] related $1/6 \langle 411 \rangle$ diamond defect nucleation in GeSi/Si heterostructures to iron contamination during growth.

Authors: Our observations show that both diamond defects and stacking fault pyramids nucleated at, or close to, the ZnTe/GaSb interface. However, we have no evidence to relate nucleation of either to impurities. For growth of diamond defects to proceed, we require an excess of vacancies during growth, which may be provided by the interfacial reaction between ZnTe and GaSb (see Discussion above). In contrast, complete stacking fault pyramids represent no net addition of point defects and have been widely observed in films in the CdTe-ZnTe-MnTe system where no diamond defects occur.

D.D. Perovic: Do the authors believe that dislocation climb could be significant at the low temperatures (240-290°C) used in the growth of the films?

Authors: Dislocation climb should take place during growth if a point defect supersaturation exists and point defects are mobile. That these conditions are met in the growth of ZnTe/GaSb is confirmed by the growth of diamond defects, which is a pure climb process. Whether climb plays an important role in the subsequent generation of $1/2 \langle 110 \rangle$ dislocations in ZnTe/GaSb, and also in CdMnTe/CdTe, is unclear at present, and we have emphasised that the interfacial configurations of $1/2 \langle 110 \rangle$ dislocations in both systems can be explained by pure glide mechanisms.