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CRYSTAL MISMATCH IN ELECTROLUMINESCENT MATERIALS. (U)
AUG 77 C LAIRD, C A BALL N00014-76-C-0360
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The results of studies of interface structure in heterojunctions having near [001] orientations are briefly reported. Observations were carried out by X-ray topography, stress-induced birefringence and transmission electron microscopy and all support glide mechanisms and sources for the origin of the dislocations which compensate the misfit of the epilayer. In order to explore the effects of choosing different orientations on the interface structure, similar studies have been carried out on heterojunctions		

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with 351 and 112 orientation. Preliminary results are reported. (Block 20)

Crystal Mismatch in Electroluminescent Materials

Task NR 372-306, #N00014-76-C-0360

A. Epitaxial Layers on 001 Surfaces. (Work carried out by R. Sankaran, J. S. Ahearn, C. A. B. Ball and C. Laird)

I. Introduction

The aim of this project was to understand the structure and origins of the dislocations required to accommodate misfit in LED-type heterojunctions. The approach was to study, at low levels of magnification, [001] oriented devices, with small misfits, and therefore small dislocation densities, using X-ray topographic and stress-induced-birefringence (SIB) techniques, in order to understand the macro arrangement of the dislocations. The micro arrangements were then studied by transmission electron microscopy (TEM) in heterojunctions of higher misfit so that their higher defect densities would allow better chances of viewing significant arrangements in the microscope.

II. Results and Discussion

The results of the X-ray topographic and SIB observations, carried out on $\text{InGa}_{1-x}\text{As}/\text{GaAs}$, $\text{InGa}_{1-x}\text{P}/\text{GaP}$, $\text{GaAsP}_{1-x}/\text{GaP}$ heterojunctions were as follows. Typical misfits studied were ~ 0.003 . Misorientations in the approximately square cross-grid of dislocations permitted the three dimensional nature of the dislocation structure in the epilayers to be studied. SIB was especially useful for thick epilayers and for viewing threading dislocations also for demonstrating long range stress fields. The evidence obtained suggested that a source other than one of those previously favored is the dominant contributor to the interfacial dislocation structure; the most likely possibility is that the majority of dislocations are introduced at near-surface sources created by interactions of gliding threading dislocations. Considerable development and theoretical work was necessary to exploit the SIB technique. These results are reported in the following papers:

- 1) J. S. Ahearn, C. Laird and C. A. B. Ball "The Misfit Dislocation Structure of an InGaAs/GaAs Heterojunction with Low Misfit", Thin Solid Films, 42, 1977, 117.
- 2) J. S. Ahearn, C. A. B. Ball and C. Laird, "Stress-Induced Birefringence of Mismatching III-V Heterojunctions", Phys. Stat. Sol., 38, 1976, 315.

The results obtained with TEM on GaAsP and InGaAs heterojunctions, using sections both parallel to, and oblique to, the interface confirmed a near surface source mechanism of dislocation multiplication. The dislocation structures were documented and the investigators were fortunate in observing how Lomer dislocations (of efficient misfit-compensating ability) were formed from 60° glide dislocations. Thus the hypothesis that all the dislocations, including the sessile types, originated from a glide

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source, was supported.

These results were published in:

- 3) J. S. Ahearn and C. Laird "Transmission Electron Microscopy Observations of Misfit Dislocations in GaAsP Epitaxial Films", J. Materials Sci., 12, 1977, 699.

In interpreting the above work, the surface dislocation source ideas of Matthews and Mader had to be considered and this called for calculations of the energy of a dislocation near an epitaxial interface. We used a stress superposition technique and solved the problem, initially, for an abrupt junction. However, since many heterojunctions involve graded layers, we felt it necessary to solve the problem for this more difficult case. These calculations spun off a number of other useful parameters, such as the critical thickness of a graded layer, which had not previously been attempted. The resulting publications are:

- 4) C. A. B. Ball and C. Laird, "Energy of a Dislocation Near an Epitaxial Interface", Thin Solid Films, 41, 1977, 9.
 - 5) C. A. B. Ball and C. Laird, "A Calculation of the Energy of Misfit Dislocations and the Critical Thickness in Graded Epitaxial Layers", Thin Solid Films, 41, 1977, 307.
- B. Graded Epitaxial Layers on (211) and (331) Surfaces.
(Work carried out by C. A. B. Ball, J. Figueroa, and C. Laird).

I. Introduction

Most III-V compound heterojunctions discussed in the literature are grown on {001} surfaces. In these, the coherency stresses (due to mismatch not accommodated by misfit dislocations) give rise to two equally stressed $\langle 110 \rangle$ {111} slip systems on each of the four {111} glide planes, and one unstressed slip system on each glide plane. The mutually perpendicular $[110]$ and $\bar{1}\bar{1}0$ dislocation lines in the interface give rise to the well known cross grid of misfit dislocations observed on (001) samples. Since the eight slip systems are equally stressed it is expected that those dislocations will occur in the cross grid in approximately equal numbers during film growth, although differences in the mobilities of α and β type dislocations in the sphalerite structure may give rise to different densities in the two perpendicular directions.

During the growth process, with dislocations gliding on all four intersecting planes the probability is high that interactions will take place, and the efficiency of misfit dislocations in accommodating the coherency stresses will probably be reduced, although the formation of highly efficient Lomer type edge dislocations has been observed, as reported above (3).

If the number of misfit dislocations is to be kept to a minimum it is desirable that fewer slip systems are operating on a reduced number of glide planes to avoid interactions. In the (331) epilayer two slip systems, namely $10\bar{1}$ (111) and $01\bar{1}$ (111), (See Table 1) on the same glide plane are the most highly stressed and little work hardening should be expected by the dislocations gliding in. The compensation should be rather complete during the early stages of film growth.

In the (211) orientation most highly stressed slip systems are extremely inefficient in misfit compensation (See tables 1 and 2) and the possibility of formation of Lomer dislocations with efficient compensation and potentially benign effects on the electrical properties is being examined. The efficiency given in Table 2 is proportional to the product of the projections of the edge component of the Burgers vector, and not the dislocation line, on to the interface.

II. Experimental Details

Liquid phase epitaxially grown In_xGa_{1-x}As layers on GaAs substrates were obtained in the (331) and ^{1-x}(211) orientations. The layer composition was graded for a thickness of approximately 8 μm with a final layer of 2 μm of constant composition with x = 0.15 corresponding to a mismatch of 1%. The surfaces of the samples showed that growth occurred along {111} planes, but below the surface the single crystal was uniform.

Electron microscope specimens were prepared by slicing with a diamond saw or spark cutter, followed by mechanical and chemical polishing. Final thinning of transmission electron microscope foils was done by jet etching (for foils parallel to the interface) or ion milling (for foils perpendicular to the interface or at an oblique angle to it; sandwiches of sample being used with the epilayers glued together to protect the area of interest). The specimens were examined in Philips EM 300 microscopes.

III. Results and Discussion

(a) (331) Orientation

A typical example of the dislocations in a (331) foil (i.e. parallel to the substrate surface) is shown in Fig. 1. The long straight parallel dislocation lines in the $[\bar{1}10]$ direction are the most highly stressed $01\bar{1}$ (111) or $10\bar{1}$ (111) type occurring in approximately equal numbers. The more efficient but less highly stressed $01\bar{1}$ (111) and $10\bar{1}$ (111) systems were not observed. The inclined dislocations of the slip systems $[\bar{1}10]$ (111) and 110 (111) were also observed. These dislocations relieve misfit parallel to the $[\bar{1}10]$ direction which is not

relieved by the long straight dislocations with dislocation line $\bar{1}10$. Regions such as that shown in Fig. 2 were observed with tangles of dislocations. This micrograph was taken of a foil perpendicular to the substrate-epilayer interface.

These observations are interpreted as follows. During the initial stages of film growth the epilayer is coherent. At a critical thickness it becomes favourable for dislocations of the 011 (111) or 101 (111) slip systems to be generated, possibly at ledges on the growth surface. These dislocations accommodate or partly accommodate the misfit perpendicular to the dislocation line $\bar{1}10$. At a greater critical thickness the unaccommodated misfit parallel to the direction $\bar{1}10$ is relieved by dislocations of the $\bar{1}10$ (111) and $\bar{1}10$ (111) slip systems gliding into the interface. It follows that if the advantages of a slip on a single glide plane are to be utilized, the thickness of the epilayer must be below the second critical thickness. The values of the critical thicknesses cannot be obtained from a grown sample, they must be obtained during the growth process. Calculations of such critical thicknesses are at present being made.

(b) (211) Orientation

This orientation is such that the glide plane ($\bar{1}11$) is perpendicular to the interface and all associated slip systems are unstressed. The (111) plane is inclined at 19° to the interface and contains the highly efficient $\bar{1}10$ (111) and 101 (111) dislocations along the line 011 . Many such dislocations were observed, an example is shown in Figure 3. It is interesting to notice that these dislocations occur in groups on the same glide plane and must have come from the same source. Also interesting is that these groups of dislocations on the same glide plane appear to pass right through the interface into the substrate region in a sort of pile-up configuration as may be seen in Fig. 4.

There are slip systems more highly stressed, but less efficient in the relief of misfit, on the ($11\bar{1}$) and ($1\bar{1}1$) planes, which are observed. These presumably occur first in the growth process. Preliminary observations have not revealed any of the Lomer type dislocations.

The initial interface of the graded region is taken to be the first line of diffraction contrast which lies in a plane parallel to the surface of the epilayer indicated in Fig. 3. These lines are observed at various distances from the epilayer surface in these samples and extend throughout the crystal in planes parallel to the surface. Preliminary results indicate that this contrast is due to elastic strain associated with an abrupt change of lattice parameter during growth. The causes of those changes are not known. This configuration would be

equivalent to a plane of infinitesimal edge dislocations as shown in Fig. 5. The contrast varies with different diffraction conditions in a way similar to that of dislocation loops. Figure 6 shows an example at higher magnification. At present calculations of expected contrast in various diffraction conditions are proceeding.

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Thanks are due to Dr. R. Sankaran of Varian Associates for preparation of samples and to the Physics Department at the University of Port Elizabeth for use of facilities.

FIGURE CAPTIONS

- Figure 1 T. E. Micrograph of dislocations in the graded region of an epilayer on (331) substrate. The foil is parallel to the substrate surface. Burgers vectors: A - 011 ; B- 101 ; C - 110 . (27,000)
- Figure 2 T. E. Micrograph of dislocations in the graded region of an epilayer on (331) substrate. The foil is perpendicular to substrate surface with normal $(11\bar{6})$. (39,000)
- Figure 3 T. E. Micrograph of dislocations in the graded region of an epilayer on (211) substrate. The foil normal is $(0\bar{1}1)$. Note the dislocations along the (111) glide planes (A) with dislocation lines parallel to $01\bar{1}$. Note the strain diffraction contrast (B). (34,000)
- Figure 4 Same as Figure 3 - note the dislocations in the substrate region. (42,000)
- Figure 5 Strain configuration in T.E.M. foil at an abrupt change in composition.
- Figure 6 Dark field T. E. Micrograph of strained region in a foil attributed to an abrupt change in composition using $(3\bar{1}\bar{1})$ reflection. Epilayer normal - (211) , foil normal $(0\bar{1}1)$. (10,300)

TABLE 1

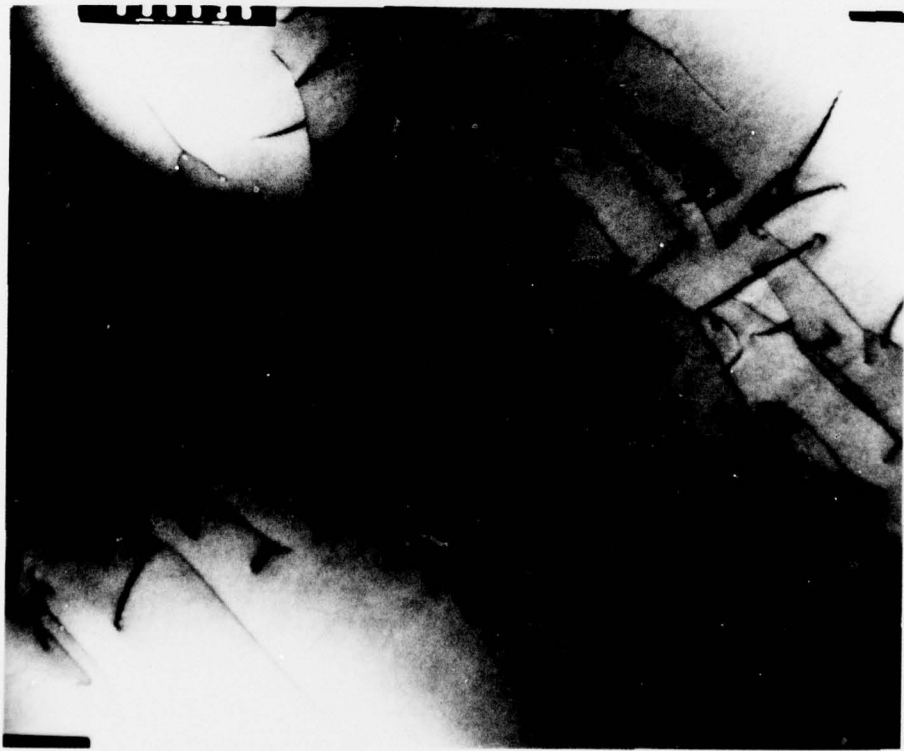
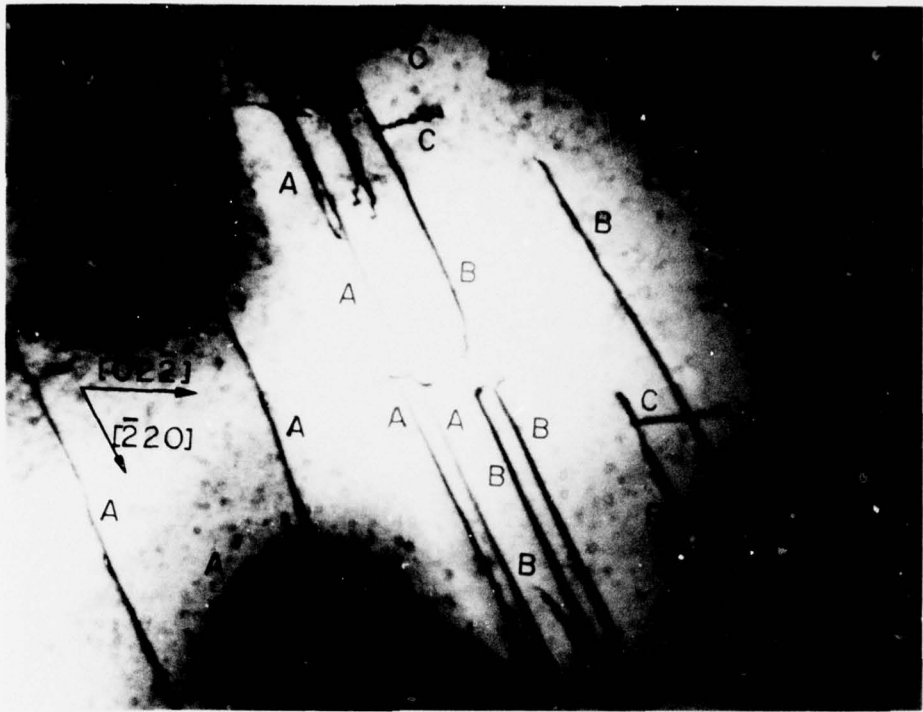
Resolved Shear Stresses in Coherent Layers With
Equal Misfits in Two Perpendicular Directions

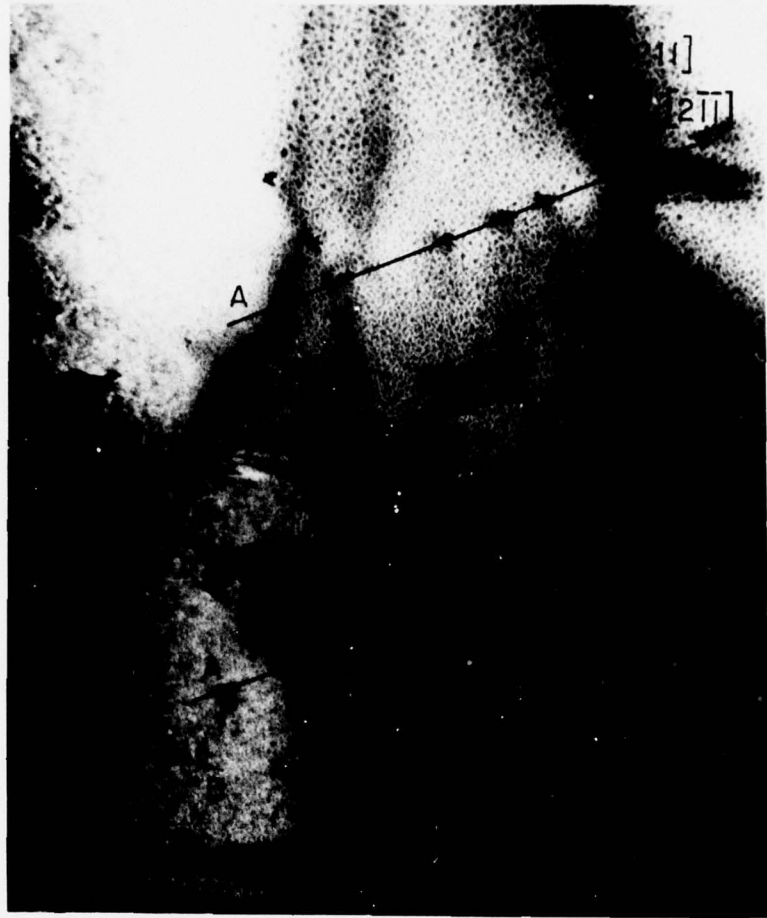
Slip System	Resolved Shear Stress in Epilayer With Normal		
	001	211	331
110 (111)	0.00	0.19	0.00
$\bar{1}01$ (111)	0.29	0.19	0.21
0 $\bar{1}1$ (111)	0.29	0.00	0.21
110 ($\bar{1}11$)	0.00	0.00	0.09
101 ($\bar{1}11$)	0.29	0.00	0.06
0 $\bar{1}1$ ($\bar{1}11$)	0.29	0.00	0.03
110 (1 $\bar{1}1$)	0.00	0.29	0.09
$\bar{1}01$ (1 $\bar{1}1$)	0.29	0.10	0.03
011 (1 $\bar{1}1$)	0.29	0.19	0.06
$\bar{1}10$ (11 $\bar{1}$)	0.00	0.10	0.00
101 (11 $\bar{1}$)	0.29	0.29	0.30
011 (11 $\bar{1}$)	0.29	0.19	0.30

TABLE 2

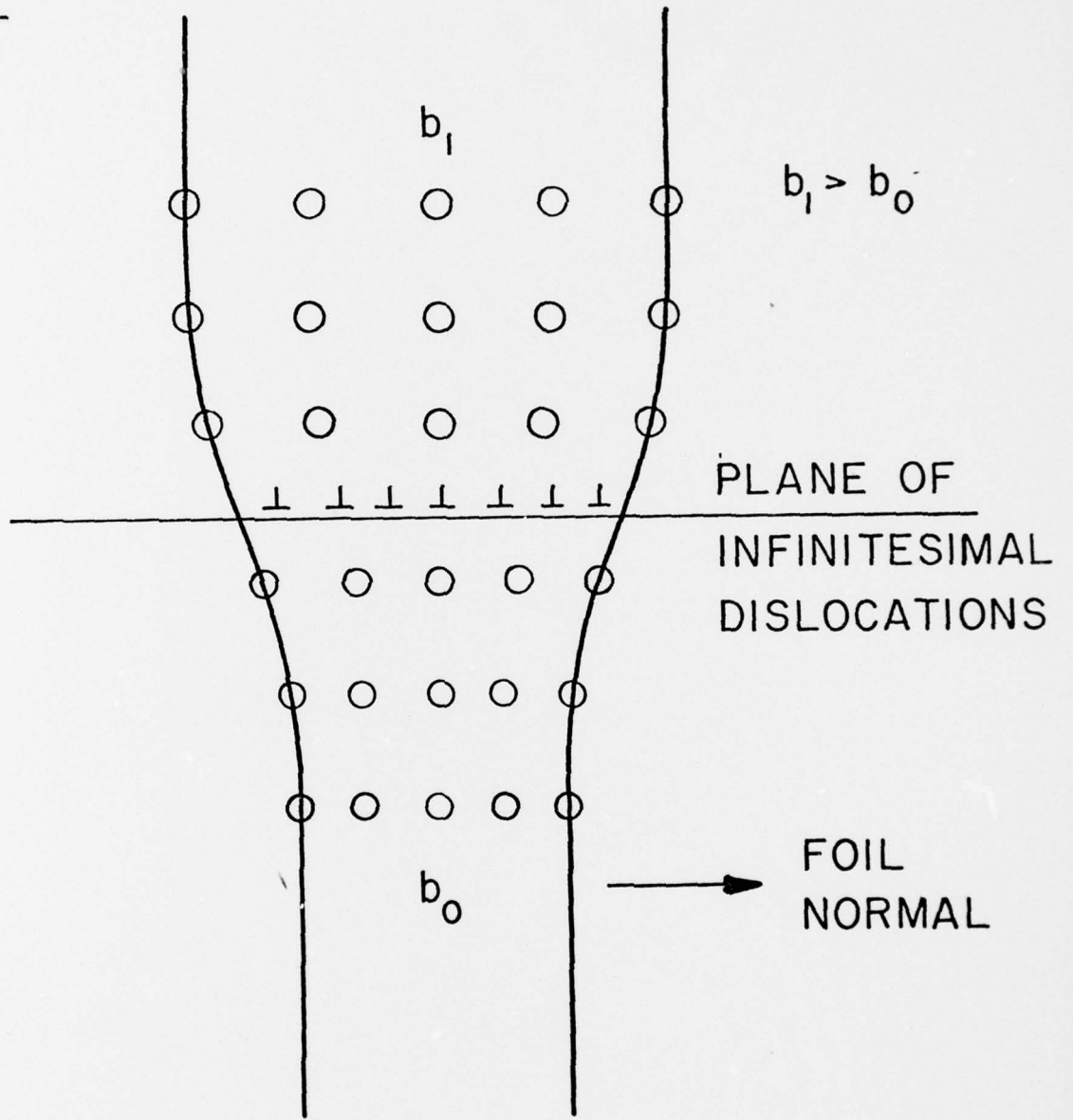
Efficiency of 60° Dislocations in the Interfacial Region

Glide Plane	Dislocation Line	Burgers Vectors	Inclination of Dislocation Line to Surface and Efficiency					
			(001)		(211)		(331)	
			Epilayer Incl	Eff	Epilayer Incl	Eff.	Epilayer Incl.	Eff
(111)	$\bar{1}10$	$\bar{1}01$, $0\bar{1}1$	0°	0.50	17°	0.39	0	0.80
(111)	$\bar{1}01$	$\bar{1}10$, $0\bar{1}1$	45°	0.18	17°	0.39	19°	0.38
(111)	$0\bar{1}1$	$\bar{1}10$, $\bar{1}01$	45°	0.18	0°	0.82	19°	0.38
($\bar{1}11$)	110	101 , $0\bar{1}1$	0°	0.50	60°	0.00	77°	0.01
($\bar{1}11$)	101	110 , $0\bar{1}1$	45°	0.18	60°	0.00	40°	0.04
($\bar{1}11$)	$0\bar{1}1$	110 , 101	45°	0.18	0°	0.00	19°	0.05
($1\bar{1}1$)	110	$\bar{1}01$, 011	0°	0.50	60°	0.10	77°	0.01
($1\bar{1}1$)	$\bar{1}01$	110 , 011	45°	0.18	17°	0.20	19°	0.05
($1\bar{1}1$)	011	110 , $\bar{1}01$	45°	0.18	35°	0.17	40°	0.04
($11\bar{1}$)	$\bar{1}10$	101 , 011	0°	0.50	17°	0.20	0°	0.57
($11\bar{1}$)	101	$\bar{1}10$, 011	45°	0.18	60°	0.10	40°	0.22
($11\bar{1}$)	011	$\bar{1}10$, 101	45°	0.18	35°	0.17	40°	0.22





HETEROJUNCTION
NORMAL



$b_1 > b_0$

PLANE OF
INFINITESIMAL
DISLOCATIONS

FOIL
NORMAL

