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DIRECT SUB-LATTICE IMAGING OF INTERFACE DISLOCATION STRUCTURES IN CdTe/GaAs(001)

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ABSTRACT

In this paper, we present directly interpretable atomic resolution images of dislocation structures at interfaces in CdTe/GaAs(001) systems. This is achieved using the technique of Z-contrast imaging in a 300kV scanning transmission electron microscope in conjunction with maximum entropy image analysis. In addition to being used to further the understanding of the relationship between growth conditions and exhibited properties, the data presented provides direct information on the atomic arrangements at dislocation cores.

INTRODUCTION

Considerable technological interest in the development of $Cd_xHg_{1-x}Te$-based infra-red optoelectronic devices grown on GaAs substrates has provoked a number of studies into the nature of interface structures in highly mismatched III-V/II-VI heteroepitaxial systems (1,2). In this regard, CdTe grown on GaAs(001) provides an ideal model system with which observed interface structures can be correlated with both growth conditions and electronic properties (3,4). Detailed analysis of both (111) and (001) oriented CdTe systems have previously been carried out using high resolution electron microscopy (HREM) (5,6). Although these studies have provided important and detailed information on, for example, the relative density of different defect structures and the angle of substrate tilt, it is not possible to provide direct structural information on the precise atomic arrangements in the sublattice at interfaces and defects. In this paper, by employing the technique of Z-contrast imaging on a 300kV scanning transmission electron microscope (STEM) we show that it is possible to acquire directly interpretable atomic resolution images of the CdTe/GaAs system. Such information can be used not only to enhance the understanding of growth process but also to yield important information on the atomic structure at dislocation cores.

DIRECT SUB-LATTICE IMAGING IN STEM

Z-contrast imaging (7,8) in STEM is an incoherent imaging technique in which, when observing crystalline specimens oriented along principal zone axes, the recorded image can be interpreted simply as a convolution between an object function (the Z-sensitive columnar scattering intensity into the high-angle electron detector) and a point spread function (the incident electron probe). In this way, the recent development of a 300kV STEM (1.3Å probe) has facilitated the direct observation of structural polarity in the sub-lattice in III-V semiconductor materials oriented along the [110] direction (9). In contrast to HREM in which image contrast can change as a function of beam defocus, Z-contrast imaging provides immediately intuitive data at atomic resolution. Furthermore, as a result of image incoherence it is possible, by applying the technique of maximum entropy, to retrieve the Z-contrast object function from each image, providing detailed information on both atomic column positions and intensities (10). Shown in Figure 1(a) is an atomic resolution Z-contrast image of a region of GaAs oriented along the [110] direction. It is clear from this image that, not only is it possible to discern individual atomic columns, relative column intensities (As brighter than Ga) reveal the structural polarity of the material. By application of maximum entropy, the corresponding 'most likely' Z-contrast object function, an array of delta functions of varying intensity located at column sites, is shown in Figure 1(b). The most readily interpretable evidence of material structure is however shown in the 'maximum entropy image' in Figure 3(c) in which the object

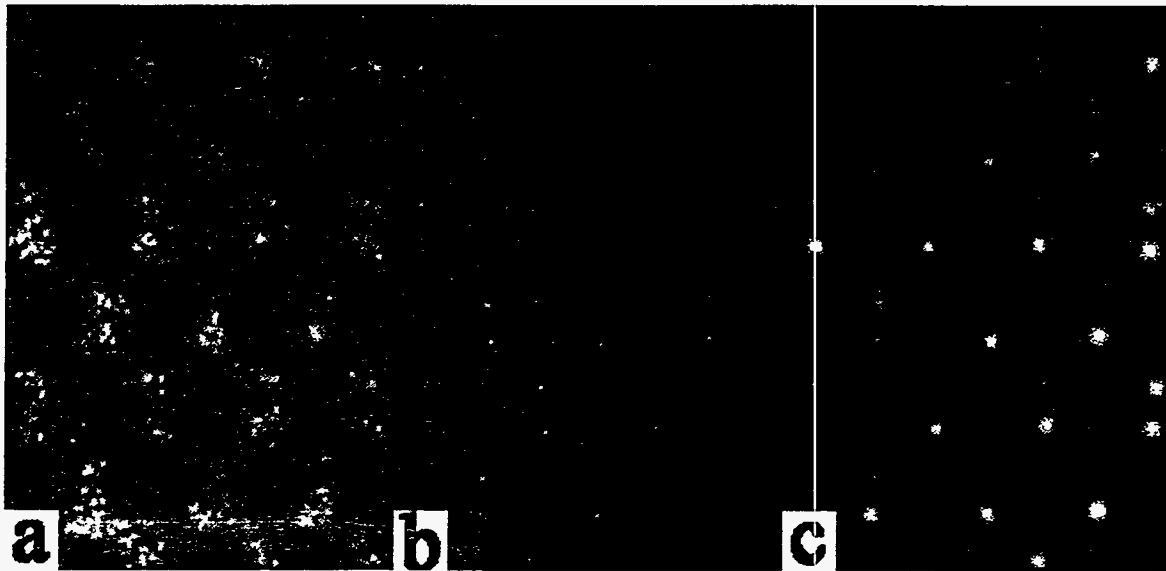

Figure 1. (a) As-acquired atomic resolution Z-contrast image of the sublattice in GaAs. (b) 'Most likely' Z-contrast object function of (a) obtained by maximum entropy. (c) Convolution of (b) with a small Gaussian point spread function. Scale: nearest neighbor separation in the GaAs [110] projection is 1.41Å.

function is convoluted with a small Gaussian probe. In this image, quantitative object function information is preserved, while it is still possible to observe structures intuitively as in Figure 1(a), but in the absence of shot noise. It is in this form that all subsequent images in this paper will be shown. In the analysis of compound semiconductors by Z-contrast imaging, GaAs is the most demanding both in lattice dimensions and relative image contrast between different atomic species. Having established that it is indeed possible to observe structural polarity in the most stringent 'perfect lattice' case, we now proceed to the investigation of more complicated and less well characterized dislocation structures.

ANALYSIS OF CdTe (111)/GaAs (001)

CdTe can be grown epitaxially on GaAs(001) in two orientations; (001) or (111). In the former, the lattice mismatch between substrate and epilayer is -14.6% in all (110) directions, while in the latter, the CdTe grows so that [110]CdTe is parallel to [110]GaAs (-14.6% misfit) but [112]CdTe is parallel to [110]GaAs (+0.7% misfit). As a step towards providing a better understanding of the resulting structures in each case, Z-contrast can be applied to provide directly interpretable information on atomic arrangements which cannot be easily achieved by other means.

A common feature (identified by HREM observation along [110]) in regions of (111) oriented CdTe is the presence of multiple twins parallel to the heteroepitaxial interface. In the same way (Figure 2), such features can also be clearly observed using Z-contrast imaging, but at a level of resolution at which individual atomic columns can be directly identified. The region in the figure consists of two twin interfaces, one of which possesses a step ~1 unit cell wide. Another feature clearly identifiable in the image is structural polarity in each layer which appears to be preserved across both boundaries shown. It should be noted that using Z-contrast, small misorientations with respect to the incident beam direction (as seen in the center layer) result in a rapid loss of spatial resolution. Thus, if the sublattice is resolved, its polarity will be directly observable.

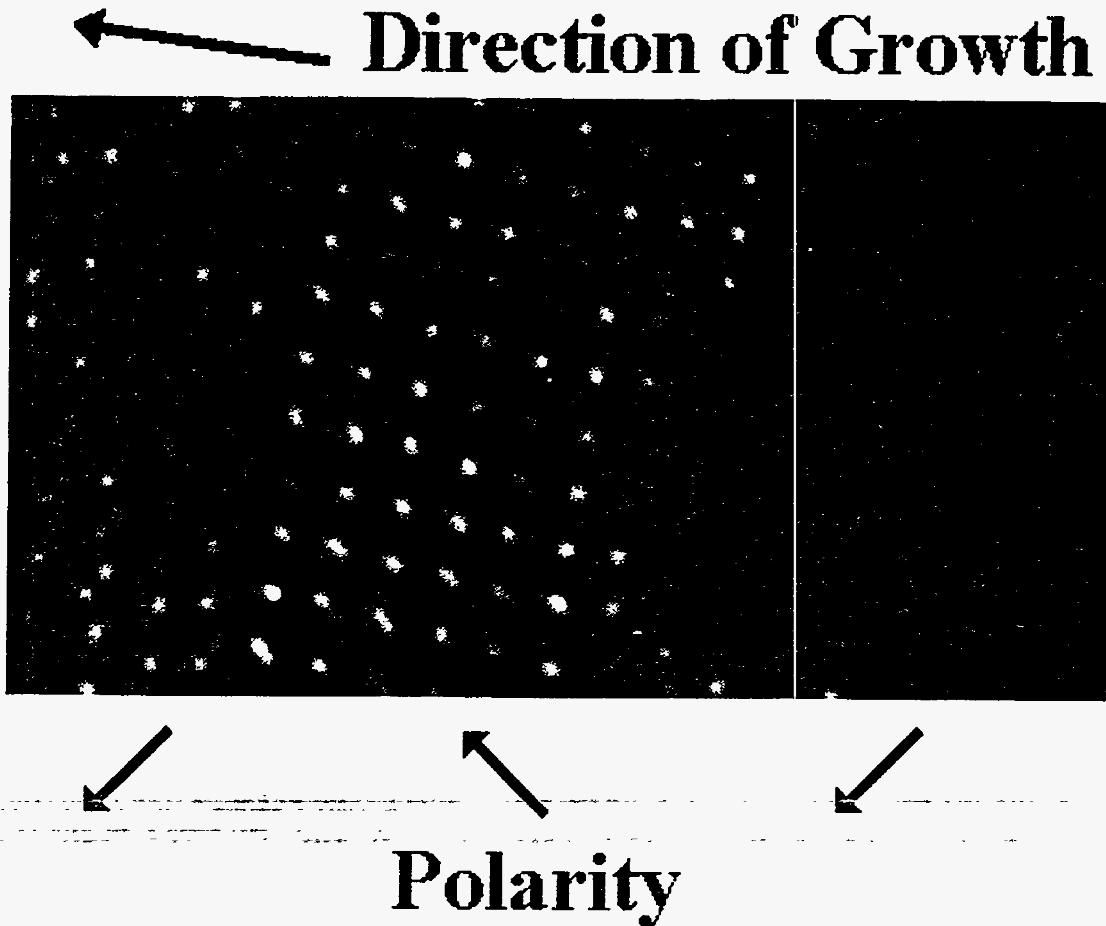

Figure 2. Region in CdTe(111)/GaAs(001) showing twins that run parallel to the interface (direction of growth marked). Scale: nearest neighbor separation in the CdTe [110] projection is 1.62Å.

ANALYSIS OF CdTe(001)/GaAs(001)

Previous investigations of the CdTe(001)/GaAs(001) system using HREM showed that the relative number of 60° and Lomer (perfect edge) dislocations at the interface can vary as a function of the misorientation of the epilayer with respect to the substrate (5). When, as a result of misorientation, the stress between the two becomes too high, planar defects such as microtwins form as a means of relaxing the stress build-up. As we show in Figures 3, 4 and 5 respectively, by employing Z-contrast imaging, it is possible to examine defect microstructure at microtwins, 60° and Lomer dislocations on a scale hitherto unattainable. In Figure 3, we show a small section of a one-half unit cell stacking fault (accommodating increased tilt-induced stress in the left hand region) that has extended into the CdTe epilayer. The atomic structure of this region is readily observed, with the structural polarity of the material retained across the fault. A schematic representation of the structure (with column positions taken directly from the image) is shown in Figure 3(b).

Of perhaps more critical importance, however, in the understanding of the way in which the CdTe accommodates the very large lattice mismatch, is the precise structure of interface dislocations. For example, shown in Figure 4(a), with a schematic representation in 4(b) is a dislocation in CdTe located one unit cell from the interface. Again, not only can individual

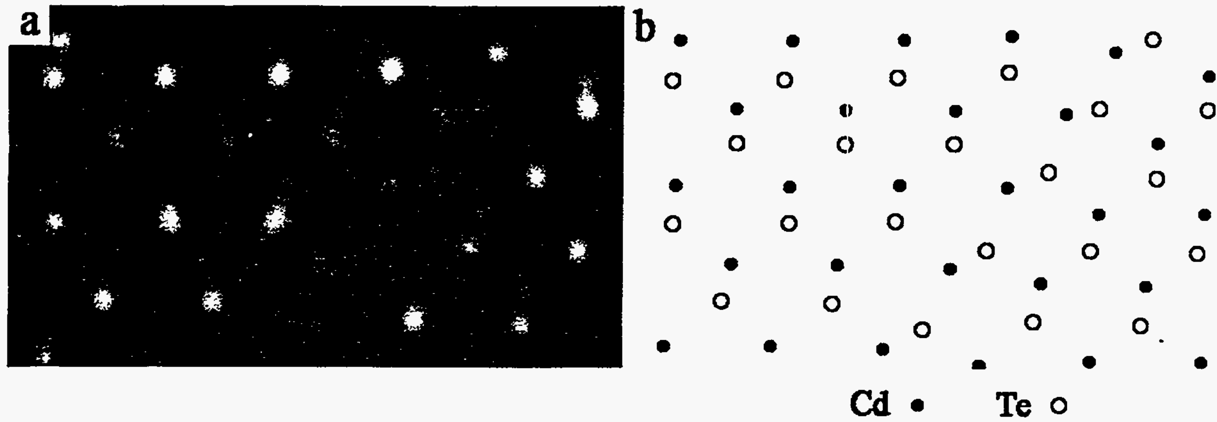

Figure 3. (a) Stacking fault in CdTe(001)/GaAs(001). (b) Schematic representation of (a). Scale: nearest neighbor separation in the CdTe [110] projection is 1.62Å.

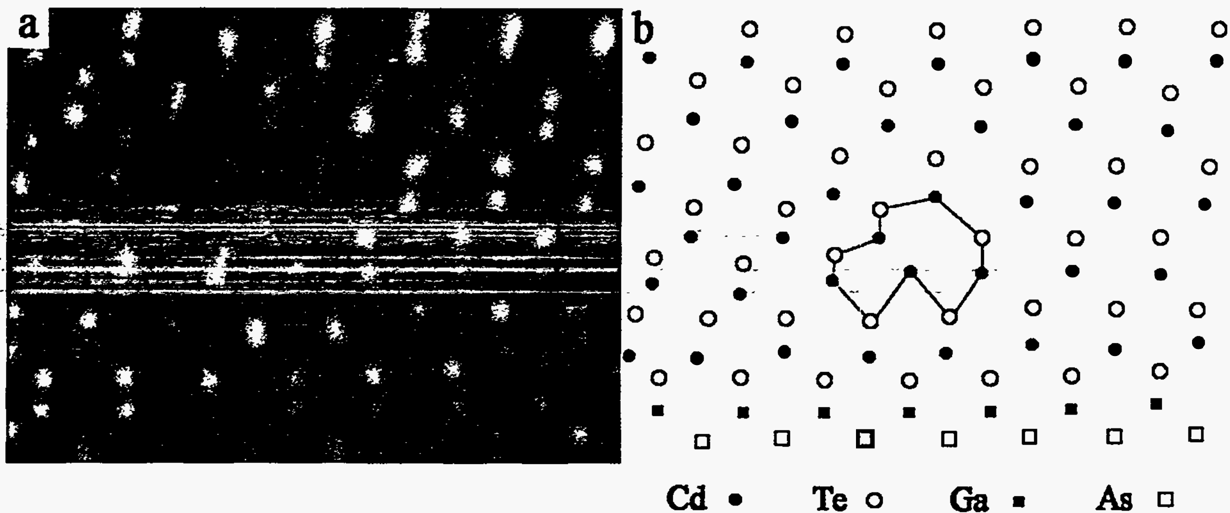

Figure 4. (a) 60° dislocation at the interface in CdTe(001)/GaAs(001). (b) Schematic representation of (a). Scale: nearest neighbor separation in the CdTe [110] projection is 1.62Å.

column sites be identified, it is possible to deduce the atomic species occupying each. From the information presented in this image, the atomic arrangements correspond to a perfect 60° dislocation of the glide set (11). The direction of tilt of the CdTe overlayer with respect to that of the substrate is again marked. In a similar manner to that of Figure 4, a Lomer dislocation situated within the first unit cell of the epilayer is shown in Figure 5. In this case, the most striking features of the core structure are that it is both Cd-rich and asymmetric, best described as consisting of 5 irregular six-fold rings surrounding a 4-fold ring. A possible explanation for this structure is that the polar nature of the material forces a 'skewing' of the atomic columns into the position observed. A clear conclusion from the experimental evidence is that the observed structure is unlike that of the Hornstra (12) model (a 7-fold ring coupled to a 5-fold ring) which posses one more column at the dislocation core. To emphasize this point, a Z-contrast image of the Hornstra structure in Ge is shown in Figure 6. The fact that the deduced structure in CdTe appears to be non-stoichiometric gives rise to a number of questions relating to, for example, the chemical bonding of this region and the possible existence of a small number of stabilizing impurity atoms at the dislocation core.

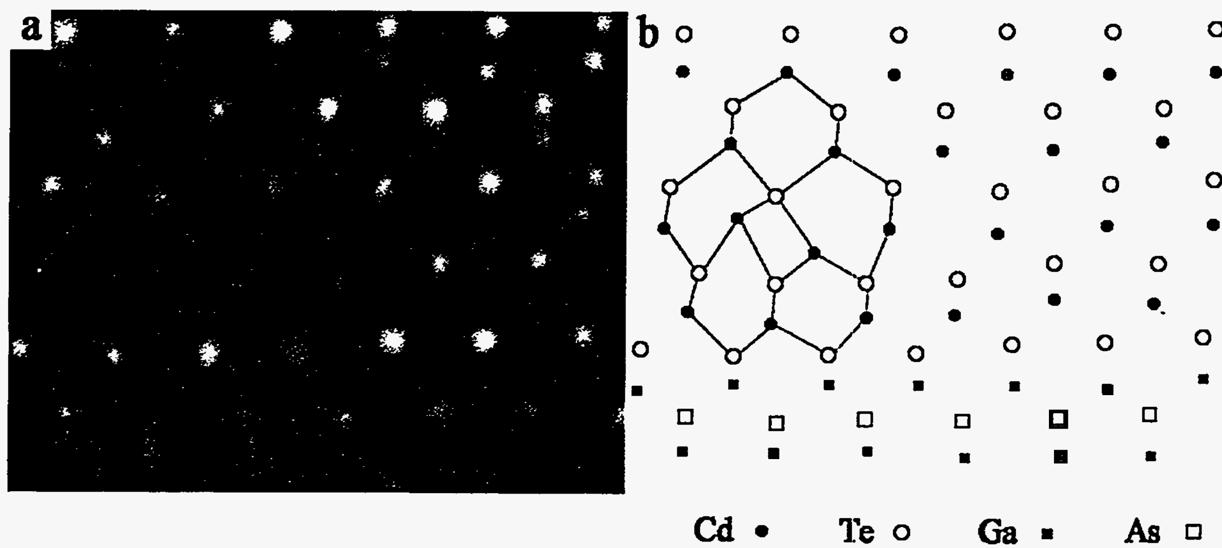

Figure 5: (a) Lomer dislocation at the interface in CdTe(001)/GaAs(001). (b) Schematic representation of (a). Scale: nearest neighbor separation in the CdTe [110] projection is 1.62Å.

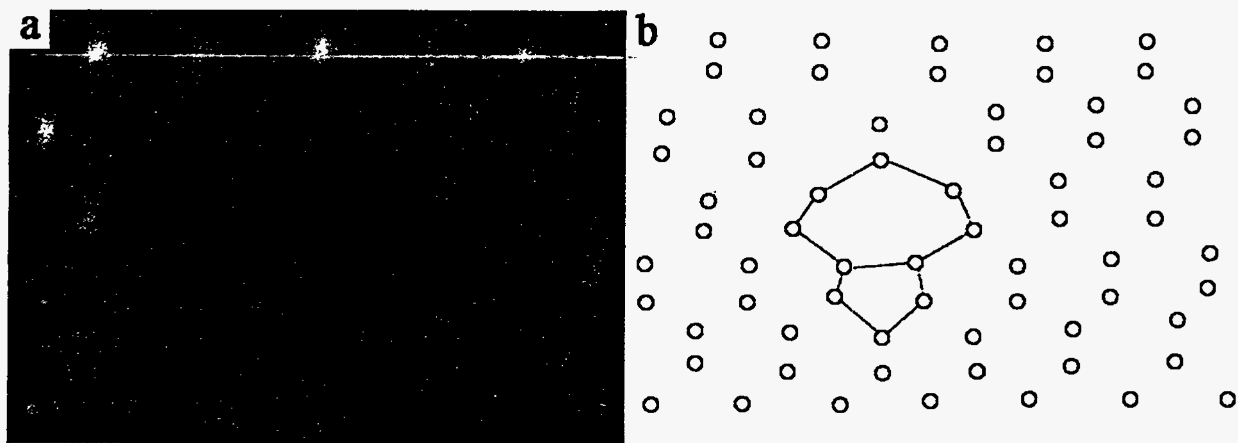

Figure 6: (a) Lomer dislocation at the interface in Ge. (b) Schematic representation of (a). Scale: nearest neighbor separation in the Ge [110] projection is 1.61Å.

Further theoretical and experimental investigations into both the structure and bonding of the observed dislocation are now underway. It should be stressed that, although asymmetric core structures (dissimilar to that observed here) in both Si (13) and compound semiconductor (14) systems have been proposed, it has not hitherto been possible to obtain direct evidence of column configurations solely from experimental data.

CONCLUSIONS

By the application of Z-contrast imaging in a 300kV STEM in conjunction with maximum entropy image analysis, it is possible to provide direct, Z-sensitive information at atomic resolution on a variety of defect structures in the CdTe/GaAs(001) system. Initial observations

of Lomer dislocations at the interface in CdTe(001)/GaAs(001) have shown evidence for the existence of an asymmetric, Cd-rich dislocation structure. Information such as this may provide valuable insight into the understanding of the structural and electronic properties of this system.

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REFERENCES

1. N.Otsuka, L. A. Kolodziejski, R. L. Gunshor, S. Datta, R. N. Bicknell and J. F. Schetzina, Appl. Phys. Lett. **48** 248 (1986)
2. S. Tatarenko, J. Cibert, Y. Gobil, G. Feuillet, K. Saminadayar, A. C. Chami and E. Ligeon, Appl. Surf. Sci. **41/42** 470 (1989)
3. G. Biasiol, L. Sorba, G. Bratina, R. Nicolini, A. Franciosi, M. Peressi, S. Baroni, R. Resta and A. Baldereschi, Phys. Rev. Lett. **69** 1283 (1992)
4. M. Marsi, S. La Rosa, Y Hwu, F. Gozzo, C. Coluzza, A. Baldereschi, G. Margaritondo, J. T. McKinley, S. Baroni and R. Resta, J. Appl. Phys. **71** 2048 (1992)
5. J. E. Angelo, W. W. Gerberich, W. M. Stobbs, G. Bratina, L. Sorba and A. Franciosi, Phil. Mag. Lett. **67** 279 (1993)
6. J. E. Angelo, W. W. Gerberich, G. Bratina, L. Sorba and A. Franciosi, J. Cryst. Growth **130** 459 (1993)
7. S. J. Pennycook and D. E. Jesson, Ultramicroscopy **37** 14 (1991)
8. S. J. Pennycook and D. E. Jesson, Acta Metall. Mater. **40** S149 (1992)
9. A. J. McGibbon, S. J. Pennycook and Z, Wasilewski, Mat. Res. Soc. Symp. Proc. **326** 299 (1994)
10. S. F. Gull and J. Skilling, IEEE Proc. **131F** 646 (1984)
11. K. Masuda, K. Kojima and T. Hoshino, Jap. J. Appl. Phys. **22** 1240 (1983)
12. J. Hornstra, J. Phys. Chem. Solids **5** 129 (1958)
13. A. Bourret, J. Desseaux and A. Renault, Phil. Mag. A **45** 1 (1982)
14. F. Louchet and J. Thibault-Desseaux, Rev. De Phys. Appl. **22** 207 (1987)

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