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DIRECT ATOMIC RESOLUTION IMAGING OF DISLOCATION CORE STRUCTURES IN A 300 kV STEM

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Direct atomic resolution imaging of dislocation core structures in a 300kV STEM

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ABSTRACT: By employing the incoherent imaging technique of Z-contrast imaging in a 300kV STEM, we show that it is possible to provide directly interpretable, atomic resolution images of the sublattice in compound semiconductors. Using this approach, analysis of dislocations at an interface in the CdTe(001)/GaAs(001) system reveals unexpected core structures at Lomer dislocations.

1. INTRODUCTION

The electronic properties of a wide range of semiconductor materials rely strongly on the precise atomic structure at interfaces, grain boundaries and dislocations. Consequently, if growth processes and device characteristics and are to be understood, controlled and, ultimately improved, a direct knowledge of atomic arrangements on the column-by-column level is essential. Such an aim can be achieved by employing the technique of atomic resolution Z-contrast imaging on a newly-developed 300kV scanning transmission electron microscope (STEM). In this paper, we apply the technique to the study of dislocation core structures and show that it is possible to retrieve important information on atomic arrangements without the need for pre-conceived structural models.

2. SUBLATTICE IMAGING

Pennycook and Jesson (1992) demonstrated that Z-contrast imaging in STEM is an incoherent imaging technique in which, when observing a crystalline specimen oriented along a principle zone axis, the recorded image can be interpreted as a convolution between an object function (the Z-sensitive columnar scattering cross-section into the high-angle annular detector) and a point spread function (the effective electron probe). Consequently, unlike data acquired using high resolution electron microscopy (HREM) in which contrast reversals can occur as a function of beam defocus, Z-contrast images can be interpreted directly. Previously carried out at 100kV, with a probe limited spatial resolution of 2.2Å, the technique can now be implemented on a VG Microscopes HB603 300kV STEM at a spatial resolution of 1.3Å. At this resolution, it is possible to resolve the nearest neighbour

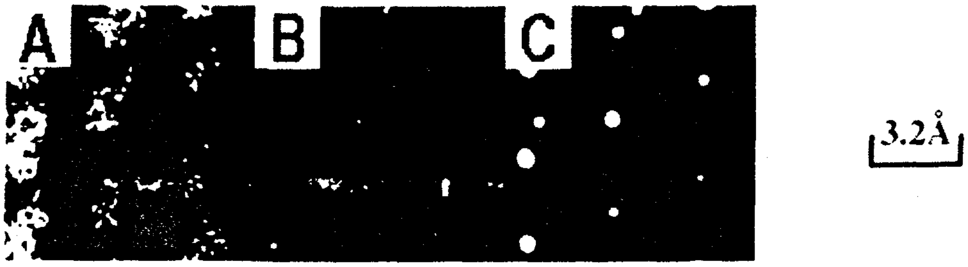

Fig. 1. A: As-acquired Z-contrast image of CdTe viewed along the [110] projection, directly revealing sublattice polarity. B: 'Most likely' Z-contrast object function of A obtained by maximum entropy analysis. C: Maximum entropy image of A.

spacing in all compound and elemental semiconductors viewed in the [110] projection (McGibbon et al. 1994). The benefits of enhanced spatial resolution is demonstrated by the as-acquired Z-contrast image of a region of CdTe shown in fig. 1A which, in addition to resolving individual atomic column positions, the sublattice polarity (Te brighter than Cd) can be seen. A further advantage of incoherent imaging in STEM is that it is ideally suited to the application of maximum entropy analysis techniques (e.g. Gull and Skilling, 1984) in which, given a knowledge of the electron probe current density distribution, a 'most likely' object function is calculated (McGibbon et al. 1995). In this way, it is possible to retrieve numerical information on both column position and composition from each Z-contrast image acquired. Using the combined Z-contrast/maximum entropy approach, the most likely object function (an array of narrow spikes located at column sites, each with a strength related to the columnar scattering power) of the region of specimen analysed in Fig. 1A is shown in Fig. 1B. This information is more readily interpreted through the convolution with a small Gaussian probe to give a 'maximum entropy image' (Fig. 1C). In this image, quantitative object function is preserved, whilst it is still possible to observe structures intuitively as in Fig. 1A, but in the absence of shot noise.

3. ANALYSIS OF DISLOCATIONS IN CdTe(001)/GaAs(001)

The full power of Z-contrast imaging can be fully utilised by the analysis of materials in which local atomic arrangements have a strong effect on bulk characteristics. An example of this is the CdTe(001)/GaAs(001) system grown by molecular beam epitaxy (MBE), which is an ideal model system in the investigation of the inter-relation between growth conditions, materials structure and electronic properties in highly mismatched III-V/II-VI heteroepitaxial materials. In this material, the lattice mismatch between substrate and epilayer is -14.6%. Previous analysis by Angelo et al. (1993) carried out using high resolution electron microscopy (HREM) has provided important and detailed information on, for example, the relative density of different defect structures and the angle of substrate tilt. However, it has not until now proved possible to provide direct structural information with Z-sensitivity on the precise sublattice arrangements at dislocations.

The dislocations shown in Figs. 2A and 2B, with schematic representations in 2C and 2D respectively are core structures in CdTe viewed along [110] (a) and [110] (b). From the information presented in these images, the atomic arrangements correspond to perfect 60° dislocations, the core of which is located in the CdTe epilayer. Furthermore, from the image data alone, it is clear that both dislocations shown here are of the glide set, indicating the

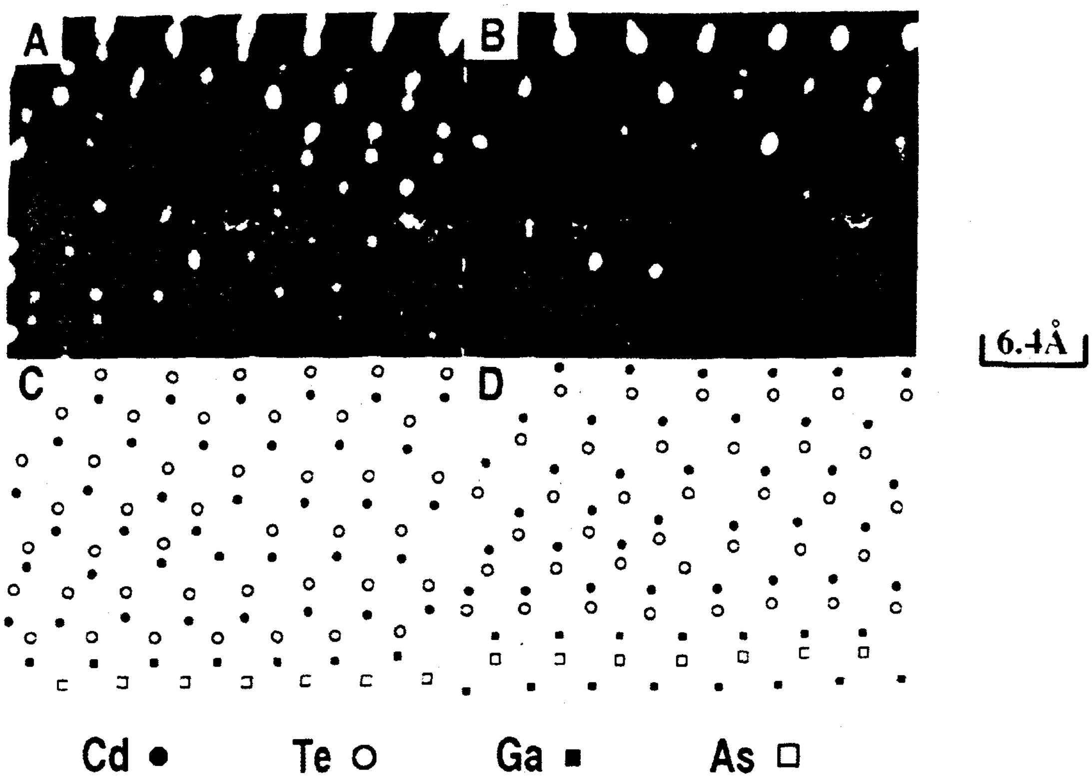

Fig. 2. 60° dislocations at the interface in CdTe(001)/GaAs(001) viewed in the [110] (A) and [110] (B) orientations, with schematic representations given in C and D respectively.

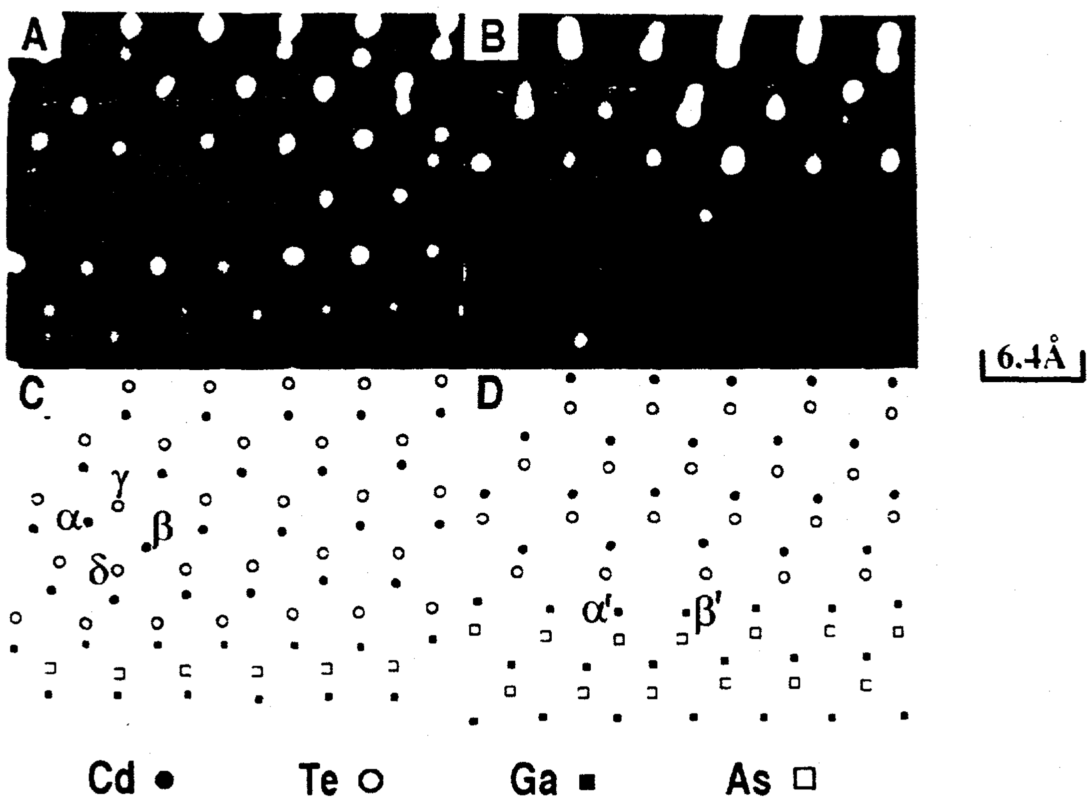

Fig. 3: Lomer dislocations at the interface in CdTe(001)/GaAs(001) viewed in the [110] (A) and [110] (B) orientations, with schematic representations given in C and D respectively.

presence of Cd-terminated dislocations along [110] and Te-terminated dislocations along [110].

In a manner similar to that of Fig. 2, Lomer dislocations viewed along [110] and [110] are shown in Figs. 3A and 3B respectively, with their corresponding core structures in Figs. 3C and 3D. In this case, it can be seen that the core structure viewed along [110] is situated above the interface and is asymmetric in nature, best described as consisting of 5 irregular six-fold rings surrounding a 4-fold ring. Clearly such a structure is unlike that predicted by Hornstra (1958) which can be described as a 7-fold ring coupled to a 5-fold ring. However, atomic arrangements similar to the Hornstra model were observed along [110], but with the dislocation located exactly at the interface, implying that the two columns common to both the 5- and 7-membered rings (marked α' and β') are occupied by Ga atoms. The most likely rationalisation of the observed atomic arrangements in the asymmetric structure is that Cd columns α and β each possess 1 dangling bond per atom and that there is also a small shear (positive for α and negative for β or vice versa) of each column along [110] (parallel to the dislocation line direction) to accommodate a 'skewed' tetrahedral bonding configuration for atoms in Te columns γ and δ. These data suggest that, possibly as a result of the highly polar nature of the CdTe, the Hornstra structure is not energetically favoured when a dislocation occurs entirely within the material.

4. CONCLUSIONS

Through the application of Z-contrast imaging in a 300kV STEM in conjuction with maximum entropy image analysis, it is possible to retrieve information on core structures of dislocations on the atomic level without the need for pre-conceived structural models. In the analysis of the CdTe(001)/GaAs(001) system, it has been possible to determine the exact nature (glide or shuffle) of 60° dislocations and to observe unexpected core structures at Lomer dislocations.

5. ACKNOWLEDGEMENTS

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