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DIRECT OBSERVATIONS OF DEFECT STRUCTURES IN OPTOELECTRONIC MATERIALS BY Z-CONTRAST STEM

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Optoelectronic semiconductor materials have wide and important technological applications. For example, wide gap nitride semiconductors have attracted significant attention recently due to their promising performance as short-wavelength light emitting diodes (LEDs) and blue lasers, while HgCdTe II-VI semiconductors are the most promising candidates for applications as infrared detectors, or large array x-ray or r-ray detectors. In this paper, two examples are given to show that high-resolution Z-contrast imaging is an effective technique to determine the atomic structures of defects in these complex semiconductor materials.

One interesting issue concerning GaN is that the material is relatively insensitive to the presence of a density of dislocations which is six orders of magnitude higher than that for III-V arsenide and phosphide based LEDs. To develop a fundamental understanding of the properties of the dislocations in GaN, the core structures are determined here by atomic-resolution Z-contrast imaging in a VG Microscopes 300kV HB603 scanning transmission electron microscope (STEM) with a resolution of 0.13nm. Figure 1a shows a high resolution Z-contrast image along <0001> of a threading edge dislocation in GaN. As the Z-contrast image is a convolution between the probe intensity profile and the specimen object function, it is possible to obtain detailed information on the atomic column positions through maximum entropy analysis (Fig. 1b). (The maximum entropy technique produces the 'most likely' object function consistent with the image). As can be clearly seen in Fig. 1b, the core structure is just an 8-fold ring, indicated by the numbers 1 to 8 in Fig. 2c. Such a structure is not expected to have deep levels in the band gap and therefore should be electrically inactive[1].

For a sphalerite semiconductor, polarity is an important issue, as the asymmetry of the structure gives rise to different physical and chemical properties. Here we show that high resolution Z-contrast imaging could be used as an effective method to determine the polarity of II-VI semiconductors without refering to reference samples or image simulations. Fig.2a is a Z-contrast image of the interface region between CdTe and HgCdTe at lower magification down [110]. Fig.2b and Fig. 2c are enlargements from the CdTe substrate and the HgCdTe layer. As the intensity of atomic columns is proportional to the mean square atomic number (Z), it is very clear that the CdTe has the {111}B polarity (ie, is Te-terminated). In the alloy, it is known that Hg replaces Cd atoms with a Hg content of 22.4%, the mixed atomic columns of Cd(Hg) image brighter than the Te columns. Therefore the epilayer maintains the same sublattice polarity as the substrate.

References:

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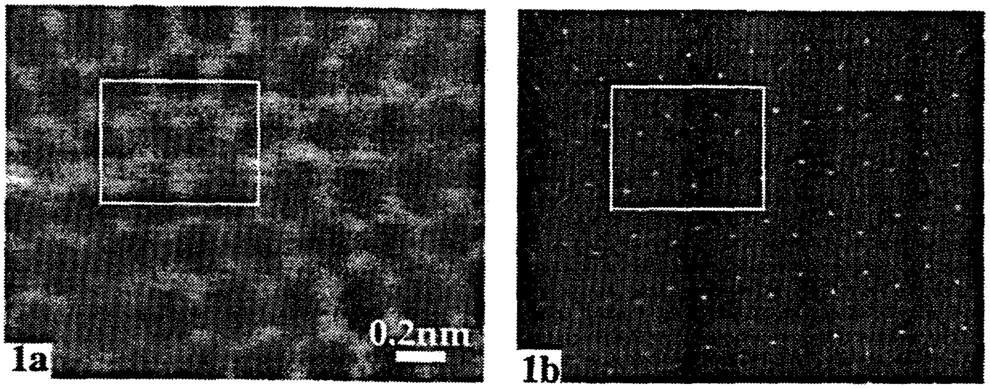

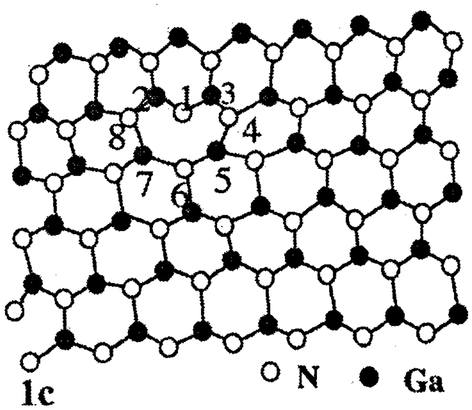

Fig.1(a) High-resolution Z-contrast image of a threading edge dislocation looking down <0001>.
(b) Maximum entropy image of (a) showing most probable column positions.
(c) Sketch of the core structure determined from the expermental data.

Fig.2 (a) High resolution Z-contrast image of interface (indicated) region of CdTe/HgCdTe down [110]. Enlargements from CdTe substrate (b) and from epilayer (c) showing the polarity.