CONF-970834--17

INTERFACES AND DEFECTS IN OPTO-ELECTRONIC SEMICONDUCTOR FILMS STUDIED BY ATOMIC RESOLUTION STEM

Y. Xin*#, D.J. Wallis#, N.D. Browning#, S. Sivananthan#, S.J. Pennycook*, C.J. Humphreys§

*Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN 37381-6031, USA
#Department of Physics, University of Illinois at Chicago, Chicago. IL 60607-7059, USA.
§Department of Materials Science and Metallurgy, University of Cambridge, CB2 3QZ, UK

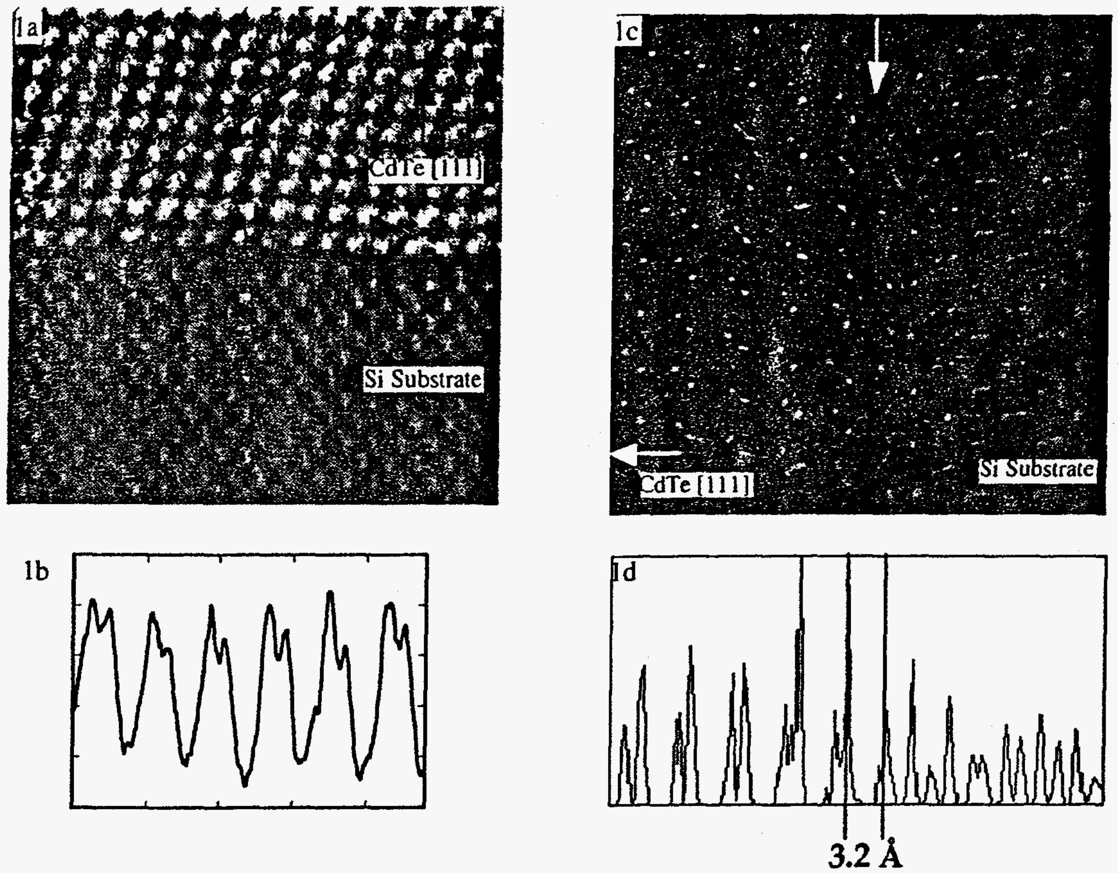
The growth of thin films on dissimilar substrates is of great technological importance for modern optoelectronic devices. However, device applications are currently limited by lattice mismatches between the film and substrate that invariably lead to defects detrimental to device performance. It is therefore of key importance that the mechanisms leading to the formation of these defects are understood on the fundamental atomic level. Correlated atomic resolution Z-contrast imaging and EELS in the STEM is a unique methodology[1] by which this information can be obtained. In this paper, the application of this methodology to determine a novel graphoepitaxial growth mechanism for CdTe on (001)Si is demonstrated, and its potential for the study of GaN is discussed.

Fig.1a shows a high resolution Z-contrast image of a cross sectional view of the CdTe/Si interface showing clearly the CdTe and Si dumbbells. Due to the differences in atomic number, the location of the interface is clear. Additionally, the first few monolayers of the substrate show some surprisingly bright atomic columns at various points along the interface. Atomic resolution EELS shows a substantial Te concentration in these layers substituted for Si atoms[2]. The polarity of the CdTe film can also be determined, as shown in Fig.1b. The line profile across the dumbbells from the boxed region of Fig.1a clearly shows the different intensity of the Cd and Te atoms, indicating a (111)A polarity for the epilayer. Furthermore, the spacing from the first Te layer of the film to the substrate is 0.32nm, determined by maximum entropy analysis[3] (Fig1d,e). This is too long for covalent bonding, but is typical of a Van der Waals interaction. This weak interaction explains the absence of localised misfit dislocations and the incommensurate nature of the interface. This growth mode, leading to excellent epitaxial alignment, is known as graphoepitaxy and results in the film having a defect density comparable to bulk crystals[2]. It is interesting to note that the initial nucleation of the CdTe layer occurs through the deposition of a Te monolayer, resulting in the Cd-terminated epilayer, a result very different from other observations[4].

Attempts are currently underway to grow GaN by this graphoepitaxial technique. An intriguing feature of GaN is its ability to function for device applications despite high defect densities. The already promising results suggest that a reduction in the defect density could lead to blue-green LEDS and reliable CW lasers being produced. Conventional HRTEM images of two commonly observed defects in GaN are shown in Fig.2; a threading dislocation viewed along <0001>, and $(1\bar{1}00)$ domain boundary along $[11\bar{2}0]$. It is hotly debated whether such defects have significant effects on the photoluminescence. Atomic resolution Z-contrast imaging and EELS performed on dedicated STEMs have the power to probe into these problems, including the determination of dislocation core structures[3], the detection or imaging of possible impurity decoration, and the atomic structure of domain boundaries, all problems difficult to solve by conventional HRTEM.

References

1. N. D. Browning, M. F. Chisholm, and S. J. Pennycook, Nature 366(1993)143
2. D.J. Wallis et al. , APL in press; S. J. Pennycook et al, these proceedings.
3. S.J. Pennycook et al., J. Electron Microsc.45(1996)36.
4. Y.P. Chen et al., J. Electronic Materials, 24(1995)475.
5. This research was sponsored by the Division of Materials Sciences, USDOE, under contract DE-AC05-96OR22464 with Lockheed Martin Energy Research Corporation, in part by DOE under grant number DOE 96ER45610.



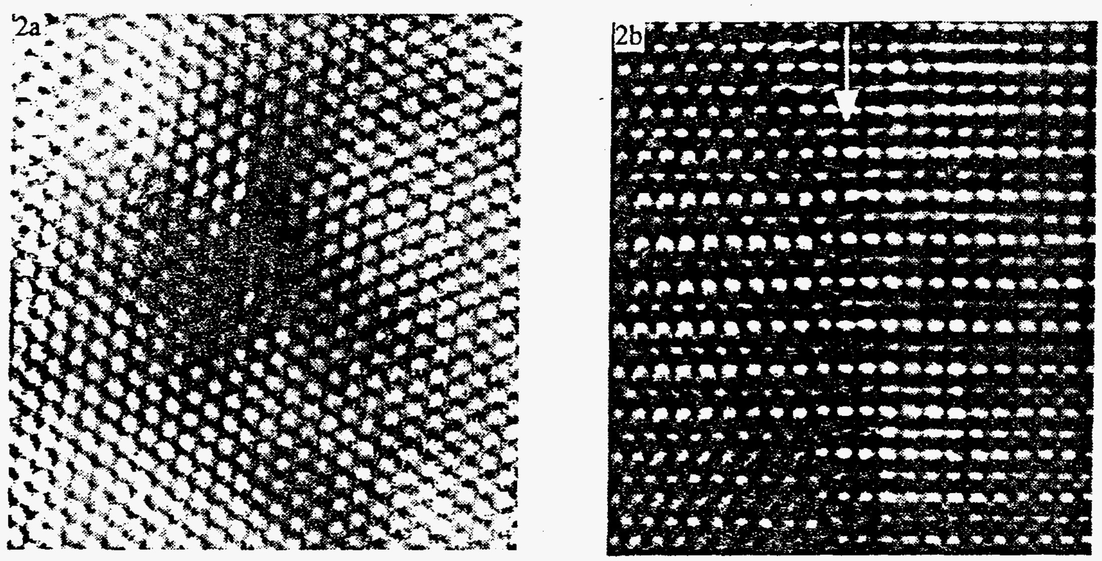


Fig. 1 (a) Atomic resolution Z-contrast image of CdTe/Si looking down [110] after low pass filtering to remove the effect of probe tails; (b) Line profile of the boxed region in (a) showing dumbbell polarity; (c) Maximum entropy image of (a) (the interface indicated by an arrow), and (d) The projected profile of the interface showing the large film/substrate separation.

Fig. 2 Conventional HRTEM images of defects in GaN, (a) Threading dislocation viewed down <0001> and (b) $(1\bar{1}00)$ domain boundary viewed down $[11\bar{2}0]$ (the boundary indicated by an arrow).