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Z-Contrast Imaging of Dislocation Cores at the Si/GaAs Interface

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The major problem in manufacturing of GaAs layers on Si substrates is the lattice mismatch of 4.1% between GaAs and Si, which leads to the creation of a large number of interfacial dislocations (misfit dislocations). By attracting impurities and other defects to the interface, nonradiative recombination centers are formed, and dislocations may affect the electronic and optical properties of the interface as well as the lifetime of the resulting GaAs based device [1]. In the present paper we study the detailed atomic structure of 60° and 90° dislocations at the Si/GaAs interface to determine their influence on the electronic and optical properties of this interface.

GaAs-thin films were grown by metal organic chemical deposition method at 650° C on a Si (001) substrate. Cross-section [110] samples were prepared by standard mechanical polishing and ion milling. The Si/GaAs interface was studied with atomic-resolution Z-contrast imaging, which provides chemical composition information and allows direct interpretation of micrographs without simulation [2]. Observations were performed in a dedicated STEM VG HB603 operating at 300 keV with probe diameter less then 0.13 nm. With such a resolution individual atomic columns (atoms) of Si or GaAs in [110] direction can be resolved and structures of interfacial dislocations can be determined directly from micrographs.

Besides the comparably small number of 60° dislocations (see fig. 3), two different types of 90° dislocations (relaxed and unrelaxed) were observed at Si/GaAs interface. The relaxed 90° dislocation is shown in fig.1. In this configuration there are no broken bonds and 5- and 7-fold rings are present. This type of dislocation is known for diamond and diamond related materials [3]. It is supposed to be more stable and in fact this type of dislocation was observed at Si/Ge interface and at low angle grain boundaries in Si and Ge.

The unrelaxed 90° dislocation consists of 6- and 8-fold rings and exhibits dangling bonds (see fig 2). It is an essentially different structure and cannot simply be transformed into relaxed 90° dislocation [4]. Unrelaxed 90° dislocations possess a line of As atoms whose coordination is different from the bulk. This results in so called broken bonds, which are supposed to cause energy levels in band gap [1]. EELS spectra from the different cores and the plane interface will be presented.

In conclusion, to the authors knowledge it is for the first time micrographs of dislocation cores structures are obtained with resolution high enough to distinguish a single atomic column in GaAs. As a result, this is the first time that the structure of unrelaxed 90° dislocation with broken bonds is reported. Since this type of 90° dislocations apparently exhibits dandling bonds, which in their turn should cause energy levels in band gap, then the presence of this dislocation type is crucial for the electrical and optical properties of the Si/GaAs interface.

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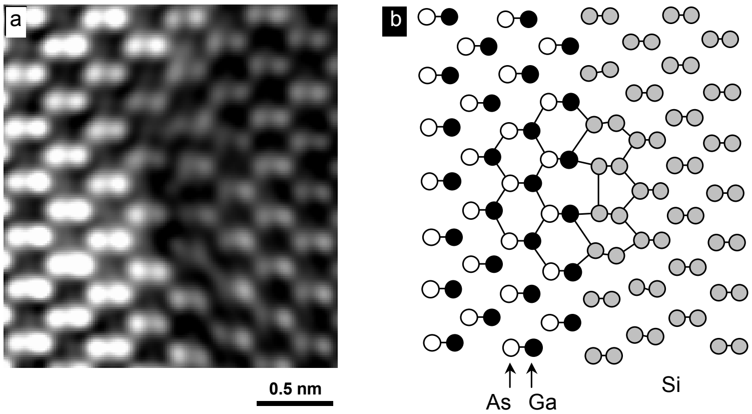

Figure 1. Z-contrast image of relaxed 90° dislocation at Si/GaAs interface (a) and dislocation core structure (b).

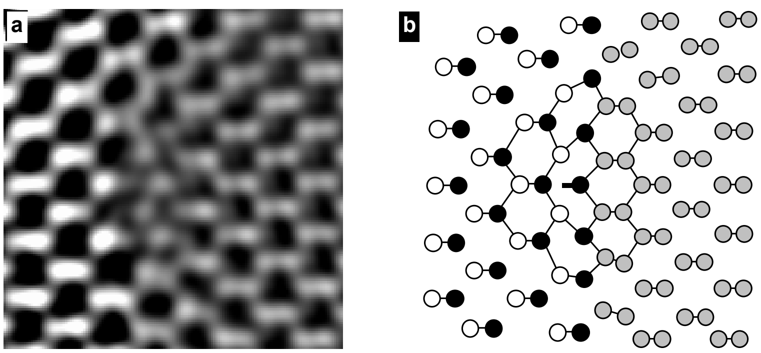

Figure 2. Z-contrast image of unrelaxed 90° dislocation at Si/GaAs interface with dangling bonds (a) and dislocation core structure (b).

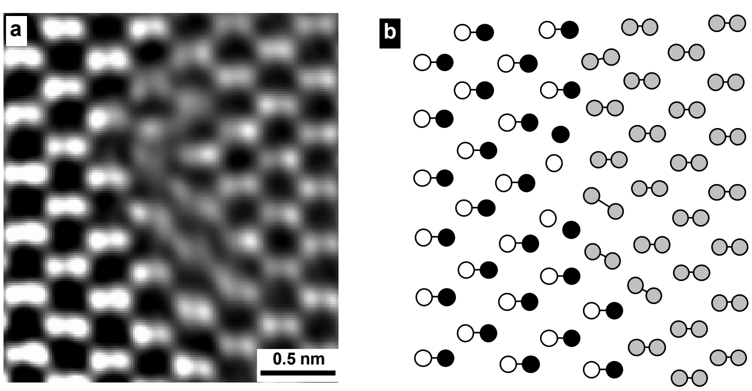

Figure 3. Z-contrast image of intersection of two 60° dislocations at the step of silicon substrate (a) and dislocation core structures (b).

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