Z-contrast Imaging and EELS of Dislocation Cores at the Si/GaAs Interface

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ABSTRACT

The interface between silicon and epitaxial GaAs thin film grown by metalorganic chemical vapor deposition was studied using atomic-resolution Z-contrast imaging and electron energy loss spectroscopy (EELS). Z-contrast imaging provides chemical composition information and allows the direct interpretation of micrographs. EELS yields a correlation between structure and chemistry. Different types of dislocations were identified at the Si/GaAs interface. The atomic structure of a non-reconstructed 90° dislocation (exhibiting a dangling bond) was refined by means of computer simulations based on density functional theory. EELS from a planar Si/GaAs interface and from the different dislocation cores was obtained and analyzed.

INTRODUCTION

One of the technological goals of the semiconductor industry is the integration of various crystalline and amorphous materials (metal, dielectrics, and semiconductors) into a single superstructure. In principle, a wide variety of devices could be manufactured on silicon substrates by the introduction of new materials into high-speed silicon integrated circuits, including majority carrier devices, field effect transistors, heterojunction bipolar transistors, and light emitting diodes [1]. The crystal lattice mismatch is the major problem in manufacturing semiconductor layers on Si substrates. This mismatch causes interfacial dislocations, which affect the electronic and optical properties of the interface and the resulting devices [2].

The presence of dislocations at the Si/ GaAs interfaces was shown experimentally in recent years. Detailed atomic structure analysis of 60° and 90° dislocations obtained by Z-contrast imaging was described in [3]. The non-reconstructed type of 90° dislocation was reported at this interface. However, the exact structure of the observed non-reconstructed 90° dislocation was left for a further clarification.

EXPERIMENTAL DETAILS

In this study, we used a dedicated scanning transmission electron microscope (STEM) for high-resolution Z-contrast imaging [4, 5] and simultaneous electron energy-loss spectroscopy (EELS) of the 90° dislocations at the GaAs/Si interface. The GaAs-

thin films were grown by MOCVD at 650° C on a Si (001) substrate. Cross-section [1$\bar{1}$0] samples were prepared by standard mechanical polishing and ion milling [6].

To obtain Z-contrast images, a crystalline sample is oriented in a low order zone axis and scanned by the focused electron probe of the STEM. While the sample is scanned, an annular detector collects electrons scattered to high-angles. Only 1s Bloch states reach the detector and contribute to the image [7], achieving, in effect, column-by-column illumination of the crystal. The image is acquired serially, and represents a map showing the location of the projected atomic columns and their relative composition (high-angle scattering is proportional to the square of the mean atomic number Z). Thus, the structure of the crystal can be obtained directly from the Z-contrast image. Electrons scattered to low-angles can be used for simultaneous electron energy-loss spectroscopy (EELS), thus providing complimentary information about chemical composition and electronic properties of the structure.

RESULTS AND DISCUSSIONS

We used a VG HB603 U dedicated STEM (300 KeV, probe diameter less then 0.13 nm) to resolve individual atomic columns in Si or GaAs in the [1$\bar{1}$0] direction. As reported in [3] a single atomic column is present at the core of the non-reconstructed 90° dislocation (see fig.1). This atomic column exhibits dangling bonds. However, the composition of this column was not determined unambiguously. The Z-contrast images could not provide this information due to insufficient difference in the atomic numbers of Ga and As. Strong stress fields around the dislocation cores also degraded the resolution. Since a layer of Ga atoms is initially deposited on Si, we first proposed that Ga atoms formed a single atomic column at the core of the non-reconstructed 90° dislocation [3].]. However, *ab initio* calculations, based on the density functional theory, showed that it is energetically more favorable for As atoms to form the single atomic

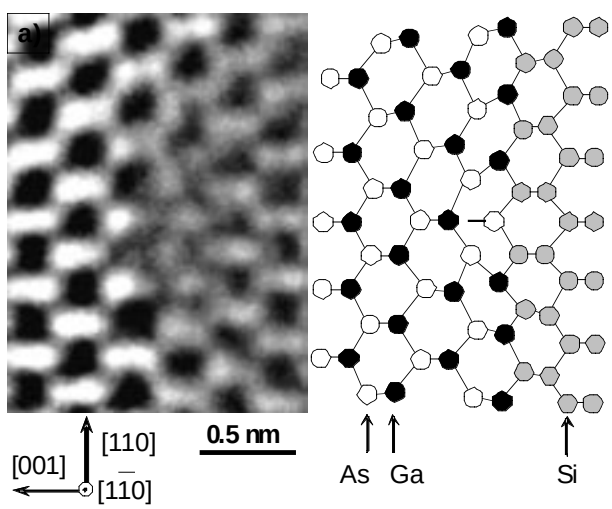

Figure1. (a) - Z-contrast image of non-reconstructed 90° dislocation at the Si/GaAs interface as obtained in [3]; (b) - structural model of the dislocation core refined after the calculations.

column at the center of this dislocation core. Thus, fig. 1.b represents a refined atomic structure of the non-reconstructed 90° dislocation. The proposed model of the dislocation core structure is consistent with atomic resolution Z-contrast imaging [8, 9], which showed a segregation of As impurities in a corresponding atomic columns in a silicon grain boundary. This segregation occurs in the form of isolated dimers.

In this study we also used the dedicated STEM VG HB501 (100 kV) for imaging of the dislocations and simultaneous EELS of the silicon edge at the dislocation cores. The latter provided correlation between structure and chemistry with atomic resolution. This was possible due to a new spherical aberration corrector installed in the VG HB501, which enabled us to achieve a spatial resolution nearly a factor of two better than before.

EELS data analysis showed a noticeable shift of 0.4 eV of the Si-$L_{2,3}$ ionization edge at the planar Si/GaAs interface (without dislocation) suggesting an opening of the Si band gap (see fig.2a). As seen from figure 2b, the analogous shift of the Si-$L_{2,3}$ ionization edge at the dislocation core is slightly smaller, but within the experimental error. The dislocation formation at the interface occurs to reduce the stress. Thus, if the stress field at the interface is the reason for the Si-$L_{2,3}$ edge shift, one would expect more significant differences between the spectra from the planar interface and from the dislocation core. Therefore, other effects such as interdiffusion are a possible explanation for this shift and further research is required to clarify this question.

CONCLUSIONS

The combination of Z-contrast imaging, EELS and functional density theory is an excellent tool for the characterization of crystalline materials and interfaces between them. It allowed us to clarify the atomic structure of the non-reconstructed 90° dislocation, as well as to analyze electronic properties of the interface. Improvements in Z-contrast imaging due to aberration correction lead to the ability “to see” a single atom and, as a result, to discover unexpected atomic structures.

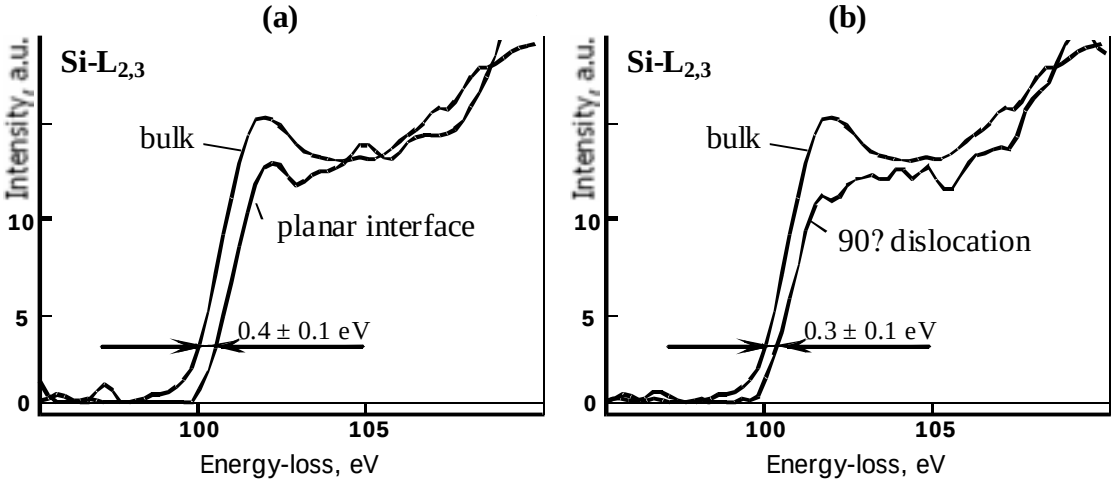

Figure 2. EELS of Si-$L_{2,3}$ edge from a) Si/GaAs planar interface; b) 90° dislocation core at the Si/GaAs interface.

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