Bragg-rod Diffraction Studies of the Gd_2O_3 – GaAs Interface

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Introduction

Two-beam coherent diffraction along Bragg rods is a powerful technique[1] for the study of two-dimensional structures such as buried interfaces and aperiodic heteroepitaxial layer structures[2,3]. Its advantage lies in the ability to extract directly both the amplitude and phase of the complex scattering factor, thereby enabling a direct determination of the structure by back Fourier transform (BFT). An important application of this method is to probe the atomic-level structure of the interface between a semiconductor wafer and a passivation layer deposited on its surface. In this particular experiment we are interested in the atomic structure of a 30Å Gd_2O_3 film epitaxially grown on the (100) surface of a GaAs single crystal[4].

Methods and Materials

The measurements were carried out in the following way: the sample was mounted on a Kappa goniometer with the undulator x-ray beam vertically focused down to about 200 microns using a Rh-coated mirror. Reflection from this mirror, together with detuning of the second monochromator crystal, practically removed the third harmonic. The goniometer, the detectors and the slits were controlled by a Labview program that we developed. Special procedures were developed to line up the goniometer to the desired accuracy. The signal was measured using a scintillator-photomultiplier combination operating in the DC mode. This allowed us to measure signals as low as 50 counts/sec and up to 300,000 counts per second. The signal was normalized with respect to a reference signal and the background was subtracted.

Results and Discussion

The diffraction intensity was measured along a number of Bragg rods: (h 1 1), (h -1 1), (h 2 0), (h 2 2), (h 3 1), (h 3 3) in the range $0.5<h<3.5$. To analyze the data we start with a model structure and adjust its parameters to provide the best fit to all the Bragg rod intensities that were measured. Any discrepancies correspond to an unknown electron density that is the difference between the true electron density of the system and that represented by the model. We then calculated the complex scattering factor of the unknown electron density using the method described in ref. 3.

The results of this structure determination procedure are shown in Fig. 1 which illustrates BFT results obtained from a single Bragg rod (h 1 –1), representing the one-dimensional electron density profile in the direction normal to the interface. The electron density exhibits oscillations on the scale of a few monolayers, probably as a result of coherency strains due to the epitaxial mismatch. The next phase of this work is to measure the diffraction along all Bragg rods within a certain range in reciprocal space and perform a three-dimensional BFT to obtain the true three-dimensional electron density of the Gd_2O_3 passivation layer.

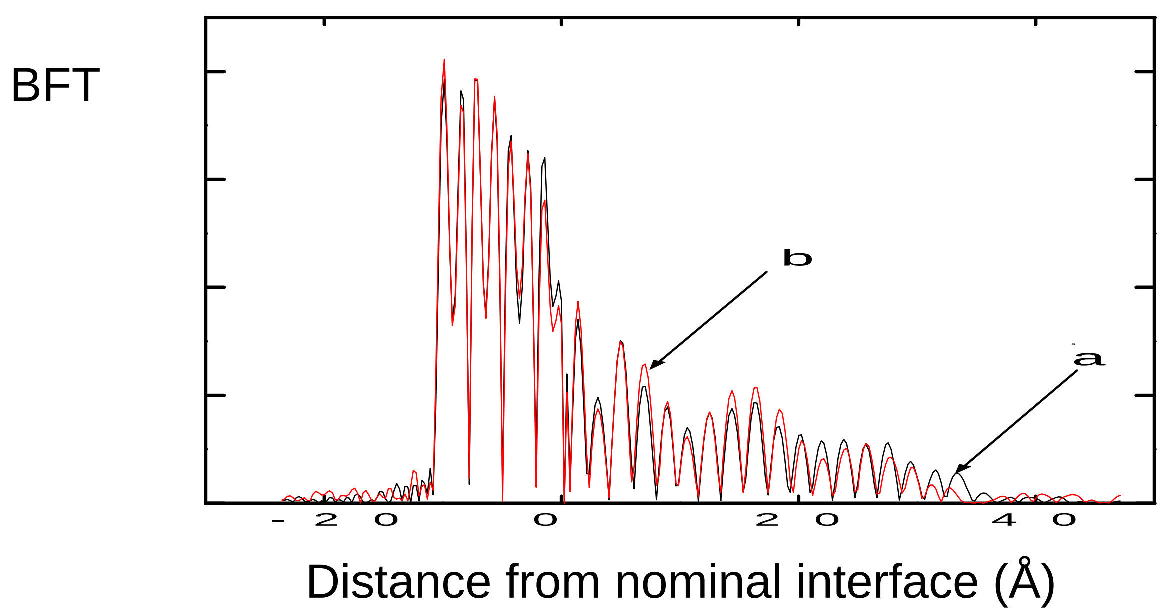

Fig. 1: Back Fourier transform of the complex structure factor of a 30 Å thick Gd_2O_3 passivation layer on (100) GaAs. Note the non-monotonic variations in the electron density to the right of the interface. The two curves (a) and (b) correspond to different starting models for the structure, illustrating that the final best fit BFT is relatively insensitive to the details of the initial reference model.

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