Determination of the Atomic Structure of a Gd_2O_3 Thin Film Epitaxially Grown on a GaAs Crystal Surface

Y. Yacoby,[1] J. O. Cross,[2] J. Pitney,[3] R. Pindak,[3] R. Clarke,[4] E. A. Stern[5]

[1] *Racah Institute of Physics, Hebrew University of Jerusalem, Israel*

[2] *Advanced Photon Source, Argonne National Laboratory, Argonne, IL, U.S.A.*

[3] *Lucent Technologies Bell Labs, Murray Hill, NJ, U.S.A.*

[4] *Department of Physics University of Michigan, Ann-Arbor, MI, U.S.A.*

[5] *Department of Physics, University of Washington, Seattle, WA, U.S.A.*

Introduction

We are in the process of determining the atomic structure of a 25 Å Gd_2O_3 film epitaxially grown on the [100] surface of a GaAs single crystal. The samples were grown by Dr. M. Hong of Lucent Technologies, Bell Labs. The structure is determined using a novel x-ray method that provides the amplitude and phase of the complex scattering factor. The real-space three-dimensional structure of the film and of the underlying GaAs crystal is then determined by back Fourier transforming the complex scattering factor into real space.

Methods and Materials

The measurements were carried out in the following way: The crystal was mounted on a 6-circle Huber goniometer. The x-ray beam was vertically focused down to about 200 microns. This together with some 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 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, consisting of radiation that was not limited to the Bragg rod, was subtracted.

Results

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. Outside this range, the intensities were too low to be measured. The data have been analyzed in the following way: We first guessed a model structure and adjusted its parameters to provide best fit to all the Bragg rod intensities that were measured. In spite of the nine adjustable parameters, the model does not fit the data well along all Bragg rods. This misfit corresponds to an unknown electron density that is the difference between the true electron density of the system and the electron density represented by the model. We then calculated the complex scattering factor of the unknown electron density using the method described in ref. 1. In this calculation the model electron density is used as a reference for the calculation of the complex scattering factor of the unknown electron density. The scattering factor of the true electron density is then the sum of the model scattering factor and the scattering factor correction.

Discussion

At this time, since we do not have data along all relevant Bragg rods, we have calculated the complex scattering factor and the back Fourier transform (BFT) of the true electron density along one Bragg rod namely [h 1 -1]. In Fig. 1 curve (a), we present the BFT of the best fit model. In Fig. 2 curve (a), we present the BFT of the true electron density. Notice that the two are quite different,

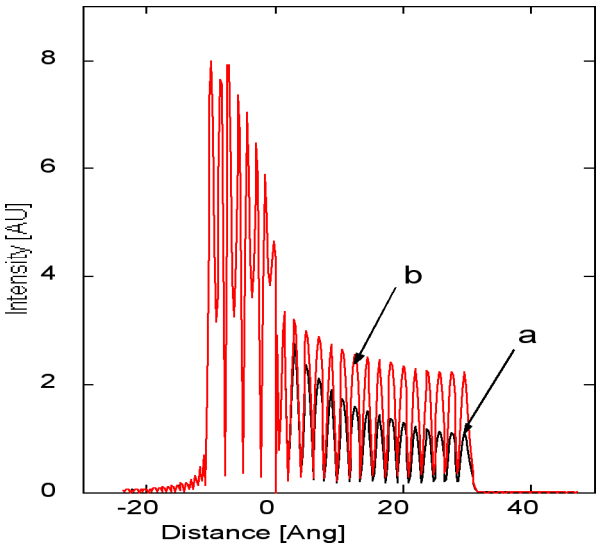

FIG. 1. BFT of the best fit model (a) and the modified model (b).

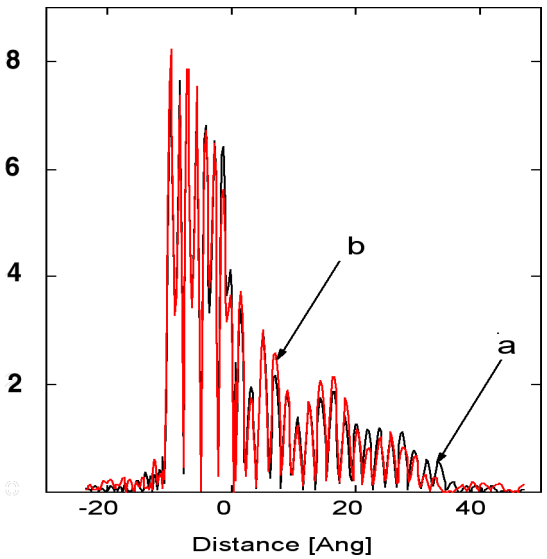

FIG. 2. BFT of the true scattering factor, (a) calculated using the best fit model, and (b) calculated using the modified model.

and it would have been difficult to guess the oscillations observed in Fig. 2. To test that the correction is not strongly dependent on the model, we used a modified reference shown by curve (b) in Fig. 1. Notice that the corresponding curve in Fig. 2 (b) is almost equal to curve (a), meaning that the final result is not strongly model dependent. Next we shall measure all Bragg point within a

certain range in reciprocal space and perform a three dimensional BFT to obtain the three dimensional true electron density.

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Reference

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