Reflection-Mode XAFS Study of 300 Å Oxidized $Al_{0.96}Ga_{0.04}As$ on a GaAs Substrate

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Introduction

New approaches for growing oxide films on AlGaAs using wet oxidation have been developed in the last several years.[1,2]

While most of the As in the semiconductor crystal leaves during oxidation, residual quantities have been correlated to bulk oxide leakage current and to interfacial traps that increase interface recombination and produce Fermi-level pinning.[3] Hydrogen liberated in the wet oxidation reaction is believed to play an important role in reducing As_2O_3 to As, and possibly As to AsH_3, volatile species that can more readily escape the oxide film.[4] Yet the degree to which, and the form in which, As remains are still not well understood. Crystalline As, amorphous As, and amorphous As_2O_3 have been observed via Raman spectroscopy in partially oxidized AlGaAs films, with As scattering dropping to barely detectable levels after full oxidation.

The reflection-mode x-ray absorption fine-structure spectroscopy (XAFS) technique is near ideal for investigating the As environment around interface between oxide and GaAs substrate. This technique is sensitive to the local structure about a chosen atomic species, revealing the types of nearby atoms and the radial distance distributions to these neighbors.

Materials and Methods

A thin 300 Å $Al_{0.94}Ga_{0.06}As$ film on a GaAs substrate is surface oxidized using the methods described previously.[5]

Reflection-mode XAFS measurements are performed at the MRCAT 10-ID line using an 8-circle Huber diffractometer over the energy range 11,667-12,900 eV for As *K* edge in fluorescence mode with the same experimental geometry as for x-ray reflectivity measurements.

Results

Figure 1 shows small-angle x-ray reflectivity data for 300 Å oxidized $Al_{0.94}Ga_{0.06}As$ / GaAs as a function of x-ray incident angle. The fluorescence data are obtained during a reflectivity scan at 300 eV above the As edge (12167 eV). At an x-ray incident angle slightly higher than the oxide critical angle, x-rays propagate through the top oxide layer (lighter layer) and totally reflect off the buried GaAs layer but can still penetrate a short distance into GaAs layer as an evanescent wave. As can be seen in Fig. 1, the fluorescence intensity increases with angle, indicating the x rays are penetrating deeper into the GaAs. Eventually the x-ray incident angle reaches the critical value for GaAs, and the fluorescence signal gets saturated. XAFS measurements were taken at four different angles between 0.15° and 0.21°.

When using glancing angles, however, the measured fluorescence signal is not linearly proportional to the absorption coefficient but includes a contribution from changes in δ with energy in the refractive index $n = 1 - \delta + i\beta$.[6] Thus, corrections need to be made before detailed XAFS analysis at glancing angles, i.e., distortions in fluorescence XAFS can be simply calculated using the density profile from the reflectivity analysis[7] and must be removed.

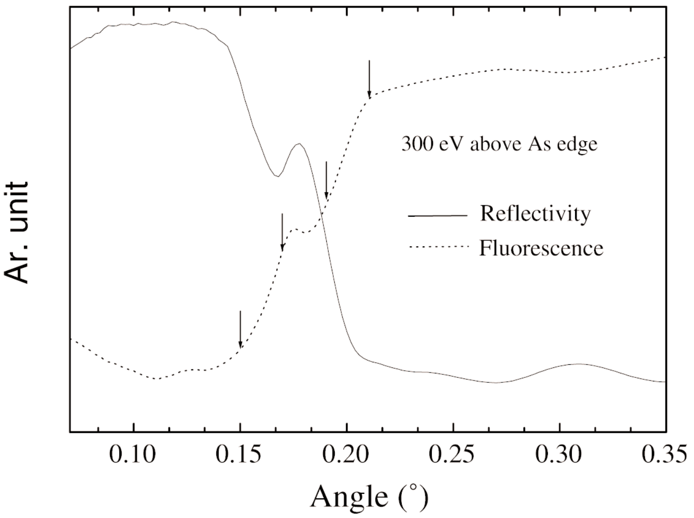

FIG. 1. Reflectivity scan as a function of x-ray incident angle (solid line). Fluorescence data were taken during a reflectivity scan (dotted line); arrows indicate the angles at which the XAFS were taken.

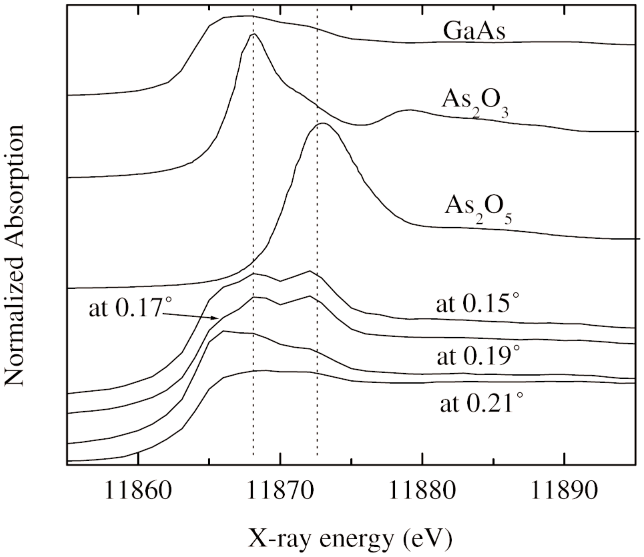

FIG. 2. XANES spectra of 300 Å oxidized $Al_{0.94}Ga_{0.06}As$ / GaAs at various x-ray incident angles. GaAs, As_2O_3, and As_2O_5 are also shown.

Figures 2 and 3 show that XANES and EXAFS data, respectively, at each angle along with several references (As_2O_3, As_2O_5, and GaAs). As can be seen features of As_2O_3, As_2O_5, and GaAs appear at the shallow angles (0.15° and 0.17°) in both XANES and EXAFS. At relatively deep angles (0.19° and 0.21°) XANES and EXAFS both show that the GaAs features become stronger due to x-ray penetration into substrate, on the other hand As oxide features becomes negligible.

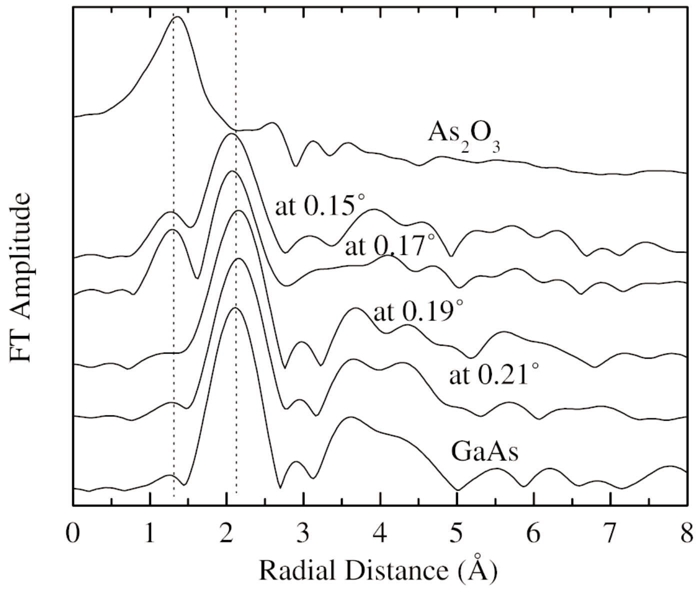

FIG. 3. Magnitudes of Fourier transform (FT) of the As K-edge data for 300 Å oxidized $Al_{0.94}Ga_{0.06}As$ */ GaAs at various x-ray incident angles. GaAs and* As_2O_3 *are also shown.*

Discussion

The reflectivity results of the same sample studied with another technique[7] show the high-density layer (close to GaAs density) with ~25 Å thickness on the surface. This GaAs presence is observed by reflection-mode XAFS. As_2O_3 and As_2O_5 are also observed in the oxide layer including the interface between oxide and GaAs substrate.

Acknowledgments

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