In situ XAFS study of Fe epitaxially grown by MBE on GaAs(001)-4x6

D.T. Jiang, R.A.Gordon, E.D.Crozier, T.L. Monchesky, B.Heinrich
Simon Fraser University, Burnaby, B.C.,Canada, V5A 1S6

Introduction

To utilize the high brilliance x-rays at the APS in studying atomic structures of ultrathin epitaxial magnetic films, we have constructed a molecular beam epitaxy (MBE) growth and analysis system at the PNC-CAT undulator beamline, sector 20. The system is designed to optimize the stability and reproducibility of sample position for glancing x-ray techniques. It consists of one single level growth/analysis UHV chamber and a sample loadlock chamber. It has a 6-degree freedom of sample manipulation: XYZ stage with ±180° polar & azimuth and 90° flip, based on Thermionics model FM103 and GB-16 components. Reflection high energy electron diffraction (RHEED, Kimball Physics EMG-14) is used to characterize the substrate crystalline state prior and during the epitaxial growth. For epitaxial growth, currently it is equipped with an Ar sputter gun (Physical Electronics 04-162), sample heating/cooling (-150 °C to 1200 °C) and three flux-controlled e-beam evaporators (Omicron EFM3). A quartz crystal thickness monitor (Leybold XTM/2) is also available for thickness calibration. The typical chamber base pressure is ~ $1x10^{-10}$ torr.

The structural analysis capabilities include conventional SEXAFS, total reflection XAFS with the x-ray electric vector being parallel or perpendicular to the sample surface, x-ray standing wave (XSW) and Reflectivity. The system is configured to simultaneously monitor glancing angle XAFS in fluorescence, total electron yield (TEY) and reflectivity. Two Ge solid state detectors (single element and 13-element, by Princeton Gamma-Tech) are available to monitor the fluorescence yield at low adsorbate coverage.

An *in situ* study of the Fe epitaxial growth on GaAs(001)-4x6 is used to illustrate the capability of the MBE/analysis facility. It has been found that room temperature growth of Fe on an As depleted GaAs(001)-4x6 surface, prepared by mild sputtering and annealing, can prevent magnetic dead layer formation [1,2]. Work has already started towards using Fe(001)/GaAs(001) as a template for further growth of giant magnetoresistance (GMR) trilayer systems [2]. Although well-defined coherent growth of Fe on GaAs(001)-4x6 has been established [1], what has yet to be determined is to what extent the Fe(001) films maintain their bulk bcc symmetry. To answer this, a distance probe along the surface normal direction is required. Polarization-dependent XAFS is well-suited to characterize the ratio between the lattice constant lying in the surface plane and that along the surface normal, giving the lattice strain in a layer-resolved manner.

Results and Discussion

The substrate surface preparation followed the procedure described in Ref. [2]. The Fe layers were grown at near room temperature and at a rate of about 0.75 ML/min. Figure 1 shows the oscillation of the RHEED specular reflection, the anti-Bragg geometry used is the same as that described previously [2]. For the first 2 monolayers the Fe growth proceeds in a 3-D island growth mode and then switches to a quasi-layer-by-layer mode.

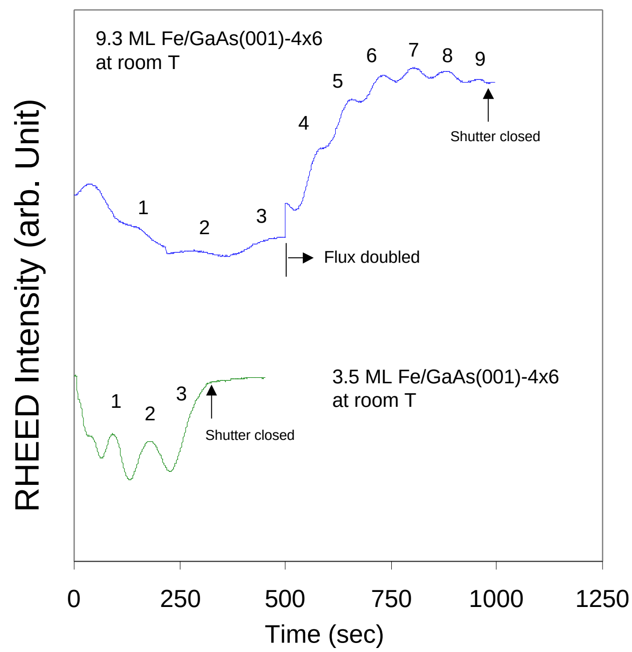

Fig. 1. RHEED specular intensity oscillations during two growths of Fe(001)/GaA(001)-4x6 at room temperature. Film thickness in monolayers is estimated from the number of oscillation periods. The first part of the 9.3 ML growth was at a slower rate and the kink between 1 and 2 ML is due to switching off an ion gauge.

The XAFS data were taken in fluorescence yield mode and with the electric vector of the x-ray perpendicular or parallel to the sample surface. The sample surface was aligned at a glancing angle of ~2/3 of the measured critical angle of each film thickness. At this angle the anomalous scattering effects in the XAFS data are small enough to neglect [3].

Figure 2 shows the XAFS interference function *c(k)* extracted from data with the electric vector of the x-ray perpendicular to the surface. As the number of monolayers increases more frequencies appear , but at 15 ML, the *c(k)* still shows significant differences compared to bulk bcc Fe. There are systematic differences between the out-of-plane and the in-plane data which resemble more closely bulk bcc Fe.

Using the *ab intio* XAFS amplitude and phase calculation package FEFF 7.02 [4] and curve-fitting the Fourier transforms of the *c(k)*, it can be shown that the differences are primarily in the photoelectron multiple scattering paths, while the basic unit cell contents (up to the second nearest neighbour) viewed from two orthogonal directions

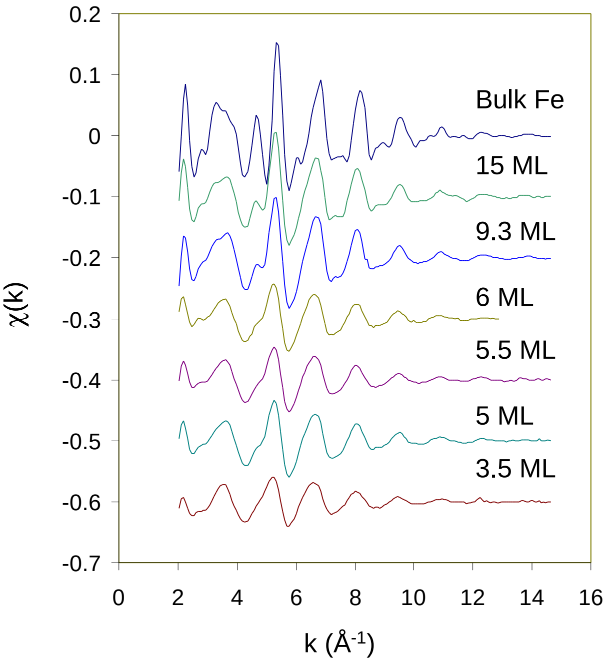

Fig. 2. Fluorescence XAFS data of Fe(001) (3.5 ML-15 ML) on GaAs(001)-4x6, with the x-ray electric vector perpendicular to the surface of the GaAs. The top trace is bcc Fe data extracted from transmission measurements on an iron foil.

are similar but with different bond length ratios. By quantitatively extracting the second nearest neighbour bond lengths, the lattice strain was obtained in terms of the c/a ratio, except for films with less than 5 ML which require further analysis.

Figure 3 shows the c/a ratio as a function of the film thickness. It is clear that the Fe films grown in the quasi-layer-by-layer mode have a bct structure, with about 3% expansion in the surface normal direction. Up to the upper thickness measured, 15 ML, there is no indication it is near the critical thickness at which the Fe film would relax back to a pure bcc structure.

Conclusions

A MBE growth/analysis system has been constructed at the PNC-CAT. As an illustration of the epitaxial growth and structure analysis capability of the system, the polarization-dependent XAFS results for Fe growth on GaAs(001)-4x6 are described. In contrast to previous perceptions about

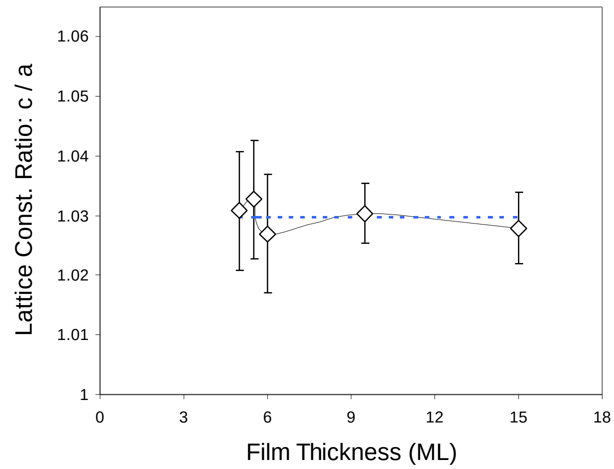

Fig. 3. The in-plane and out-of-plane lattice constant ratio c/a. Results are for five samples grown at room temperature on four individually prepared GaAs(001)-4x6 substrates (15 ML sample was grown on top of the 5.5 ML sample). The dashed line indicates a ratio of 1.03. The ratio for bulk bcc Fe is unity.

the 3-D structure of this system, films with 5 to 15 ML of Fe still possess a significant strain as indicated by the 3% c/a ratio expansion. The Fe on GaAs(001)-4x6 system is better described as a bct structure. The same conclusion was reached in our *ex situ* XAFS study of Fe/GaAs(001)-4 x6 capped with 20 ML of Au [5]. Thus a strain-induced magneto-elastic anisotropy contribution due to this type of vertical lattice expansion should be considered when intepreting magnetic properties of this system.

Acknowledgements

The Natural Sciences and Engineering Research Council of Canada provided support through an operating grant and a major facility access grant. Experiments at the PNC-CAT beamline, Advanced Photon Source, Argonne National Laboratory are also supported by the U.S. Department of Energy, Basic Energy Sciences, Office of Science, under Contract No. W-31-109-Eng-38 (APS) and DE.FG03-97ER45628 (PNC-CAT).

References.

[1] M. Zölfl, M. Brockmann, M. Köhler, S. Kreuzer, T. Schwenböck, S. Miethaner, F. Bensch, and G. Bayreuther, J. Magn. Magn. Mater.175, 16(1997).

[2] T.L. Monchesky, B. Heinrich, R. Urban, and K. Myrtle, Phys. Rev. B. 60,10242 (1999).

[3] D.T. Jiang and E.D. Crozier, Can. J. Phys. 76, 621(1998).

[4] S.I. Zabinsky, J.J. Rehr, A. Ankudinov, R.C. Albers, and M.J. Eller, Phys. Rev. B52, 2995(1995).

[5] R.A. Gordon, E.D.Crozier, D.T. Jiang, T.L. Monchesky, B. Heinrich, APS User Activity Report, 2000.