



Investigating In-plane Structural Anisotropy of Ultra-thin Fe Films on GaAs(001)-4x6

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PNC-CAT

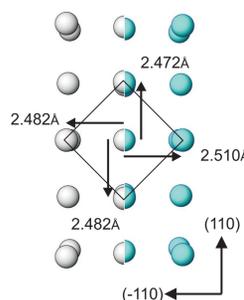


INTRODUCTION

Iron films on gallium arsenide substrates, with the small mismatch (1.4%) between lattices, are subjected to extensive experimental and theoretical examination in an effort to understand the magnetic behavior and the role of the interface in influencing the magnetic anisotropy. Bulk body-centred-cubic (bcc) iron deposited on the Ga-terminated 4x6 reconstructed surface of GaAs will grow epitaxially, but strained due to the mismatch in lattices, with layer-by-layer growth occurring above 3 - 4 monolayers (ML) thickness and island growth below.

Our detailed *in-situ* X-ray Absorption Fine Structure (XAFS) study on films up to 30ML thick [1] indicated a distortion to a body-centred-tetragonal (bct) structure, with a *c/a* ratio essentially constant from 5 to 30 ML at 1.03(1). This study, however, did not fully examine any potential in-plane structural anisotropy. First-principles density-functional calculations by Mirbt et al. [2] on the Fe-GaAs interface, for films up to 5 ML thick, indicated a *c/a* ratio consistent with the XAFS work, but also suggested an in-plane distortion was possible. We have returned to this system to examine further this possibility by studying films of 2 and 5 ML thickness using polarization-dependent XAFS with an emphasis on the in-plane (110) and (-110) directions.

Theoretical In-plane Distortion

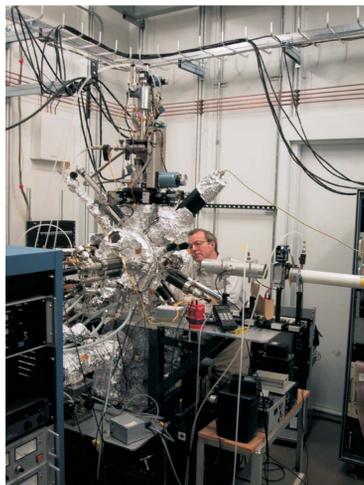


A comparison of bcc Fe (gray/white spheres) and the distortion calculated by Mirbt et al. (Blue) for 5ML Fe with 1ML As overlayer. The original bcc unit cell is outlined. Nearest-neighbour distances are shown.

The calculations by Mirbt et al, indicated that the films distort along both the (110) and (-110) directions in-plane as well as in the (001) out-of-plane direction. The extent of distortion is dependent on the amount of arsenic that segregates to the surface of the film and the thickness of the film itself.

From Table 1 in Mirbt et al, the distortions can be used to calculate revised near-neighbour distances for comparison to bcc Fe.

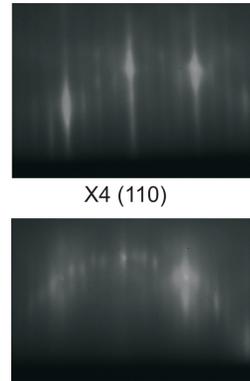
Film	As-overlayer	NN-(110)/Å	NN-(-110)/Å
Bulk Fe	None	2.482	2.482
2ML	0.5ML	2.447	2.524
	1.0ML	2.471	2.531
5ML	0.5ML	2.454	2.480
	1.0ML	2.472	2.510



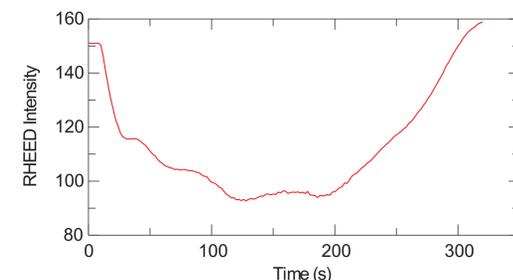
Sample Preparation

Thin film samples were prepared and examined *in-situ* using the MBE1 facility at the Pacific Northwest Consortium beamline, sector 20 at the APS. The system has a base pressure near 2×10^{-10} Torr, possesses 3 Omicron EFM3 evaporators for metal deposition and uses a custom sample goniometer (Thermionics Northwest GB-16) for sample positioning. Cleaved sections of n-type GaAs(001) substrates (American Xtal Tech.) were given a thermal desorption treatment near 600 °C, then sputtered at room temperature using 500eV Ar⁺ ions for 3 hours. Substrates were then annealed to achieve the 4x6 reconstructed surface over the course of 30 minutes.

LEFT: The MBE1 endstation in 20-ID-C set up for X-ray measurements.

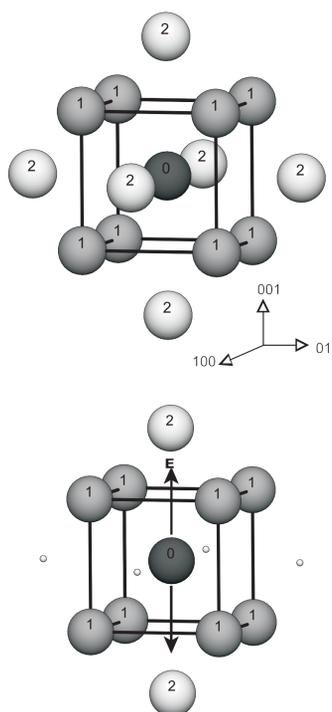


RHEED images of the 4x6 reconstruction of GaAs



Iron film thickness as determined by monitoring oscillations in the Reflection High Energy Electron Diffraction (RHEED) intensity of the specular spot from an electron beam as shown above for the deposition of 5 ML of iron.

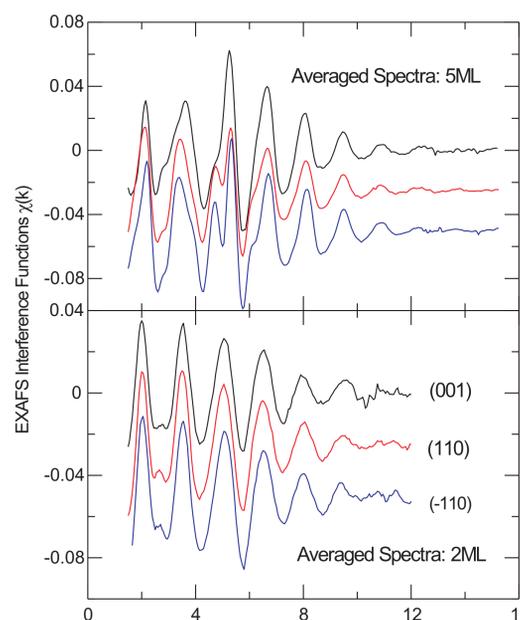
Polarization-Dependent XAFS



A small splitting of distances within an XAFS "shell" can be difficult to resolve. The body-centred geometry (left), however, with the linearly polarized X-rays permits the split distances to be analyzed separately. Atoms perpendicular to the X-ray polarization contribute little to the XAFS.

Second-near neighbours can be separated by orienting the X-ray electric field vector along (001) or in-plane (below left and right)

First-near neighbours can be separated by using X-rays polarized along (110) and (-110) (below).



Fit Results

Data Fourier-transformed and fit in R-space using FEFF[3] and WinXAS[4].

First-near-neighbour results:

5ML
(001) 2.485(11) Å
(110) 2.491(10) Å
(-110) 2.484(10) Å

These are essentially the same.

2ML
(001) 2.471(10) Å
(110) 2.461(10) Å
(-110) 2.478(10) Å

There is a sufficient difference between (110) and (-110) to suggest an in-plane distortion is present, but smaller than calculated.

Conclusions

There is evidence for an in-plane distortion at 2 monolayer thickness, below the transition from island to layer growth modes. The first-principles calculations of Mirbt et al. overestimates the magnitude of the distortion.

At 5 monolayers, where epitaxial layer-by-layer growth is occurring, no conclusive evidence for a distortion was observed. From an XAFS perspective, 5ML iron films on GaAs(001)-4x6 are indistinguishable from a body-centred tetragonal structure.

Acknowledgments

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References
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