

Distorted Iron Films on GaAs (001)-(4x6)

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Introduction

Significant efforts have been made to understand the physical and magnetic behavior of iron films on gallium arsenide [1-4]. The appeal of this system is the very small lattice mismatch between body-centered cubic (bcc) iron ($a = 2.866\text{\AA}$) and GaAs ($a/2 = 2.827\text{\AA}$). Having only a 1.4% mismatch should facilitate the growth of bcc-like Fe films on the GaAs substrate, making this system ideal for testing new thin-film structures for magnetoelectronic applications [5,6].

Complications to studies of this system, in the form of magnetically-dead layers arise from reaction of the iron with the GaAs to form a solid solution, $\text{Fe}_3\text{Ga}_{2-x}\text{As}_x$ [7,8] at the interface and, depending on preparation conditions, to several tens of monolayers in thickness [7]. Two approaches exist to avoid forming this ternary phase at the interface: sulphur passivation [9,10] and Ga-enrichment of the GaAs surface by using the (4x6) reconstruction [11,12]. Both are aimed at reducing the availability of As for reaction with the Fe and at producing bcc-structured Fe films.

We have used polarisation-dependent XAFS to determine the in-plane and out-of-plane lattice parameters of three iron films. We have examined *ex-situ* a 10 monolayer iron film on GaAs(001)-(4x6) capped with 20 monolayers of gold (20Au/10Fe/GaAs(001)-(4x6)) and compared it to *in-situ* results on a 9.3 ML sample (9.3Fe/GaAs(001)-(4x6)) that are preliminary to an extended *in-situ* study [13]. Measurements for further comparison have also been made on a 5 ML gold-capped iron film on a sulphur-passivated GaAs(001) substrate (20Au/5Fe/GaAs-S-pass.).

Experimental

Samples on (4x6)-GaAs were prepared by molecular beam epitaxy on epitaxially grown GaAs (American Xtal Technology) as described in reference 14. The *in situ* sample was grown in MBE-1 [13] located on the PNC-CAT undulator beamline [15], sector 20, APS. The sulphur-passivated sample was prepared by treatment with aqueous ammonium sulphide, rinsed and dried prior to introduction to the vacuum system as described in reference 10. The samples for *ex-situ* measurements also had 20 monolayers of gold epitaxially grown on top of the iron for protection from the atmosphere.

Fe K-edge fluorescence XAFS measurements were made with linearly polarised X-rays from a Si-(111) double crystal monochromator (60% tune at 7500eV). The x-rays were incident on the films at 0.25° ($\sim 5/8$ the critical angle for total reflection) for *in-situ* or near glancing angle ($\leq 2^\circ$) for *ex-situ* measurements. The electric field vector of the X-rays was within 2° of the (001) direction for out-of-plane measurements on the three samples. In-plane measurements

were done roughly along the (110) and (010) directions for *ex-situ* and *in-situ* samples, respectively.

Results

The polarisation-dependent XANES for the 5ML of Fe on sulphur-passivated GaAs resembles quite strongly that for the iron foil. The XANES for the samples on (4x6)-GaAs, while exhibiting features similar to those for polycrystalline Fe foil, do show some differences that are more pronounced for the out-of-plane measurements than those for the measurements made with the X-ray electric field vector in the plane of the film. This suggests that the structure of the iron films is similar to that for bcc iron, with some distortion for the samples on (4x6)-GaAs.

The effects of the distortion are evident in the XAFS interference function, $\chi(k)$, with the most obvious differences between either the polycrystalline Fe foil or the in-plane film and the out-of-plane film data occurring in the range 2.5\AA^{-1} to 10\AA^{-1} , Fig.1. To obtain quantitative structural parameters, the Fourier transforms Fig. 1, were fit over the R-space range 1.6\AA to 4.1\AA . The polarisation-

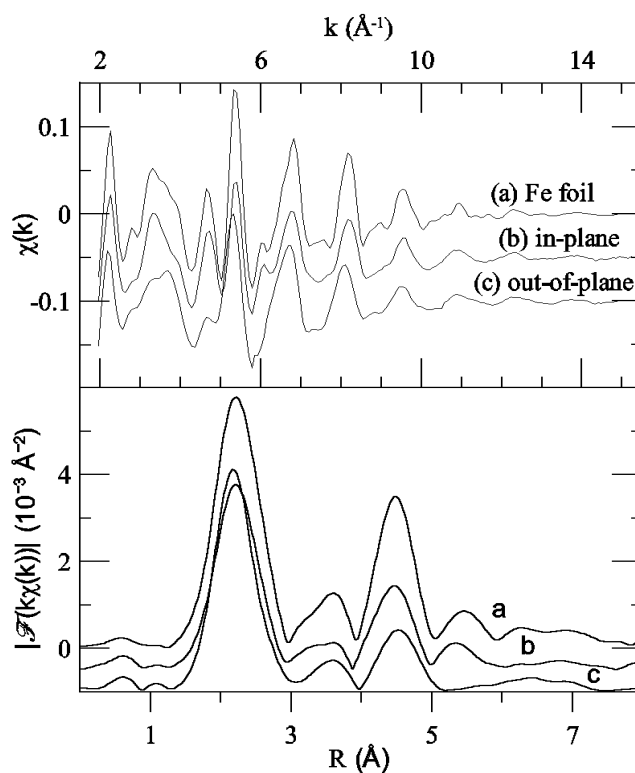


Fig.1. The XAFS interference function, $\chi(k)$, and the magnitude of the Fourier transform $F(k\chi(k))$ of polycrystalline Fe foil and 10 monolayers of Fe in 20Au/10Fe/GaAs(001)(4x6). The transform was taken over the range 3\AA^{-1} to 15\AA^{-1} with a 10% Gaussian window applied.

dependent multiple scattering formalism of Rehr and Albers implemented in the computer program FEFF7 [16] permitted analysis of the first three shells - nearest neighbour, lattice parameter and face diagonal positions of a body centered tetragonal unit cell. The main objective of the fitting was to obtain the in-plane and out-of-plane lattice parameters. These are tabulated in Table 1. for all three films as well as iron foil.

An in-plane contraction can be understood as an effort to lattice match to the underlying GaAs ($a/2 = 2.827\text{\AA}$) and the expansion an effort to conserve cell volume (a^2c , Table 1.) or nearest-neighbour distance. According to elasticity theory, the ratio of the out-of-plane to in-plane strain $\Delta c/\Delta a = -2c_{12}/c_{11}$. Using the known elastic constants c_{ij} [17], the ratio should be -1.212. The experimental strains for the films, defined by subtracting the lattice parameter of the bcc Fe foil, are tabulated in Table 1. Although the errors associated with the small differences are large, for the *ex situ* 10ML film $\Delta c/\Delta a = -2.0 \pm 1.0$ is noticeably offset from the bulk iron value of -1.212. However, for the *in-situ* 9.3 ML film and the 5ML film on sulphur-passivated GaAs, no disagreement with macroscopic elasticity theory can be claimed.

Table 1. Comparison of lattice constants and uniaxial strain for epitaxial iron films on GaAs (001)(4x6) and GaAs(001)-S-passivated.

Parameter	Fe crystal	20 Au/10Fe	9.3Fe	20Au/5Fe(S)
a (Å)	2.8664	2.834(2)	2.837(2)	2.862(2)
c (Å)	2.8664	2.93(3)	2.91(50)	2.858(20)
c/a	1.000	1.034(11)	1.026(18)	0.999(1)
a^2c (Å ³)	23.55	23.5(3)	23.4(4)	23.41(5)
Δa (Å)	0.000	-0.032(2)	-0.029(2)	-0.004(2)
Δc (Å)	0.000	0.064(30)	0.044(50)	-0.008(2)
$\Delta c / \Delta a$	-1.2128*	-2.0 ± 1.0	-1.5 ± 1.8	2 ± 1
* $\Delta c / \Delta a = -2c_{12} / c_{11}$ $\Delta a = a - a_{crysta}$ $\Delta c = c - c_{crystal}$				

In the analysis it was necessary to consider the possibility of the formation of the “Fe₃Ga_{2-x}As_x” compound. From simulations using FEFF7 [16] we were able to conclude that the films are dominated by a Fe bct-like structure and are not Fe₃Ga_{2-x}As_x. We cannot, however, rule out some small mixture of phases. The simulations indicated that EXAFS would be insensitive to any alloying less than 20%.

Conclusions

We have used polarised-XAFS studies to examine the structures of two iron films deposited on GaAs(001)-(4x6) surfaces and one on sulphur-passivated GaAs(001), and compared them to the body-centred cubic structure of an iron foil. The 5ML sample on sulphur-passivated GaAs exhibits a nearly cubic structure with $c/a = 0.999(1)$. The

structures of the 10ML (*ex-situ*) and 9.3ML (*in-situ*) samples on (4x6)-GaAs can be modeled by a tetragonal distortion away from bcc with an in-plane contraction that improves (lessens) the lattice mismatch with GaAs and an out-of-plane expansion that nearly conserves cell volume to give a c/a ratio of 1.03(1).

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