Distorted iron films on GaAs(001)-(4×6)

Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6
(Received 27 December 1999)

Polarized K-edge x-ray absorption fine structure spectroscopy (XAFS) studies were performed both in and ex situ on iron films deposited on GaAs substrates. Samples with 5 and 10 ML (monolayers) of iron deposited on sulfur-passivated and (4×6)-reconstructed GaAs(001) surfaces, respectively, were studied ex situ (capped with 20 ML of gold) and compared with 9.3 ML on GaAs(001)-(4×6) measured in situ. Analysis of XAFS spectra for both samples on (4×6)-GaAs reveals a tetragonal distortion of the iron film relative to bulk body-centered-cubic iron. The distortion involves an in-plane contraction and an expansion perpendicular to the GaAs surface to give a c/a ratio of 1.03(1), with a comparable to half the bulk lattice constant of GaAs. The sample on sulfur-passivated GaAs did not exhibit this distortion.

I. INTRODUCTION

Significant efforts have been made to understand the physical and magnetic behavior of iron films on gallium arsenide.1–6 The appeal of this system is the very small lattice mismatch between body-centered-cubic (bcc) iron (a = 2.866 Å) and GaAs (a/2 = 2.827 Å). 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.7,8 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, Fe3Ga2(Asx), with a1 001 comparable to half the bulk lattice constant of GaAs.9,10 at the interface and, depending on preparation conditions, to several tens of monolayers in thickness.9 Two approaches exist to avoid forming this ternary phase at the interface: sulphur passivation11,12 and Ga enrichment of the GaAs surface by using the (4×6) reconstruction.13,14 Both are aimed at reducing the availability of As for reaction with the Fe and at producing bcc-structured Fe films.

Recently, Monchesky et al.15 described a method, modified from Zöllf et al.13 for preparing high-quality Fe films on GaAs(001)-(4×6) for iron thicknesses greater than 4 ML (monolayers). Using polarization-dependent x-ray absorption fine-structure spectroscopy (XAFS),16–21 we can examine the structure of the iron film both in plane, and extract information complimentary to the electron diffraction techniques, reflection high-energy electron diffraction (RHEED) or low-energy electron diffraction and perpendicular to the surface, a direction in which interpreting results from the electron techniques is more involved. We have examined ex situ a 10 ML iron film on GaAs(001)-(4×6) capped with 20 ML of gold [20Au/10Fe/GaAs(001)-(4×6)] using polarized XAFS and compared it to in situ results on a 9.3 ML sample [9.3Fe/GaAs(001)-(4×6)] that are preliminary to an extended in situ study.22 Measurements for further comparison have also been made on a 5 ML gold-capped iron film on a sulfur-passivated GaAs(001) substrate (20Au/5Fe/GaAs-S-pass).

II. EXPERIMENT

Samples on (4×6)-GaAs were prepared by molecular-beam epitaxy on epiready GaAs (American Xtal Technol-
III. RESULTS

Figure 1 shows the x-ray absorption near-edge structure (XANES) for the three samples 20Au/10Fe/GaAs(001)-S-passivated (ex situ), 20Au/5Fe/GaAs(001)-(4×6), and 20Au/10Fe/GaAs(001)-(4×6). The monochromator was calibrated such that the onset for the edge (first maximum in the derivative) in the foil \( E_0 \) was defined to be 7112 eV. The edge energies for the thin-film samples are consistent with the foil’s edge energy, indicating no change in valence for the iron in the thin films. Above the edge, the XANES for the 5 ML of Fe on sulfur-passivated GaAs resembles quite strongly that for the iron foil. The XANES for the samples on (4×6)-GaAs, while exhibiting features similar to those for the 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 all suggests that the structure of the iron films is similar to that for bcc iron, with some distortion for the samples on (4×6)-GaAs.

The EXAFS interference functions \( \chi(k) \), shown in Figs. 2 through 4 were extracted from the \( \mu(E) \) data of individual scans using a polynomial background subtraction and normalization to edge jump.\(^{25}\) The \( \chi(k) \) shown are averages of five scans for out-of-plane, three for in-plane measurements, and one for ex situ, as shown in Figs. 1(a), 1(b), and 1(c).

FIG. 1. Polarization dependent Fe K-edge XANES of (a) 20Au/10Fe/GaAs(001)-(4×6) (ex situ), (b) 9.3Fe/GaAs(001)-(4×6) (in situ), and (c) 20Au/5Fe/GaAs(001) (S passivated, ex situ) samples compared with iron foil. The electric-field vector of the x-rays was either parallel (in-plane) or perpendicular (out-of-plane) to the substrate. Data has been offset vertically in 0.1 increments for clarity.

FIG. 2. Counterclockwise from top: XAFS \( \chi(k) \), magnitude of the Fourier transform, \( \mathcal{F}[k\chi(k)] \), and the derivative of the phase of the inverse transform of the first peak for 20Au/10Fe/GaAs(001)-(4×6).

FIG. 3. Counterclockwise from top: XAFS \( \chi(k) \), magnitude of the Fourier transform, \( \mathcal{F}[k\chi(k)] \), and the derivative of the phase of the inverse transform of the first peak for 9.3Fe/GaAs(001)-(4×6).
and two for the foil. Fourier transforms in these figures were
taken with \( k^1 \) weighting and a 10\% Gaussian window over
the \( k \)-space range using the nearest zero crossings to 3 and 15
Å\(^{-1} \). Inverse transforms of the first peak were taken typically
over the range 1.65 to 2.85 Å to examine interference effects
(beating) between the nearest and second-nearest neighbors.
The phases of the inverse transform have been differentiated
with respect to \( k \) \( = h^{-1}\sqrt{2m(E-E_0)} \) and plotted with
the EXAFS spectra and Fourier transforms for beating analysis.\(^{26,27} \)

The first- and second-nearest neighbors in bcc iron (Fig.
5), at \( R_1 = 2.4824 \) Å and \( R_2 = 2.8664 \) Å (note: \( R_2 = a \),
the lattice parameter), cause the beating observed from the first
peak in the Fourier transform of \( k \chi(k) \). The \( k \) values corre-
spending to the minima in the derivatives of the phase shown in
Figs. 2-4 are related approximately to the separations be-
 tween \( R_1 \) and \( R_2 \) for the foil and samples by the relation\(^{26,27} \)

\[
k_{min} \times (R_2 - R_1) = \text{const}
\]  

provided the two neighbors are the same element. Ideally,
the constant would be \( \pi/2 \), however, the transform range,
disorder, alloying, the presence of a substrate, and a passiva-
tion layer or capping layer may all influence the difference in
distances for our samples.

![FIG. 5. bcc iron unit cell showing representative atoms for the first three backscattering paths: \( R_1 \)---nearest neighbor, \( R_2 \)---lattice parameter, and \( R_3 \)---face-diagonal distances.](image-url)

Taking the iron foil as a reference to give the \textit{constant}
term, and \( k_{min} \) from the derivatives of the phase, \( d\phi/dk \),
shown in Figs. 2–4, we obtain the values listed in Table I for
the differences in distance. Also listed in Table I are esti-
mates of the lattice parameters using the bulk-iron crystallo-
graphic value of \( R_1 \). Consistent with the XANES, the 5 ML
sample on S-passivated GaAs shows little difference (possibly
a slight in-plane expansion and out-of-plane contraction)
from bcc iron while the samples on (4\times6) GaAs exhibit a
small in-plane contraction and larger out-of-plane expansion.
The beating analysis provides an initial model for further
analysis: a body-centered-tetragonal (bct) distortion from
body-centered-cubic iron with space group I4/mmm, \( a = 2.84 \) Å and \( c = 2.92 \) Å for the samples on (4\times6) GaAs,
and no distortion from bcc for the 5 ML sample on S-passivated GaAs.

Before continuing the analysis, and even though the \( \chi(k) \)
bears a strong resemblance to that for bulk iron, it was nec-
necessary to consider the possibility of the formation of the
‘\text{Fe}_{x}\text{Ga}_{y}\text{As}_{z}’ compound. Using the computer program,
\text{FEFF7,28} \) to generate electron-scattering amplitudes and phase
shifts, EXAFS simulations were made of both bcc iron and a
representative composition of the ternary solid solution
\text{Fe}_{0.72}\text{Ga}_{0.28}\text{As}_{0.32}.\) \(^{29} \) To prepare the simulations, a Deby
 temperature of 470 K corresponding to bulk iron, was used
with the temperature set at 300 K. The final \( \chi(k) \) for the
ternary composition was a weighted sum of the contributions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Fe foil</th>
<th>20Au/10Fe</th>
<th>9.3Fe</th>
<th>20Au/5Fe (S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_{min} ) (in plane, Å(^{-1} ))</td>
<td>4.003(5)</td>
<td>4.332(5)</td>
<td>4.132(8)</td>
<td>3.961(8)</td>
</tr>
<tr>
<td>( R_2 - R_1 ) (Å)</td>
<td>0.3840</td>
<td>0.355(1)</td>
<td>0.372(1)</td>
<td>0.388(1)</td>
</tr>
<tr>
<td>( R_2 = a ) (Å)</td>
<td>2.8664</td>
<td>2.837(1)</td>
<td>2.854(1)</td>
<td>2.870(1)</td>
</tr>
<tr>
<td>( k_{min} ) (out-of-plane)</td>
<td>4.003(5)</td>
<td>3.519(6)</td>
<td>3.409(7)</td>
<td>4.036(9)</td>
</tr>
<tr>
<td>( R_2 - R_1 ) (Å)</td>
<td>0.3840</td>
<td>0.437(2)</td>
<td>0.451(1)</td>
<td>0.381(1)</td>
</tr>
<tr>
<td>( R_2 = c ) (Å)</td>
<td>2.8664</td>
<td>2.919(2)</td>
<td>2.933(1)</td>
<td>2.863(1)</td>
</tr>
<tr>
<td>( c/a )</td>
<td>1.000</td>
<td>1.029(1)</td>
<td>1.028(1)</td>
<td>0.9976(7)</td>
</tr>
</tbody>
</table>

Table I. Beating analysis results for samples 20Au/10Fe/(4\times6)-GaAs, 9.3Fe/(4\times6)-GaAs, and 20 Au/5Fe/GaAs (S passivated) referenced to iron foil. The known crystallographic distances were used for iron foil \( R \) values. In all cases, \( R_1 \) was taken to be that for iron foil (2.4824 Å). Random errors quoted come from locating \( k_{min} \) and do not include other sources.
from the three iron sites. The results of the simulations, transformed as per the real data, are compared in Fig. 6(a).

The most significant difference, apart from scale, lies in the scattering paths

Due to differences in backscattering. The presence of some substrate effects on the nearest and second-nearest neighbor changes at low k due to differences in backscattering. The effects on the nearest and second-nearest neighbor (R1 and R2 in Fig. 5) contributions were small, but for higher shells, and particularly for the multiple scattering, the effects were noticeable. In that light, it is possible the differences in the polarization-dependent XANES may be also due to the presence of the substrate (and Au or floating-As capping layers).

The data were fit in R space with FEFF7 simulations using the program WINXAS,30 WINXAS uses the generated Fef- fnan.dat files for each selected scattering path of a particular structural model and generates a $\chi(k)$ using the XAFS function (neglecting cumulants):

$$\chi_{model}(k) = \sum S_{g}^{2} N_{j} F_{j}(k) e^{-2k^{2}R_{j}^{2}}$$

$$\times e^{[-(2R_{j}/\lambda)]} \sin[2kR_{j} + \delta_{j}(k)].$$ (2)

The resulting $\chi_{model}(k)$ is transformed to R space and compared to the transform of the data.

Fits in R space were done over the range 1.6 to 4.1 Å with the aim of extracting the distances for the first three shells—nearest neighbor, lattice parameter, and face-diagonal positions. The main objective of fitting is to obtain the in-plane and out-of-plane lattice parameters. The iron foil data is again used as a reference to determine offsets in R and to set the FEFF $E_{0}$ shift for the film data. Coordination numbers $N_{j}$ were fixed according to the models used. While correlations exist between the $S^{2}_{g}$, $N_{j}$, and Debye-Waller terms $[\exp(-\sigma^{2}_{j}k^{2})]$, no significant correlation exists between these terms and the $R_{j}$ values. For the foil, no polarization dependence was used in FEFF7 and bulk values for $N_{j}$ were used ($N_{1}=8$, $N_{2}=6$, $N_{3}=12$). For the films, polarization dependence was used.

Polarization dependence in XAFS reduces the degeneracy of some scattering paths (as does the reduction in symmetry from bcc to bct) in a crystalline material. This occurs because of a cosine-squared dependence of the XAFS interference function $\chi(k)$ on the angle, $\alpha_{j}$, between the interatomic bond direction $R_{j}$ and the x-ray polarization vector and causes atoms perpendicular to the polarization vector to contribute little to the backscattering.31 For polarization along the c axis in bcc iron, for example, the six atoms in the second shell ($N_{c}$) are no longer equivalent backscatterers. Instead, the two atoms at (0,0,±a) dominate. For the rest of this paper, we only enumerate the dominant backscattering atoms in the shells being fit. These values ($N_{dom,j} = 1,2,3$) are reduced from the unpolarized values (8,6,12) of bcc iron to (8,2,8) for polarization along (001) or (010) directions and to (4,4,10) for polarization along (110).

Although the terrace sizes are large,15 being greater than 60×100 Å², the average coordination numbers may be further reduced due to finite thickness.32 In considering an isolated infinite bcc crystalline sheet and polarization along (001), for example, the numbers are reduced to $N_{1dom}=7.2$, $N_{2dom}=1.6$, and $N_{3dom}=6.4$ for 10 isolated monolayers. Scattering from substrate and capping layers, however, will

Auger results14,15 for films on (4×6)-GaAs have indicated the presence of some (≤1 ML)15 arsenic in the film or floating on its surface after iron deposition. FEFF7 simulations of a 10% random inclusion of arsenic in iron indicate some changes at low k due to differences in backscattering. The effects on the nearest and second-nearest neighbor ($R_{1}$ and $R_{2}$ in Fig. 5) contributions were small, but for higher shells, and particularly for the multiple scattering, the effects were noticeable. In that light, it is possible the differences in the polarization-dependent XANES may be also due to the presence of the substrate (and Au or floating-As capping layers).

The data were fit in R space with FEFF7 simulations using the program WINXAS,30 WINXAS uses the generated Fef-fmnn.dat files for each selected scattering path of a particular structural model and generates a $\chi(k)$ using the XAFS function (neglecting cumulants):

$$\chi_{model}(k) = \sum S_{g}^{2} N_{j} F_{j}(k) e^{-2k^{2}R_{j}^{2}}$$

$$\times e^{[-(2R_{j}/\lambda)]} \sin[2kR_{j} + \delta_{j}(k)].$$ (2)

The resulting $\chi_{model}(k)$ is transformed to R space and compared to the transform of the data.

Fits in R space were done over the range 1.6 to 4.1 Å with the aim of extracting the distances for the first three shells—nearest neighbor, lattice parameter, and face-diagonal positions. The main objective of fitting is to obtain the in-plane and out-of-plane lattice parameters. The iron foil data is again used as a reference to determine offsets in R and to set the FEFF $E_{0}$ shift for the film data. Coordination numbers $N_{j}$ were fixed according to the models used. While correlations exist between the $S^{2}_{g}$, $N_{j}$, and Debye-Waller terms $[\exp(-\sigma^{2}_{j}k^{2})]$, no significant correlation exists between these terms and the $R_{j}$ values. For the foil, no polarization dependence was used in FEFF7 and bulk values for $N_{j}$ were used ($N_{1}=8$, $N_{2}=6$, $N_{3}=12$). For the films, polarization dependence was used.

Polarization dependence in XAFS reduces the degeneracy of some scattering paths (as does the reduction in symmetry from bcc to bct) in a crystalline material. This occurs because of a cosine-squared dependence of the XAFS interference function $\chi(k)$ on the angle, $\alpha_{j}$, between the interatomic bond direction $R_{j}$ and the x-ray polarization vector and causes atoms perpendicular to the polarization vector to contribute little to the backscattering.31 For polarization along the c axis in bcc iron, for example, the six atoms in the second shell ($N_{c}$) are no longer equivalent backscatterers. Instead, the two atoms at (0,0,±a) dominate. For the rest of this paper, we only enumerate the dominant backscattering atoms in the shells being fit. These values ($N_{dom,j} = 1,2,3$) are reduced from the unpolarized values (8,6,12) of bcc iron to (8,2,8) for polarization along (001) or (010) directions and to (4,4,10) for polarization along (110).

Although the terrace sizes are large,15 being greater than 60×100 Å², the average coordination numbers may be further reduced due to finite thickness.32 In considering an isolated infinite bcc crystalline sheet and polarization along (001), for example, the numbers are reduced to $N_{1dom}=7.2$, $N_{2dom}=1.6$, and $N_{3dom}=6.4$ for 10 isolated monolayers. Scattering from substrate and capping layers, however, will

![Fig. 6. FEFF7 simulations: (a) R-space transforms for bulk iron (solid line) and Fe_{72}Ga_{43}As_{8} ternary compound (dashed line) at 300 K and a Debye temperature of 740 K, and (b) k-space EXAFS simulations of bcc Fe, bct Fe, an 80% bcc/20% ternary alloy, and the ternary compound.](image-url)
TABLE II. Summary of fit results for the first three backscattering paths: nearest neighbor, lattice parameter, and face diagonal. An offset correction based on the difference between the foil and bcc crystal R values has been applied to the film fit results. Errors reported were obtained from a doubling of the residual sum of squares from the minimum value. For the third shell of the bct structure, $N_{3\text{dom}}$ has been split into in-plane and out-of-plane values.

<table>
<thead>
<tr>
<th>Sample</th>
<th>$N_{1\text{dom}}$</th>
<th>$R_1$ (Å)</th>
<th>$\sigma_1^2$ ($10^{-4}$ Å²)</th>
<th>$N_{2\text{dom}}$</th>
<th>$R_2$ (Å)</th>
<th>$\sigma_2^2$ ($10^{-4}$ Å²)</th>
<th>$N_{3\text{dom}}$</th>
<th>$R_3$ (Å)</th>
<th>$\sigma_3^2$ ($10^{-4}$ Å²)</th>
<th>$\Delta E_0$ (eV)</th>
<th>Residual%</th>
</tr>
</thead>
<tbody>
<tr>
<td>bcc Fe crystal</td>
<td>8</td>
<td>2.4824</td>
<td>6</td>
<td>2.8664</td>
<td>12</td>
<td>4.0537</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fe foil</td>
<td>8</td>
<td>2.462(4)</td>
<td>46(3)</td>
<td>2.839(8)</td>
<td>52(6)</td>
<td>12</td>
<td>4.035(17)</td>
<td>95(20)</td>
<td>2.64(50)</td>
<td>2.8</td>
<td></td>
</tr>
<tr>
<td>Offset</td>
<td>0.020(4)</td>
<td>0.027(8)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>bct Fe model crystal</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>In-plane (110) 20Au/10Fe</td>
<td>4</td>
<td>2.4828</td>
<td>4</td>
<td>2.8400</td>
<td>2</td>
<td>4.0164</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Out-of-plane (001)</td>
<td>8</td>
<td>2.495(8)</td>
<td>52(3)</td>
<td>2.834(14)</td>
<td>54(4)</td>
<td>2</td>
<td>4.02(5)</td>
<td>79(20)</td>
<td>2.64</td>
<td>3.1</td>
<td></td>
</tr>
<tr>
<td>In-plane (010) 20Au/5Fe ($S$)</td>
<td>8</td>
<td>2.493(9)</td>
<td>40(3)</td>
<td>2.837(20)</td>
<td>79(20)</td>
<td>4</td>
<td>4.02(6)</td>
<td>95(40)</td>
<td>2.64</td>
<td>2.6</td>
<td></td>
</tr>
<tr>
<td>Out-of-plane (001)</td>
<td>8</td>
<td>2.497(10)</td>
<td>53(26)</td>
<td>2.91(5)</td>
<td>142(82)</td>
<td>8</td>
<td>4.08(6)</td>
<td>166(73)</td>
<td>2.64</td>
<td>3.1</td>
<td></td>
</tr>
<tr>
<td>In-plane (110) 9.3Fe</td>
<td>4</td>
<td>2.490(10)</td>
<td>45(3)</td>
<td>2.862(20)</td>
<td>70(10)</td>
<td>10</td>
<td>4.08(5)</td>
<td>91(30)</td>
<td>2.64</td>
<td>2.8</td>
<td></td>
</tr>
<tr>
<td>Out-of-plane (001)</td>
<td>8</td>
<td>2.494(10)</td>
<td>52(10)</td>
<td>2.858(23)</td>
<td>75(20)</td>
<td>8</td>
<td>4.05(5)</td>
<td>118(30)</td>
<td>2.64</td>
<td>3.6</td>
<td></td>
</tr>
</tbody>
</table>

*a Residual(%) = $\frac{\sum|y_{\text{exp}}(i) - y_{\text{calc}}(i)|}{\sum|y_{\text{exp}}(i)|} \times 100.$

Contribute with different atom type having more effect on the higher shells and on the multiple scattering than on the $R_1$ and $R_2$ shells. This will effectively increase the coordination numbers towards bulk (with polarization) crystalline values. We therefore consider a capped infinite sheet model with parameters $S_0^5$ (scale factor), $\{R_j\}$ (distances), and $\{\sigma_j^2\}$ (mean-square relative displacement) to be fit and $N_j’s$ fixed to the bulk, polarization-dependent values.

Table II contains the results of the fits to each sample and orientation. Shells from one orientation required for multiple scattering and face-diagonal paths in the other were fixed to the appropriate fit values and the fitting iterated until stable. The triangular multiple-scattering paths on the low-R side of the $R_1$ peak were constrained in WIXAS using the parameters for the first and second shells. For the foil, it is evident in Fig. 7(a) that the multiple-scattering region is not being fit perfectly. The fit is worse in this region for the thin-film samples, with the worst case (largest residual) shown for the 5 ML sample (polarization out-of-plane) in Fig. 7(b), presumably due to non-iron atoms contributing to the (multiple) scattering.

The fitted foil $R$ values listed in Table II differ from the crystallographic values due to a small systematic offset from using FEFF7. An offset correction equal to the difference between the foil fit and crystal $R$ values was applied to obtain the film $R$ values listed in the table. The resulting $R_2$ values for the 5 ML sample on sulfur-passivated GaAs, indicate a nearly cubic material with a $c/a$ ratio from the 5 ML sample on sulfur-passivated GaAs, indicate a nearly cubic material with a $c/a$ ratio of 1.00(1). The in-plane and out-of-plane $R_2$ values for the films on (4×6) GaAs are different, as expected from the beating analysis, with an in-plane contraction and out-of-plane expansion. Some small additional offset due to Ga and As backscattering contributions must also be present. The contraction to 2.834 Å in-plane in the 10 ML film gives a closer match to the underlying GaAs ($a/2 = 2.827$ Å) than assumed in the starting model (2.84 Å). The out-of-plane expansion is slightly different between in and ex situ samples, but within error. The $c/a$ ratio (Table III) from the 10 ML ex situ measurements is 1.03(1) and the ratio from the in situ sample is 1.03(2). Both are in agreement and consistent with the value obtained from beating analysis.

An in-plane contraction can be understood as an effort to lattice match to the underlying GaAs ($a/2 = 2.827$ Å) and the expansion an effort to conserve cell volume (Table III) or nearest-neighbor distance (Table II). According to elasticity theory, the ratio of the out-of-plane to in-plane strain is $\Delta c/\Delta a = -2c_{12}/c_{11}$. Using the known elastic constants $c_{ij}$, 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 III. Although the errors
TABLE III. Comparison of lattice constants and uniaxial strain for epitaxial iron films on GaAs(001) \((4 \times 10^{-6})\) and GaAs(001)-S, passivated using results from the FEFF fitting.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Fe crystal</th>
<th>20Au/10Fe</th>
<th>9.3Fe</th>
<th>20Au/5Fe (S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a (\text{Å}))</td>
<td>2.8664</td>
<td>2.834(14)</td>
<td>2.837(20)</td>
<td>2.862(20)</td>
</tr>
<tr>
<td>(c (\text{Å}))</td>
<td>2.8664</td>
<td>2.93(3)</td>
<td>2.91(5)</td>
<td>2.858(23)</td>
</tr>
<tr>
<td>(c/a)</td>
<td>1.000</td>
<td>1.034(12)</td>
<td>1.026(19)</td>
<td>1.00(1)</td>
</tr>
<tr>
<td>Volume ((a^2 c, \text{Å}^3))</td>
<td>23.55</td>
<td>23.5(3)</td>
<td>23.4(5)</td>
<td>23.4(3)</td>
</tr>
<tr>
<td>(\Delta a = a - a_{\text{crystal}} (\text{Å}))</td>
<td>0.000</td>
<td>-0.032(14)</td>
<td>-0.029(20)</td>
<td>-0.004(20)</td>
</tr>
<tr>
<td>(\Delta c = c - c_{\text{crystal}} (\text{Å}))</td>
<td>0.000</td>
<td>0.064(30)</td>
<td>0.044(50)</td>
<td>-0.008(23)</td>
</tr>
<tr>
<td>(\Delta c/\Delta a = -2c_{12}/c_{11})</td>
<td>-1.212</td>
<td>-2.0 ± 1.3</td>
<td>-1.5 ± 2.0</td>
<td>(ill-defined)</td>
</tr>
</tbody>
</table>

associated with the small differences are large, for the \textit{ex situ} 10 ML film, \(\Delta c/\Delta a = -2.0 \pm 1.3\) is noticeably offset from the bulk-iron value of \(-1.212\). However, for the \textit{in situ} 9.3-ML film and the 5-ML film on sulfur-passivated GaAs no disagreement with macroscopic elasticity theory can be claimed. How does knowledge of a structural anisotropy or strain affect the potential application of iron films on GaAs for magnetoelectronics? The existence of this strain will affect the interpretation of the uniaxial surface anisotropy. The tetragonal distortion of nickel films on copper, for example, has been shown to dramatically affect the magnetic anisotropy energy.\(^{30}\) The uniaxial surface anisotropy is typically measured by ferromagnetic resonance and magnetometry. In the saturated state, the effective demagnetizing field perpendicular to the film surface depends on the strain as

\[
4 \pi M_{\text{eff}} = 4 \pi DM_s + \frac{2K_u}{M_s d} \frac{2B_1(e_i - e_s)}{M_s},
\]

where \(M_s\) is the bulk magnetization, \(D\) is the demagnetization factor, \(d\) is the film thickness, \(B_1\) is the magnetoelastic coupling coefficient (\(-3.44 \times 10^{-12} \text{erg/cm}^2\) for Fe), \(e_i\), and \(e_s\) are the strains parallel and perpendicular to the substrate, and \(K_u\) is the perpendicular surface anisotropy. Measurements of \(K_u\) have yielded a value of 1.1 erg/cm\(^2\) (Ref. 15) but this value may have to be modified by a 22% increase if the strain relaxes as \(1/d\). Further detailed study of the thickness dependence of the lattice strain is in progress.

IV. CONCLUSIONS

We have used polarized-XAFS studies to examine the structures of two iron films deposited on GaAs(001)-(4 \times 6) surfaces and one on sulfur-passivated GaAs(001), and compared them to the body-centered-cubic structure of an iron foil. The 5 ML sample on sulfur-passivated GaAs exhibits a nearly cubic structure with \(c/a = 1.00(1)\). The structures of the 10 ML \(\textit{ex situ}\) and 9.3 ML \(\textit{in situ}\) samples on \(4 \times 6\)-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).

ACKNOWLEDGMENTS

The Natural Sciences and Engineering Research Council of Canada provided support through operating grants and a major facility access grant. Experiments at the PNC-CAT beamline, Advanced Photon Source, Argonne National Laboratory are also supported by the United States Department of Energy, Basic Energy Sciences, Office of Science under Contract Nos. W-31-109-Eng-38 (APS) and DE-FG03-97ER45628 (PNC-CAT). The authors would also like to thank S. Watkins for the sulfur-passivated substrate.

\(^{9}\) Corresponding author.


The FEFF7 computer code uses the Rehr–Albers formalism to include in the XAFS interference function $\chi(k)$ the contribution of the polarization dependence for each scattering path (Ref. 28) and the equation for $\chi(k)$ does not include the $\cos^2 \alpha_j$ factor explicitly. This differs from earlier treatments (see, for example, Sec. 10.4.1 of Ref. 16) in which the equation for $\chi(k)$ for a $K$ edge contains a multiplicative factor of $3 \cos^2 \alpha_j$ where $\alpha_j$ is the angle between a particular bond $R_j$ and the electric vector of the incident x ray.

References: