Structural studies of Fe 0.81 Ga 0.19 by reciprocal space mapping

D. Viehland, J. F. Li, T. A. Lograsso, A. Ross, and Manfred Wuttig

Citation: Applied Physics Letters **81**, 3185 (2002); doi: 10.1063/1.1516231
View online: http://dx.doi.org/10.1063/1.1516231
View Table of Contents: http://scitation.aip.org/content/aip/journal/apl/81/17?ver=pdfcov
Published by the AIP Publishing

Structural studies of $Fe_{0.81}Ga_{0.19}$ by reciprocal space mapping

D. Viehland[a] and J. F. Li
Department of Materials Science and Engineering, Virginia Tech, Blacksburg, Virginia 24061

T. A. Lograsso and A. Ross
Metals and Ceramic Sciences, Ames Laboratory, Ames, Iowa 50011

Manfred Wuttig
Department of Materials and Nuclear Engineering, University of Maryland, College Park, Maryland 20742

(Received 24 June 2002; accepted 29 August 2002)

Reciprocal lattice mapping has been performed on $Fe_{0.81}Ga_{0.19}$ crystals by $\omega-\omega/2\theta$, $\Psi-\phi$, and $\omega-\phi$ scans. A strong elongation of the $\langle 001\rangle_c$ peak was found along the $\langle 110\rangle_c$ direction. ω scans revealed short lateral correlation lengths ξ along $\langle 110\rangle_c$ and strong diffuse scattering along the $\langle 001\rangle_c$. Multiple domains with monoclinic symmetry (angle $\sim 190°$) were observed by $\Psi-\phi$ and $\omega-\phi$ scans on the $(001)_c$ face, and were also tilted with respect to each other. The results show an average cubic structure with orthorhombic structural modulations, and two structural domain states that result in a limiting monoclinic symmetry. © *2002 American Institute of Physics.*
[DOI: 10.1063/1.1516231]

The magnetostrictive strain $(3/2)\lambda_{100}$ of Fe is well known to be small, on the order of 30 ppm. Introduction of Ga into crystalline solution with Fe results in pronounced increases in $(3/2)\lambda_{100}$,[1–3] as long as the BCC phase remains stable for the $Fe_{1-x}Ga_x$ solution,[2] even though Ga is nonmagnetic. For gallium concentrations $x>0.15$, this crystalline solution is not stable in the annealed condition.[4] However, rapid quenching of specimens is known to extend the limit of stability up to $x=0.19$.[2] The highest magnetostriction reported to date for any material is found for $Fe_{0.81}Ga_{0.19}$, with $(3/2)\lambda_{100}\sim 400$ ppm. Even though the magnetic moment is being diluted, an enhancement of the magnetostriction occurs.

The magnetostriction is strongly peaked near $x=0.19$.[3] At higher and lower Ga contents (i.e., $\Delta x\sim\pm 0.02$), $(3/2)\lambda_{100}$ is decreased by $\sim$50%. The anomalous magnetostriction cannot be due to a conventional mechanism. It has been conjectured that short-range ordering of Ga atoms occurs along the [100] in the α-Fe structure.[2,5] Wuttig *et al.*[5] have developed a model to explain this unique magnetostriction based upon Ga pairs. Accordingly, the magnetostriction would increase quadratically as a function of Ga concentration and decrease at higher Ga contents due to the formation of DO_3 or B2 ordered states.[2]

Previous elastic constant measurements have shown a significant decrease in Young's modulus with increasing Ga,[5,6] indicating that the lattice is softening as the magnetostriction is increasing. However, a structural understanding of this decrease, and hence the increase of the magnetostriction, remains lacking. Therefore, the purpose of this study was to investigate $Fe_{0.81}Ga_{0.19}$ crystals using reciprocal space mapping and texture analysis. The results show an average cubic structure, which has orthorhombic structural modulations, and two structural domain states that result in a limiting monoclinic symmetry.

[a]Electronic mail: viehland@mse.vt.edu

$Fe_{0.81}Ga_{0.19}$ crystals were grown by a Bridgman method, as previously described.[3] The crystals were homogenized at 900 °C and rapidly quenched to stabilize the BCC α-Fe structure.[2,3] The crystal was oriented along the $\langle 001\rangle_c$ and was cut to dimensions $10\times 10\times 2$ mm^3. A Philips MPD high resolution diffractometer equipped with an open Eulerian cradle was used for structural investigations. The $\langle 001\rangle_c$ face was investigated by $\omega-\omega/2\theta$, $\Psi-\phi$, and $\omega-\phi$ scans.

Angular $\omega-\omega/2\theta$ scans are done by measuring numerous coupled $\omega/2\theta$ Bragg scans for a range of incident angles ω as starting values by cradle rocking. The angle Ψ is the angular position of the sample surface normal in the direction perpendicular to the diffraction plane, whereas ϕ is the rotation angle perpendicular to the plane of diffraction. A $\Psi-\phi$ scan performs a series of coupled rotations about the two axes perpendicular to $\omega/2\theta$, while maintaining a constant 2θ.[7] This gives the integration volume of reciprocal space on a plane perpendicular to the plane of diffraction. Rotation of this perpendicular plane yields the three-dimensional spatial distribution of the diffraction intensity (or texture) at constant Bragg conditions. A $\omega-\phi$ scan utilizes a series of ω curves taken at different ϕ positions, at constant 2θ. The integration volume of reciprocal space appears as thin rods perpendicular to the diffraction plane, as the instrument broadening is quite large in this direction.[5] From these data, detailed information concerning the average crystal structure, domain texture, lateral coherency, and mosaicity can be obtained.

Figure 1(a) shows a $\omega-\omega/2\theta$ scan. A single diffraction peak was found along $\omega/2\theta$, and splitting was not observed along ω. Thus, the structure is clearly cubic, with $a=b=c=2.906$ Å and $\alpha=\beta=\gamma=90°$. This is consistent with the BCC α-Fe structure. However, the peak was strongly elongated along the $\langle 110\rangle_c$, shifting significantly in ω with changes in $\omega/2\theta$. The diffraction intensity along the $\langle 110\rangle_c$ elongation was very strong and could only be determined by rocking the sample.

Reciprocal lattice plots were calculated, as shown in Fig.

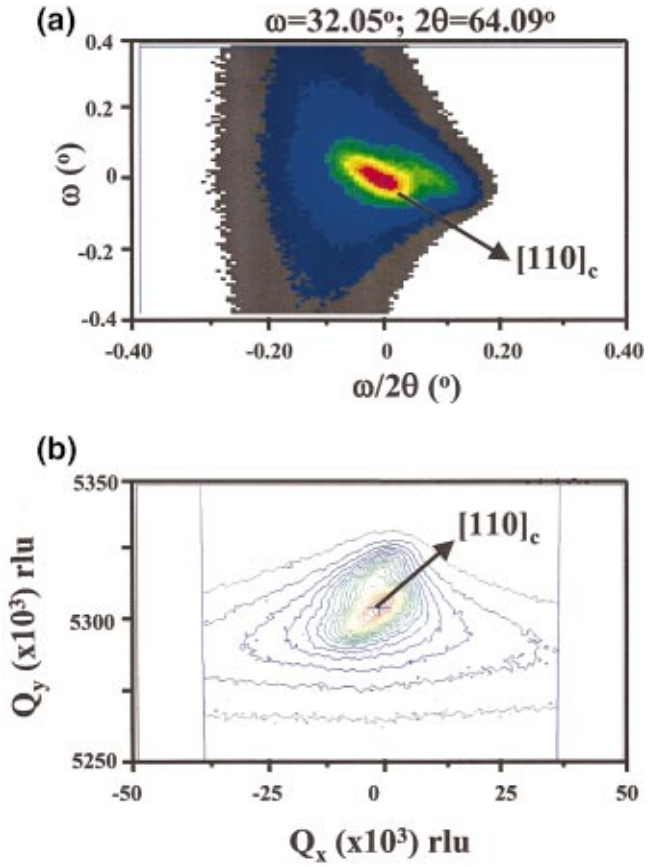

FIG. 1. (Color) X-ray diffraction data for a $\langle 001\rangle_c$ oriented $Fe_{0.81}Ga_{0.19}$ single crystal, which had been rapidly quenched. (a) $\omega-\omega/2\theta$ scan, and (b) reciprocal lattice map.

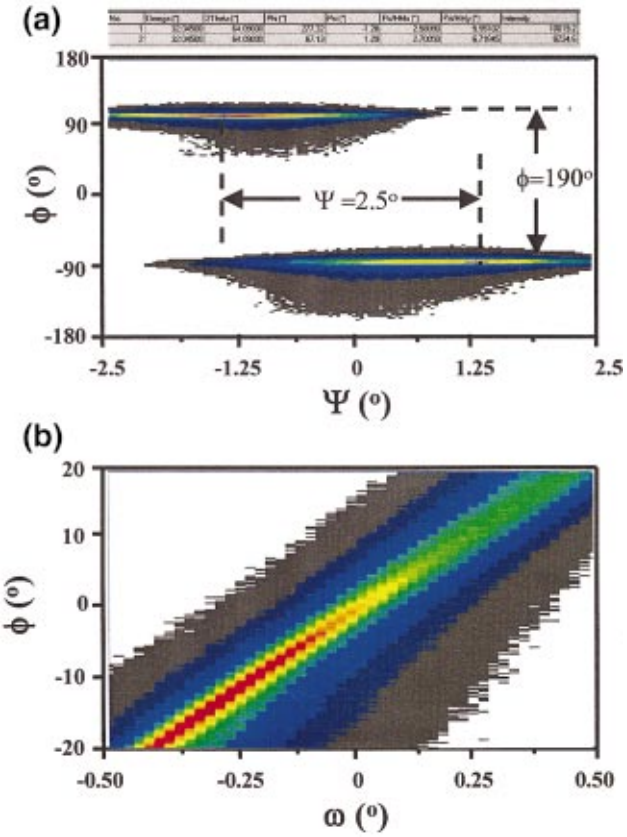

FIG. 2. (Color) X-ray diffraction data taken at constant Bragg conditions for a $\langle 001\rangle_c$ oriented $Fe_{0.81}Ga_{0.19}$ single crystal. (a) ω-ψ scan. (b) ω-ϕ scan.

1(b). In this figure, the peak was elongated along both Q_x and Q_y. The $\langle 110\rangle_c$ orientation of the elongation is marked in the figure. The $\langle 110\rangle_c$ directionality demonstrates the presence of pseudo-orthorhombic symmetry. The broadness of this peak demonstrates that the pseudo-orthorhombic symmetry has significant structural irregularity. The line broadening along the ω direction yields the lateral correlation length ξ. The Scherrer equation[8] $\xi = \lambda/[2\,\mathrm{FWHM}_\omega \cos(2\theta/2)]$ can be used to determine ξ, where FWHM is the full width at half maximum, λ is the wavelength of the Cu K_α radiation (1.5406 Å) and $(2\theta/2)$ is the peak position of the principle peak occurring at 64.094°. The FWHM_ω was $\sim 0.15°$ $(2.62\times10^{-3}$ rad), thus $\xi < 300$ Å.

In addition, Fig. 1(a) exhibits strong diffuse scattering along $\langle 001\rangle_c$, as can be seen from the dark colored contour regions. The diffuse scattering along this direction was much more broad in ω than that along the $\langle 110\rangle_c$. The results demonstrate strong structural irregularity along both $\langle 001\rangle_c$ and $\langle 110\rangle_c$; however, that along the $\langle 001\rangle_c$ did not possess any significant lateral correlation. This is consistent with the reports of short-range chemical ordering along the $\langle 001\rangle_c$ in $Fe_{0.81}Ga_{0.19}$.[2,5] It appears that $Fe_{0.81}Ga_{0.19}$ is structurally frustrated, containing elements of both the BCC α-Fe and DO_3 or B2 structures. In this structurally inhomogeneous state, anomalous magnetostriction may exist due to a large elastic compliance of elastic microtwins under magnetic field, during magnetization rotation.

Figure 2(a) shows a ψ–ϕ scan. This data demonstrates two preferred orientations that are rotated in ϕ by 190°, and are tilted in ψ by $\sim 2.5°$ with respect to each other. This rotation produces monoclinic symmetry, as ϕ is noticeably greater than 180°. The results unambiguously demonstrate the presence of two domain states whose *c*-axes are slightly tilted away from the $[001]_c$. This is directly revealed from the symmetry in the diffraction intensity of the ψ–ϕ scan. The average crystal symmetry remains cubic consistent with the bcc α-Fe structure. However the domain-averaged limiting symmetry is monoclinic. Neumann's law will then require that the property tensor matrices have monoclinic (point group) symmetry.[9]

The resolution of our instrument in the ϕ-direction is significantly higher than that in the ψ-direction. Thus, the ω–ϕ scan will offer better resolution when mapping of the spatial distribution of domains. Figure 2(b) shows an ω–ϕ scans taken along the $(001)_c$. A single thin rod can be seen that has nonuniform intensity. This demonstrates that the domain state is spatially nonuniform. The relative intensity of the rod can be seen to vary as a function of ϕ. At some ϕ-positions, the intensity was much stronger than at others. These results are consistent with a stacking of microtwins, resulting in a domain-averaged monoclinic limiting symmetry.

The results of this investigation for $Fe_{0.81}Ga_{0.19}$ crystals can be summarized as (i) the average crystal structure is cubic, with a domain-averaged monoclinic limiting symmetry; (ii) structural nonuniformity exists along both the $\langle 110\rangle_c$ and $\langle 001\rangle_c$; and (iii) orthorhombic structural modulations exist with a short lateral correlation length.

The research was supported by the Office of Naval Research under grants N000140210340, N000140210126, and MURI N000140110761. One of the authors (T. A. L.) acknowledges the support of the Office of Basic Energy Sciences, Materials Sciences Division, of the U.S. Department of Energy under Contract No. W-7405-ENG-82.

[1] A. E. Clark, J. B. Restorff, M. Wun-Fogle, T. A. Lograsso, and D. L. Schlagel, IEEE Trans. Magn. **36**, 3238 (2000); A. E. Clark, M. Wun-Fogle, J. B. Restorff, T. A. Lograsso, A. R. Ross, and D. Schlagel, *Proceedings of the Actuator 2000 Conference*, Bremen, Germany, June 2000.
[2] A. E. Clark, M. Wun-Fogle, J. B. Restorff, T. Lograsso, J. R. Cullen, IEEE Trans. Magn. **37**, 2678 (2001).
[3] A. E. Clark, M. Wun-Fogle, J. B. Restorff, T. Lograsso, *Proceedings of the Fourth Pacific Rim International Conference on Advanced Materials and Processing (PRICM4)*, edited by S. Hanada, Z. Zhong, S. Nam, and R. Wright, (The Japan Institute of Metals ..., 2001), p. 1711.
[4] See for example: *Binary Alloy Phase Diagrams*, 2nd ed., edited by T. B. Massalski (ASM International, Materials Park, OH, 1990).
[5] M. Wuttig, L. Dai, and J. Cullen, Appl. Phys. Lett. **80**, 1135 (2002).
[6] Liyang Dai, M. S. Thesis, University of Maryland, 2002.
[7] Xin Wang, Ph.D. Dissertation No. 557, Linkoping University, 1998.
[8] B. D. Cullity, Elements of X-ray Diffraction (Addison-Wesley, Reading, MA, 1978).
[9] J. F. Nye, *Physical Properties of Crystals: Their Representation by Tensors and Matrices* (Oxford University Press, Oxford, 1985).