Elemental moment variation of bcc Fe_xMn_{1-x} on MgO(001)

H. Bhatkar¹, R. J. Snow¹, E. Arenholz², Y. U. Idzerda^{1*}

¹Department of Physics, Montana State University, Bozeman, MT 59717, USA

²Advanced Light Source, Lawrence Berkeley National Laboratories, Berkeley, CA 94720, USA

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ABSTRACT

We report the growth, structural characterization, and electronic structure evolution of epitaxially grown bcc Fe_xMn_{1-x} on MgO(001). It is observed that the 20 nm thick Fe_xMn_{1-x} alloy films remained bcc from $0.65 \leq x \leq 1$, much beyond the bulk stability range of $0.88 \leq x \leq 1$. X-ray absorption spectroscopy and X-ray magnetic circular dichroism show that both the Fe and Mn L₃ binding energies slightly increase with Mn incorporation and that the elemental moment of Fe in the 20 nm crystalline bcc alloy film remain nearly constant, then shows a dramatic collapse near $x \sim 0.84$. The Mn MCD intensity is found to be small at all compositions that exhibit ferromagnetism

1. Introduction

Thin films of fcc Fe_xMn_{1-x} have been of excitement in the area of magnetic storage for a considerable time due to their application as the alloy of choice in multilayer systems that form magnetoresistive read heads [1]. In terms of the exchange-biasing achieved using the Fe_xMn_{1-x} materials, it was observed that the fcc Fe_{0.5}Mn_{0.5} ($x = 0.5$ or 50% Mn lattice site occupancy - all percentages are lattice site occupations) was stable and antiferromagnetic (AFM) in thin film form at room temperature [2], which became the key motivation to study FeMn in various structures and in thin films. The antiferromagnetic Fe_xMn_{1-x} alloy in fcc phase have been stabilized in the $0.5 \leq x \leq 0.7$ range [3] on various substrates such as copper [4]. Crystalline thin films reduce the complexity of the possible magnetic structures allowing for a clearer identification of the magnetic structure associated with the alloy. Since the fcc Fe is AFM [5] and bcc Fe is ferromagnetic (FM) [6], determining the mechanism of the magnetic moment variation in the ferromagnetic phase becomes of interest not only for moment control, but as guidance for applications that take advantage of exchange bias of fcc FeMn layers where the magnitude of the elemental moments at the AF interface plays an important role.

The bulk bcc Fe_xMn_{1-x} alloy is intriguing because of its departure from the Slater-Pauling curve [7, 8]. The average moment per atom of nearly all transition metal binary alloys is found to first increase with the electron

filling, then decrease above a critical value. For FeMn, the average alloy moment follows this trend only for the high Fe concentrations (see Figure 1). At $x = 0.88$ (12% Mn lattice site occupancy), the bulk average moment rapidly vanishes, suggesting the onset of a magnetic phase transition. Earlier works reported that the low concentration of Mn are stable in the bcc structure only up to 5% Mn [9], then later revised up to $x = 0.88$ (12% Mn) [10]. In many cases, substrate stabilization have allowed for the stabilization of unfavored structures beyond the bulk limit and have even stabilized crystal structures not found in the bulk [11].

Some binary alloys that seem to deviate from the Slater-Pauling behavior of Figure 1 are actually in agreement with Friedel's interpretation [12] of the Slater-Pauling behavior. This can be visualized if the magnetic moment per atom is plotted as a function of the average magnetic valence [13] resulting in a straight line, in contrast to the conventionally plotted volcano shaped Slater-Pauling curve [14]. Some alloy systems involving AFM-FM transition metal alloys that are identified as departures in the conventional plot, become regularly behaved points around the central trend-line [13]. Plotting the FeMn data in this manner again shows a marked departure from the anticipated straight line (due to the abrupt loss of magnetization).

The reported growth of bcc Fe_xMn_{1-x} films is limited. The structure was first stabilized as 2.5 nm thick films as Fe_{0.9}Mn_{0.1}/Ir(001) superlattices [15], then stabilized with a slight tetragonal distortion on GaAs(001) substrates to $x = 0.8$ (20% Mn) for films less than 3 nm thick [16],

* Corresponding author. Tel.: +1 406 994 7838; fax: +1 406 994 4452.

E-mail address: idzerda@montana.edu.

Fig. 1 - Slater-Pauling curve of measured bulk atomic moments for different transition metal alloys as a function of electron filling (from Ref. 8).

and subsequently stabilized as ultrathin films (<6 ML) on Ag(001) to $x = 0.72$ (28% Mn) [17]. Here we report the growth and magnetic moment variation of bcc $\text{Fe}_x\text{Mn}_{1-x}$ single crystal films on MgO(100). Interfaces with MgO are of particular interest for TMR devices [18, 19]. Only states that can exist on both sides of the interface of Fe-MgO control the coherent tunneling current in these devices [20]. Such matching of states across the interface is a very sensitive function of parameters like crystallinity and the abruptness of the interface. Mixing of Fe and Mg at the interface can strongly affect the filtering effect across the barrier [21] and has been attributed to reduction of the predicted value of 1500% TMR of Fe/MgO/Fe magnetic tunnel junctions to experimentally achieved one of 180% [19].

2. Experimental details

Using Molecular Beam Epitaxy (MBE), single crystal films of $\text{Fe}_x\text{Mn}_{1-x}$ were deposited on polished single crystal MgO(001) substrates. The MgO substrate cleaning procedure consisted of sonication of the MgO substrate in acetone followed by sonication in methanol for 5 minutes. Usually, as the third step in the triple-wash technique, substrates are rinsed in de-ionized water, but due to the hygroscopic nature of MgO, this final step was avoided. After flowing dry nitrogen over the freshly sonicated MgO, these substrates were quickly mounted onto a molybdenum holder using indium solder and loaded into high vacuum. The substrates were then heat-treated to clean any possible adsorbed contaminants by annealing in vacuum at 800°C (1073 K) for 2 minutes. This cleaning procedure has been shown to produce single crystal epitaxial growth with minimal interfacial oxidation of the Fe [22, 23].

The base pressure just prior to growth was $\sim 1.0 \times 10^{-9}$ Torr and during film growth with all Knudsen Cell sources at their operating temperatures, the pressure raised to $\sim 2.5 \times 10^{-9}$ Torr. For all growths, the Fe source was always maintained at constant temperature of $\sim 1400^\circ\text{C}$ (1673 K) assuring a constant rate of Fe deposition while the Mn source was held at various temperatures to achieve different Mn flux rates and therefore different alloy stoichiometries for the films. The films were deposited with the substrate held at 150 – 160°C (423–433 K) to ensure good quality, ~ 20 nm thick films [24]. Deposition fluxes were monitored by quadrupole mass spectrometry (QMS). A layer of amorphous aluminum of thickness 3.5

nm was deposited as a capping layer. Substrates were cooled to 70°C (343 K) before deposition of Al capping layer to minimize any interlayer mixing between the FeMn film and Al capping layer. Film compositions were verified by comparison of the Fe and Mn integrated $L_{2,3}$ -edge XAS intensities and film thicknesses were calibrated by Rutherford Backscattering Spectrometry (RBS).

3. Results and Discussion

The bare MgO(001) substrate surface quality was first characterized in ultra-high vacuum using *in-situ* Reflection High Energy Electron Diffraction (RHEED) imaged immediately after heat treatment. Since MgO is an insulating material, substrate charging can distort the diffraction pattern, resulting in broad fuzzy lines as seen in the left panel of **Figure 2**. RHEED was also used to confirm that the growth of $\text{Fe}_x\text{Mn}_{1-x}$ films remained epitaxial and in the bcc phase up to $x = 0.65$ with an in-plane lattice constant identical to the MgO(001) surface net. Due to the lattice mismatch these films are strained bcc films and most likely tetragonally distorted. Representative RHEED images along high symmetry directions of MgO substrate for the $\text{Fe}_x\text{Mn}_{1-x}$ are shown in the center and right panel of **Figure 2**. The absence of any additional RHEED features suggests that less than 10% of the film is present in an ordered secondary phase. Higher Mn concentrations ($x < 0.65$) showed complex RHEED patterns indicating the loss of bcc epitaxy. It should be noted that the bcc growth of $\text{Fe}_x\text{Mn}_{1-x}$ films is similar to pure Fe films deposited on MgO where the bcc Fe lattice is rotated 45° from the MgO surface net [25]. Thus the (100) direction of the MgO(001) surface coincides with (110) direction of the epitaxial bcc $\text{Fe}_x\text{Mn}_{1-x}$ lattice.

Fig. 2 - RHEED images (LEFT) from the bare MgO(001) substrate taken along the $\langle 100 \rangle$ direction, (CENTER) for a 20 nm pure Fe film on MgO(001) along the $\langle 100 \rangle$ direction of the MgO substrate, and (RIGHT) for a 20 nm $\text{Fe}_{0.8}\text{Mn}_{0.2}$ film on MgO(001) along the $\langle 110 \rangle$ direction of the MgO substrate.

To investigate the elemental moment variation and to examine whether ultrathin films behave similarly to the bulk, X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (MCD) of 20 nm $\text{Fe}_x\text{Mn}_{1-x}$ films were acquired. Both were measured in sample current configuration at Beamline 6.3.1 of the Advanced Light Source of Lawrence Berkeley National Laboratories. By comparing the integrated $L_{2,3}$ -edge XAS intensities of Fe and Mn, the Mn source temperature can be correlated with the Mn flux and therefore the concentration of Mn in the films. Precise film alloy compositions could be targeted by control of the Mn flux via the Mn source temperature by using a thermocouple in direct contact with the Mn Knudsen cell crucible. Mn Source temperature was varied from 680°C for the lowest Mn concentration films to 852°C for the highest concentration of Mn in the $\text{Fe}_x\text{Mn}_{1-x}$ films. **Figure 3**

displays the log (base 10) of the integrated Mn XAS intensity (after normalization by the integrated Fe XAS intensity) as a function of the inverse Mn source temperature for many of the FeMn samples. Due to this normalization, the reported Mn XAS intensity is now proportional to the Mn flux rate (since the Fe flux rate is constant). The straight-line is a fit using the August equation. The August equation is similar to Antoine equation which describes vapor pressure and temperature relation for pure liquids and gasses [26, 27]. From the extracted parameters of the August equation and the Rutherford backscattering data, the Mn flux rate and film composition can be determined.

Fig. 3 - The log of the integrated Mn XAS normalized by the integrated Fe XAS (Mn flux) as a function of the inverse of the Mn source temperature (filled triangles). The straight-line is a fit to the data using the August equation.

The evolution of the electronic structure with alloy composition was monitored by XAS which measures the element-resolved unfilled density of states above the Fermi level. **Figures 4 and 5** display representative

Fig. 4 - Normalized Fe L_{23} -edge XAS spectra for various Mn concentrations. INSET: Fe L_3 -peak energy as a function of Mn concentration.

extremes of the evolution of the peak normalized Fe L_{23} -edge XAS and Mn L_{23} -edge XAS with Mn concentration using linear polarized X-rays, respectively. The evolution is gradual and only the limiting spectra are shown for clarity. The energies are calibrated by comparison with reference powders that are measured immediately before and after all the Fe_xMn_{1-x} films. The Fe energies are calibrated using a $ZnFe_2O_4$ powder with an L_3 -peak energy of 708.22 eV and the Mn energies are calibrated by comparison with a $MnTiO_3$ powder with an L_3 -peak energy of 637.90 eV. The peak energy values are determined by fitting a Gaussian to the data points near the peak energy. Additionally, new fast scan capabilities at beamline 6.3.1 minimize the time between subsequent XAS scans, resulting in more reliable energy calibration values. For the lowest Mn concentrations, the small features at energies beyond the L_2 -peak beginning at 651.5 eV are from Mg K-edge absorption features (1303 eV) from the underlying MgO substrate due to 2nd harmonic light passed by the X-ray monochromator.

The Fe L_3 -peak energy (inset of **Figure 4**) shows a small shift to higher binding energy with increasing Mn concentrations to $x = 0.65$ (35% Mn). For $x < 0.65$ (above 35% Mn), where the RHEED images show a change in crystal structure, the L_3 -peak energy rapidly returns to its original value. This small shift (0.18 eV overall) can be accurately determined because of this robust energy calibration procedure. The Fe XAS spectra also exhibit an increased broadening in the L_3 -peak and a slight change in the branching ratio (L_3 -to- L_2 peak ratio). For this reason, integrated XAS values for the entire L_{23} -edge energy region are used for composition determination.

Fig. 5 - Normalized Mn L_{23} -edge XAS spectra for various Mn concentrations. INSET: Mn L_3 -peak energy as a function of Mn concentration.

The Mn L_3 -peak energy (inset of **Figure 5**) shows a similar energy shift with increasing Mn concentration. The similarity in binding energy shifts between Fe and Mn suggests that either an increase of the Fermi level with increasing Mn incorporation is responsible for the increase in the measured binding energies, unlikely from strictly electron filling arguments, or the unfilled Mn and Fe 3d bands above the Fermi level move to higher energies. Spin polarized electronic structure calculations using the coherent potential approximation within the Korringa-Kohn-Rostoker (KKR-CPA) method [28], the Augmented Space Recursion coupled with tight-binding linearized muffin tin orbital (TB-LMTO) method [29], and the all-electron full-potential linearized augmented wave approximation within the generalized gradient approximation (FPLAPW) method [30] qualitatively support this latter conclusion.

We have used the projector augmented wave basis for the application of density functional theory with the Abinit code [31, 32] to determine trends in the magnetic ground state and in the magnetic moments. We have addressed the concentration of $x=0.875$ with one Mn and 7 Fe atoms in a bcc supercell, investigating the total energies and magnetic moments as a function of cell volume as determined within the generalized gradient approximation (GGA) [33], and comparing Mn in the parallel and anti-parallel configurations. Total energies were converged to within 0.1 mRy/atom with respect to the number of k-points and to within 1 mRy/atom with respect to the energy cutoff, while magnetic moments are roughly approximated by an integration of spin densities in spheres of radius 1.16 Å around each atom.

As seen in **Figure 6a**, the ground state magnetic structure changes from parallel to anti-parallel alignment at 2.9 Å (near the Fe experimental lattice constant), peaks near the MgO coherent growth volume, and then changes back again to parallel alignment at large volume. Additionally, in **Figure 6b** the Mn moment in the anti-aligned case varies more strongly with cell volume than the Fe moment, and in the parallel case has a sharp rise at 2.9 Å (although antiparallel order is expected here). For reference, the Fe bcc lattice constant according to our calculation was 2.829 Å, while the experimental constant is 2.87 Å, and an equivalent lattice parameter for pseudomorphic growth on the MgO substrate would be 2.98 Å. These calculations suggest the anti-parallel alignment of Mn magnetic moments with respect to Fe for pseudomorphic growth on MgO. As the alloy approaches the Fe lattice constant, however, the GGA total energy favors parallel alignment, although the energy difference is rather small, suggesting the possibility of frustration or a mixture of aligned and anti-aligned Mn moments. In both cases, however, the Mn moments remain far from zero, and demonstrate some instability with volume.

Fig. 6 - The effect of cell volume on **a**) Total energy difference of magnetic configurations with Mn parallel and anti-parallel and **b**) the magnetic moments of the atoms, encompassing the Fe lattice constant of 2.87 Å and that of bcc pseudomorphic growth on MgO, 2.98 Å.

By using circular polarized X-rays and reversing the magnetization direction at each photon energy through application of a ± 500 Oe magnetic field applied along the photon propagation direction, the MCD spectra of Fe and Mn were obtained. After correction for the incident beam direction, incomplete polarization, and a slight out-of-plane magnetization from the variation in perpendicular magnetic anisotropy (both M_s and magnetocrystalline), the evolution of the MCD with composition can be determined. Due to the availability of high *in-situ* fields and the experimental restriction of applying fields out of the film plane and along the photon propagation direction in most MCD endstations, the correction of the small out-of-plane component of the

magnetization is important in determining the actual elemental moment behavior, but is often not accounted for.

The evolution of the elemental magnetic moments can be determined by the evolution of the Fe and Mn L_{23} -edge MCD spectra. In **Figure 7** are shown representative Fe L_{23} -edge MCD spectra (after corrections) for different alloy compositions. As the Fe content is decreased to $x = 0.86$, the Fe moment is very slightly reduced. For compositions $x < 0.86$, no dichroism is visible. The **INSET** of Figure 7 shows the evolution of the small positive going peak immediately following the large negative peak of the Fe L_{3} -edge MCD spectra in this limited composition range of $0.86 \leq x \leq 1.0$. The peak is seen to decrease slightly in intensity, consistent with the shifting and filling of the Fe minority band associated with alloying [34].

Fig. 7 - Fe L_{23} -edge MCD spectra for various alloy compositions after corrections (see text). For concentrations below $x = 0.86$, there is no dichroism signal. **INSET**: Evolution of post- L_{3} -edge region as a function of Mn concentration indicating band-filling and alloy formation.

Figure 8 shows representative Mn L_{23} -edge MCD spectra (after corrections) for different alloy compositions. Intriguingly, the Mn shows a small MCD signal ($< 2\%$) at all concentrations suggesting that the net Mn moment is small, probably due to moment cancellation from spin frustration while the individual Mn moments may remain large. Calculations reported in this paper support larger values of moments for Mn. This small dichroism signal persists even at Mn concentrations as low as 1% ($x = 0.99$) and for low temperature depositions (substrate held at RT) to reduce the Mn mobility and prevent Mn clustering.

Fig. 8 - Mn L_{23} -edge MCD spectra for various Mn concentrations.

In the absence of Mn clustering, the Mn atom is present as an impurity in a ferromagnetic host. If the Mn-site is centro-symmetric, the resulting exchange coupling with the Fe host results in a Mn moment that must be either aligned or anti-aligned to the host moment, neither of which leads to spin frustration. This has been observed in other host materials such as $\text{Ni}_x\text{Mn}_{1-x}$, $\text{Co}_x\text{Mn}_{1-x}$ [35], and 2 ML Mn/Fe(001) [36] where the Mn displays a large (5-15%) dichroism spectra typical of a metal with a single L_3 peak and a single, although oppositely directed, L_2 peak. This Mn lineshape is also present in Mn-doped GaAs [37], a magnetic semiconductor. It is significant to note that the MCD spectrum for Mn in the bcc $\text{Fe}_x\text{Mn}_{1-x}$ alloy is quite different. Not only is it small, but the L_2 -edge displays a derivative-like feature instead of a single peak. This suggests that the Mn magnetic structure is more complicated and that perhaps the Mn-site in the $\text{Fe}_x\text{Mn}_{1-x}$ alloy is not centro-symmetric, but is distorted from the typical bcc structure.

The average Fe atomic moment was then determined from the peak of the L_3 -edge MCD spectra at each composition for comparison with the bulk behavior as determined by Gumlich [7, 38] (Fig. 7-32 in ref. 7) which is displayed in the compilation shown in **Figure 1**. Since the Mn net

Fig. 9 - Average atomic moment as a function of composition for alloy films (solid triangles) and the bulk average moment (open circles from Gumlich in ref. 39).

moment is very small, the average moment per atom can be found by scaling the average Fe moment by a dilution factor ($1/x$). The result (shown in **Figure 9**) shows good agreement between the bulk behavior (open circles) and the thin film behavior (filled triangles) although the thin film moment persists to a slightly higher concentration ($x = 0.86$).

The thin film data displays a gradual reduction in the average moment with composition followed by an abrupt decrease at $x \sim 0.86$ which occurs at a slightly higher composition and looks to be much more abrupt than moment reduction in the bulk data. Note that the Fe L_3 binding energy shift shows no dramatic change at this composition suggesting that this moment loss is due to an abrupt magnetic structure change even though the crystal structure remains bcc. (The abruptness of this transition was investigated using a compositional wedge sample and reported elsewhere. [39])

4. Conclusion

In summary, the growth of bcc $\text{Fe}_x\text{Mn}_{1-x}$ is pseudomorphic to the MgO(001) surface with a 45° rotation and stable up to $x = 0.65$. The elemental magnetic moment of Fe shows a behavior very similar to bulk as the Mn content is varied from $0.65 < x < 1$, consistent with the Slater-Pauling behavior with a sudden deviation from the linear trend at $x = 0.86$. The elemental moment of Mn in bcc $\text{Fe}_x\text{Mn}_{1-x}$ alloys is very small and showed no significant variation with composition.

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REFERENCES

- [1] B. Dieny, V.S. Speriosu, S.S.P. Parkin, B.A. Gurney, D.R. Wilhoit, and D. Mauri, *Physical Review B*, **43** (1991) 1297.
- [2] R.D. Hempstead, S. Krongelb, and D.A. Thompson, *IEEE Trans. Mag.*, **14** (1978) 521.
- [3] H. Umebayas and Y. Ishikawa, *J. Phys. Soc. Jpn.*, **21** (1966) 1281.
- [4] C. Tsang, N. Heiman, and K. Lee, *J. of Appl. Phys.*, **52** (1981) 2471.
- [5] H. Hasegawa and D.G. Pettifor, *Phys. Rev. Lett.*, **50** (1983) 130.
- [6] J.H. Park, S.K. Kwon, B.I. Min, and H.S. Cho, *J. Korean Phys. Soc.*, **37** (2000) 109.
- [7] R.M. Bozorth, *Ferromagnetism*, IEEE Press, New York, 1951.
- [8] R. O'Hanley, *Modern Magnetic Materials: Principles and Applications*, John Wiley & Sons, New York, NY, 2000.
- [9] M. Hansen, *Constitution of binary alloys*, 2d ed., New York, McGraw-Hill, New York, 1958.
- [10] H. Yamauchi, H. Watanabe, Y. Suzuki, and H. Saito, *J. Phys. Soc. Jpn.*, **36** (1974) 971.
- [11] G.A. Prinz, *Phys. Rev. Lett.*, **54** (1985) 1051.
- [12] J. Friedel, *Nuovo Cim.*, **7** (1958) 287.
- [13] A.R. Williams, A.P. Malozemoff, V.L. Moruzzi, and M. Matsui, *J. Appl. Phys.*, **55** (1984) 2353.
- [14] A.R. Williams, V.L. Moruzzi, A.P. Malozemoff, and K. Terakura, *IEEE Trans. Mag.*, **19** (1983) 1983.
- [15] H. Fischer, S. Andrieu, P. Bauer, and M. Piecuch, *MRS Proceedings*, **384** (1995) 271.
- [16] C. Jing, Y.Z. Wu, Z.X. Yang, G.S. Dong, and X.F. Jin, *J. Magn. Mater.*, **198-99** (1999) 270.

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- [17] R. Paniago, J. L. López, and H.-D. Pfannes, in *Hyperfine Interactions (C): Proceedings of the International Conference on the Applications of the Mössbauer Effect, (ICAME 2001) September 2–7, 2001, Oxford, U.K.*, edited by M. F. Thomas, J. M. Williams and T. C. Gibb (Springer Netherlands, Dordrecht, 2002), p. 595.
- [18] S.S.P. Parkin, C. Kaiser, A. Panchula, P.M. Rice, B. Hughes, M. Samant, and S.H. Yang, *Nature materials*, **3** (2004) 862.
- [19] S. Yuasa, T. Nagahama, A. Fukushima, Y. Suzuki, and K. Ando, *Nature materials*, **3** (2004) 868.
- [20] W.H. Butler, X.G. Zhang, T.C. Schulthess, and J.M. MacLaren, *Phys. Rev. B*, **63** (2001) 054416.
- [21] J. Mathon and A. Umerski, *Phys. Rev. B*, **74** (2006) 140404.
- [22] Y.U. Idzerda, H. Bhatkar, and E. Arenholz, *J. of Appl. Phys.*, **117** (2015) 17A721.
- [23] R. Bertacco, S. De Rossi and F. Ciccacci, *J. Vac. Sci. Technol. A* **16** (1998) 2277 .
- [24] A. McClure, E. Arenholz, and Y.U. Idzerda, *J. Vac. Sci. Tech A*, **28** (2010) 969.
- [25] T. Urano and T. Kanaji, *J. Phys. Soc. Jpn.*, **57** (1988) 3403.
- [26] A. Zehe, A. Ramírez, and B. W. Müller, *Superficies y Vacío* **13** (2001) 72.
- [27] G.W. Thomson, *Chemical reviews*, **38** (1946) 1.
- [28] N.I. Kulikov and C. Demangeat, *Phys. Rev. B*, **55** (1997) 3533.
- [29] S. Ghosh, B. Sanyal, C.B. Chaudhuri, and A. Mookerjee, *Eur. Phys. J. B*, **23** (2001) 455.
- [30] G. Rahman, I.G. Kim, H. Bhadeshia, and A.J. Freeman, *Phys. Rev. B*, **81** (2010) 11.
- [31] M. Torrent, F. Jollet, F. Bottin, G. Zerah, and X. Gonze, *Comp. Mat. Sci.*, **42** (2008) 337.
- [32] P.E. Blochl, *Phys. Rev. B*, **50** (1994) 17953.
- [33] J.P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.*, **77** (1996) 3865.
- [34] E. Arenholz, G. van der Laan, A. McClure, and Y. Idzerda, *Phys. Rev. B*, **82** (2010) 4.
- [35] J.W. Cable and Y. Tsunoda, *J. Magn. Magn. Mater.*, **140–144**, (1995) 93.
- [36] S. Andrieu, M. Finazzi, F. Yubero, H.M. Fischer, A. Ph, F. Chevrier, L. Hennen, K. Hricovini, G. Krill, and M. Piecuch, *Europhysics Letters*, **38** (1997) 459.
- [37] D.J. Keavney, D. Wu, J.W. Freeland, E. Johnston-Halperin, D.D. Awschalom, and J. Shi, *Phys. Rev. Lett.*, **91** (2003) 187203.
- [38] E. Gumlich, *Wiss. Abhandl. Physik-tech. Reichsanstalt.*, **4** (1918) 267.
- [39] Y.U. Idzerda, H. Bhatkar, and E. Arenholz, *J. Appl. Phys.*, **117** (2015) 17A721.