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Textured growth of the high moment material Gd(0001)/Cr(001)/Fe(001)

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Abstract. By magnetic coupling of Fe and Gd via Cr interlayers, the large local moment of Gd can be combined with the high Curie temperature of Fe. The epitaxial growth of a Gd film is studied here by preparing trilayer systems of Fe/Cr/Gd on MgO(100) substrates by molecular-beam epitaxy (MBE). The thickness of the Cr interlayer was varied between 3-5 monolayers. The structural quality of the samples was confirmed by in-situ RHEED and ex-situ XRD measurements. Epitaxial Cr(001)/Fe(001) growth was observed, as expected. By use of ⁵⁷Fe-CEMS (Conversion Electron Mössbauer Spectroscopy) in combination with the ⁵⁷Fe tracer layer method the Fe/Cr interface could be examined on an atomic scale and well separated Fe/Gd layers for all Cr thicknesses were confirmed. The unusual Gd/Cr crystallographic relationship of Gd(0001)||Cr(001), with domains of the hexagonal Gd basal planes randomly oriented in the sample plane and not in registry with the underlying Cr(001) lattice, was found from combined RHEED and X-ray measurements. Annealing of the samples resulted in a remarkable improvement of the crystalline structure of the Gd layers. On the other hand, the appearance of a single line in the CEM spectrum leads to the conclusion that during annealing a small amount of Fe diffuses into the Cr layer. The electronic structure and magnetism of this system is investigated by first principles theory.

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1. Introduction

Materials with high saturation magnetization are important in microelectronic devices such as read heads for high density magnetic recording. The highest magnetic moment per atom among the 3d metals is known for Fe_xCo_{1-x} alloys, where $x \sim 0.65$, as predicted by the Slater-Pauling curve [1]. An important combination of high frequency response with high magnetization is realized, for example, in nanogranular systems of the type [2] $(Fe_xCo_{1-x})-Al-O$. Other materials, which follow the Slater-Pauling behavior, are full Heusler alloys containing Co, Fe, Rh and Ru [3]. A combination of 4f and 3d metals, which are coupled via a Cr interlayer, may lead to still observable huge magnetic moments on the rare earth atoms even at RT. Through coupling of Gd to a 3d ferromagnet like Fe it was possible to observe nearly temperature independent Gd moments of $6.2-7.2 \mu_B$ at the Gd/Fe interfaces in Fe/Gd multilayers and a modified Curie temperature with nearly the same value as for Fe ($T_C = 1043$ K) [4]. It was also shown that the Fe and Gd moments at the interfaces are antiparallel at RT. One idea to align the Fe and Gd moments is to insert the correct number of monolayers (ML) of Cr between Fe and Gd. Cr is an antiferromagnet with a Néel temperature T_N of 313 K [5], below which it attains a state of static spin density waves (SDW) along the [001]-direction, which can have complex variations [6]. In bulk Cr the AF order leads to an incommensurate spin density wave (ISDW) with a periodic modulation of the Cr magnetic moment. Since the Fe, Gd and Cr magnetic moments couple antiferromagnetically with each other [7, 8], one can achieve a parallel alignment of the Fe and Gd moments by choosing the correct number of Cr ML, i.e. $(2n+1)$, where n is zero or an integer. We have shown recently the parallel coupling of Fe and Gd by Cr interlayers. The results of element specific measurements on this system via XMCD (X-ray Magnetic Circular Dichroism) and the theoretical framework concerning the coupling of Fe/Cr/RE (RE: Rare Earth) have been published recently [9]. This work focuses on the structural characterization of Fe/Cr/Gd trilayers. In the past, the common epitaxial relationships for hexagonal (hcp) and body-centered cubic (bcc) systems were reported. Depending on the extent of the lattice mismatch two different epitaxial relationships were found. If the hcp lattice is larger by 13% compared to the bcc lattice constant, the hcp[1 $\bar{1}$ 00] direction is parallel to bcc[1 $\bar{1}$ 0] and hcp[11 $\bar{2}$ 0]||bcc[001]. This is designated as Nishiyama-Wassermann (NW) orientation [10–13]. This type of epitaxy is also found for the growth of rare earths on W(110) [14]. On the other hand, if the lattice mismatch is larger than 35%, the [11 $\bar{2}$ 0] direction is either parallel [1 $\bar{1}$ 1] or $\bar{1}$ 11]. This is the so called Kurdjumov-Sachs (KS) orientation [15, 16]. Studies on the growth of Gd on Cr(001) are very rare. The only study which is known to the authors examined Gd/Cr multilayers on MgO(001) and it was found that Gd grows polycrystalline [17]. In the present work we investigate growth and structure of Gd thin films (a hexagonal system) deposited onto the surface of Cr(001) which has 4-fold symmetry. An unusual crystallographic relationship is observed. The electronic and magnetic structure of this system is also reported here, using first-principles theory.

2. Experimental Procedure

Trilayer systems of the type Fe/Cr/Gd with 3.5 monolayer (ML) thick $^{57}\text{Fe}(001)$ tracer layers have been grown on commercial MgO(001) substrates by molecular-beam epitaxy (MBE). The sample structure was MgO(001)/15 ML ^{nat}Fe /3.5 ML ^{57}Fe /x ML Cr/15 ML Gd, with x=3, 4, 5, respectively (^{nat}Fe =iron of natural ($\sim 2\%$) ^{57}Fe isotopic abundance). The MgO substrates were rinsed in propanol and dry-cleaned with N_2 before loading into the UHV chamber. Subsequently they were cleaned by low-energy Ar ions (ion energy 0.5 keV, current density $1 \mu\text{A}/\text{cm}^2$, $5.5 \cdot 10^{-5}$ mbar) for times ≥ 1 h at 700 °C. After this treatment almost all of the carbon impurities were removed, as confirmed by Auger electron spectroscopy (AES). Reflection high-energy electron diffraction (RHEED) images of the clean substrates proved that the surface was flat and well ordered with no superstructures due to surface impurities. The ^{57}Fe (95% enriched in ^{57}Fe), ^{nat}Fe (purity of 99.9985 at.%) and Cr (purity of 99.995 at.%) films were deposited by thermal evaporation from Al_2O_3 crucibles. The Gd (purity of 99.9 at.%) films were evaporated from an Al_2O_3 crucible, which was lined on the inside with a Mo-sheet. The pressure during ^{57}Fe and ^{nat}Fe deposition was $8 \cdot 10^{-10}$ mbar (base pressure of $2 \cdot 10^{-10}$ mbar), with a deposition rate of 0.03 Å/s at a nominal substrate temperature of $T_s = 350$ °C, which leads to a minimum surface roughness and large island sizes [18]. The pressure during Cr-evaporation was $4 \cdot 10^{-10}$ mbar with a deposition rate of 0.02 Å/s and $T_s \leq 60$ °C. Finally, the Gd-films were evaporated at $4.5 \cdot 10^{-10}$ mbar, with a deposition rate of 0.03 Å/s at $T_s \leq 53$ °C. If not otherwise stated, all samples had a Gd thickness of 15 ML, corresponding to $15 \cdot c_{Gd}/2 = 43.4$ Å and $c_{Gd} = 5.781$ Å. The deposition rates were monitored with calibrated quartz-crystal oscillators. The 3.5 ML tracer layers of ^{57}Fe were deposited onto the surface of the 11.5 ML thick ^{nat}Fe layers, in order to examine the Fe/Cr interfaces with ^{57}Fe CEMS (conversion electron Mössbauer spectroscopy) [19]. For protection the samples were covered with 40 Å thick Au or 50 Å Cr layers.

The epitaxial growth of the Fe, Cr and Gd layers during growth was investigated by RHEED with the electron beam (15 keV, 30 μA) incident at about 2-3 ° relative to the sample plane and along the [100] azimuthal direction of the MgO(100) substrate. The RHEED patterns during the growth process were recorded in real time by a CCD camera for data evaluation. Ex-situ x-ray diffraction (XRD) in $\theta - 2\theta$ geometry was used to study the epitaxial nature of the samples. ^{57}Fe CEMS spectra were measured at RT using a homemade He/ CH_4 -gas-flow proportional counter. A Mössbauer drive system operated in constant acceleration mode combined with conventional electronics and a ^{57}Co (Rh matrix) source of ≈ 50 mCi activity were used. The least-squares fitting procedure of the CEM spectra was performed with the NORMOS program package by R. A. Brand [20]. Due to the high enrichment of the ^{57}Fe probe layer (95%) and the low ^{57}Fe content of the ^{nat}Fe layer ($\sim 2\%$) the CEMS signal originates predominantly from the interfacial ^{57}Fe probe layer.

3. Results and Discussion

The RHEED patterns of the Fe, Cr and Gd layers taken along the $[100]$ azimuth of $MgO(001)$ are shown in figure 1. Fe and Cr show well defined streaks, which confirm the epitaxy and the flatness of the surface. As additionally confirmed by LEED, $Fe(001)$ on $MgO(100)$ grows with the relationship $Fe[110]||MgO[100]$ (rotation by 45°). The Cr film shows the same orientation as the $Fe(001)$ film and even sharper RHEED streaks (figure 1 (b)). The most interesting RHEED pattern is exhibited by Gd (figure 1 (c) and (e)). We observe broadened and faint (but clearly visible) streaks indicating preferential crystallographic growth of Gd. No LEED pattern could be detected for these Gd films. Strikingly, the RHEED pattern from the Gd films was found to be nearly unaffected by azimuthal rotation of the sample (figure 2). This leads us to the assumption that the Gd film consists of tiny (0001) -oriented crystallites, with their c -axes preferentially oriented perpendicular to the film plane (as proven by XRD, see below) and with their hexagonal basal planes randomly oriented in the film plane and not in registry with the underlying $Cr(001)$ lattice. In order to test this assumption we have simulated a RHEED pattern within the kinematic scattering approximation. Figure 1 (d) represents the simulated RHEED pattern from a flat 2-ML thick hexagonal $Gd(0001)$ crystallite of 19 Gd atoms (bottom layer: 12 Gd atoms; top layer: hexagon of 7 Gd atoms; assuming lattice parameters of bulk Gd) that was rotated about the c -axis (perpendicular to the sample plane) in steps of 1° from an azimuthal angle of 0° to 59° , and the obtained 60 individual diffraction patterns were incoherently superimposed. This simplified model simulates the case of tiny $Gd(0001)$ crystallites with their c -axes perpendicular to the film plane and with their hcp basal planes randomly oriented in the film plane. It can be seen that the resulting simulated RHEED pattern (figure 1 (d)) is in fair agreement with the experimental RHEED patterns (figure 1 (c), (e)). This provides evidence that our assumption on the Gd-film structure is justified. The RHEED intensity of the $(0,0)$ streak showed no oscillations during Fe or Gd growth, which is indicative of a Volmer-Weber (island) growth mode. During evaporation of Cr, weak RHEED oscillations could be detected (not shown), which were maintained until 4-5 ML. For higher thicknesses the oscillations faded away. This indicates a Stranski-Krastanov growth mode for Cr with a layer-by-layer growth for the first few ML. The in-plane interplanar distances of all films were evaluated by the simple relationship derived from the Bragg formula $d_f = (k_s/k_f)d_s$, where d_f and d_s are the in-plane interplanar distances of film and substrate perpendicular to the RHEED beam, respectively, and k_f and k_s are the position in k -space of the first-order diffraction spots relative to the zero-order reflection of film and substrate, respectively. We used a value of $d_s = 2.105 \text{ \AA}$ for bulk MgO . k_f and k_s were measured in pixels from a recorded video during film growth. The evolution of the obtained in-plane interplanar distances is shown in figure 3. It is observed that the in-plane atomic distance, d_{Fe} , of Fe decreases to a minimum of $1.95 \text{ \AA}$ after evaporation of 3.5 ML Fe. This is followed by a slow increase up to $1.99 \text{ \AA}$ after a total of 12 ML Fe. Considering a value of $a_{Fe}/\sqrt{2} = 2.027 \text{ \AA}$ in Fe bulk, this

Figure 1. Typical RHEED patterns taken with the beam along the $[100]$ azimuthal direction of $MgO(001)$ of 15 ML ($21.5 \text{ \AA}$) Fe (a), followed by 4 ML ($5.8 \text{ \AA}$) Cr (b), followed by 15 ML ($43.4 \text{ \AA}$) Gd (c), and 15ML Gd after annealing at 210°C in UHV (e). (d) shows a simulated RHEED pattern from a 2-ML thick $Gd(0001)$ crystallite consisting of 19 atoms (12 atoms in the bottom layer, 7 atoms in the top layer). In order to simulate the random in-plane orientation of the hexagonal basal plane, the $Gd(0001)$ crystallite was rotated in the film plane relative to the beam direction from 0° to 59° in steps of 1° , and the obtained 60 diffraction patterns were incoherently superimposed.

corresponds to a relative difference of -1.33% . Cr shows negligible changes (not shown) and attains an in-plane value of $d_{Cr} = 2.00 \text{ \AA}$ after 4 ML. This results in a difference of -1.8% compared to $a_{Cr}/\sqrt{2} = 2.037 \text{ \AA}$ in bulk Cr. Starting with the evaporation of Gd on Cr, the RHEED pattern showed a transition with additional broad reflections, which were superimposed on the Cr pattern. Therefore, a quantitative evaluation of the Gd reflections was only possible after 8 ML Gd (figure 3). X-ray diffraction indicates that the c-axis of Gd is preferentially oriented perpendicular to the sample surface (figure 4). The in-plane atomic distance of Gd after evaporation of $24.5 \text{ \AA}$ of Gd is $3.32 \text{ \AA}$ (figure 3 (b)). Although this is close to $3.14 \text{ \AA}$, which would be expected for $Gd[11\bar{2}0]||Cr[110]$, azimuthal rotation of the sample relative to the RHEED beam produced only slight changes in the RHEED pattern (figure 2), and the observed interplanar distance for an azimuthal direction of 45° relative to the RHEED beam (i.e. along $Cr[100]$) was $3.31 \text{ \AA}$ (figure 3 (c)) which is nearly identical to the previous value of $3.32 \text{ \AA}$. This demonstrates that the average in-plane interplanar distance of the Gd film is isotropic. This implies that the Gd film consists of randomly oriented tiny grains with a c-axis texture perpendicular to the film surface. The interplanar distance from the simulated RHEED pattern of figure 1 (d) was $3.2 \text{ \AA}$. Compared to this value we observe an in-plane lattice expansion in the Gd film of about 4% .

The $\theta - 2\theta$ x-ray diffraction (XRD) diagrams of the as grown trilayers indicate a

Figure 2. RHEED patterns of a 45 Å thick Gd film taken with the beam along different azimuthal directions: (a) 0°, (b) 15°, (c) 30°, (d) 45°. The angles refer to the [100] azimuthal direction of MgO(001).

high crystallographic order for the Fe and Cr films. Figure 4(a) exhibits the diffraction pattern of a sample with a 5 ML Cr interlayer and a Gd thickness of 43.38 Å, corresponding to $15 \cdot c_{Gd}/2$, with $c_{Gd} = 5.783$ Å. The diffraction peaks at 29.4° and 65.5° correspond to the Gd(0002) and Fe(200), Cr(200) planes. Here it must be mentioned that in an earlier publication [9] we stated that the Gd c-axis lies in the sample plane, which was apparently a misinterpretation of our data. As one can see more clearly for thicker Gd-films (figure 4(d)) the main Gd-reflection must be indexed (0002) and not (10 $\bar{1}$ 0). Fitting the reflections with Gaussian profiles in order to determine their widths and applying the Scherrer formula provides average crystallite sizes of 16.5 Å for Gd and 34 Å for Fe plus Cr. The latter value is in good accordance with the total thickness of the first two layers. The low value of 16.5 Å for Gd as compared to 43.4 Å can be attributed to poor crystallinity perpendicular to the sample surface. Additionally the roughness of the Gd surface can lead to a reduction of the apparent average particle size. The position of the XRD peaks provided lattice constants of 6.081 Å for 43.4 Å Gd and 2.852 Å for Fe(Cr), respectively. The first one corresponds to a perpendicular lattice expansion of Gd (relative to the bulk) of +5%, the last one to a tiny contraction of -0.5% for Fe(Cr). The XRD pattern of an annealed sample is shown in figure 4 (b). It was carefully annealed in UHV up to 210 °C. Compared to the non-annealed sample the ratio of the intensities of the Fe(200) to the Gd(0002) reflection changes

Figure 3. In-plane interplanar distances as a function of film thickness of Fe (a) and Gd (b),(c): The RHEED beam was parallel to the $[100]$ azimuthal direction of $MgO(001)$ in (a) and (b), and parallel to $[110]$ of $MgO(001)$ in (c). The value of $4.211 \text{ \AA}$ of bulk MgO [21] was considered as reference for the following evaluation of the in-plane atomic distance in the films.

from $I_{Fe/Gd} = 2.5$ to $I_{Fe/Gd} = 0.46$. This indicates that the annealing largely improved the structural quality of the Gd layer. Application of the Scherrer formula results in average Gd grain sizes of $25.6 \text{ \AA}$ for the annealed sample, which has to be compared with $16.5 \text{ \AA}$ for the non-annealed sample. The annealing process did not change the lattice constant of Gd. The RHEED pattern of the annealed sample shows an improvement from a rough towards a smooth Gd surface, which can be inferred from the appearance of the streaks in figure 1 (d). XRD rocking curves around the (0002) -reflection of $200 \text{ \AA}$ thick Gd-films (figure 5 (a)) show substantial broadening with a full width at half maximum (FWHM) of 11.5° . For the thinner films ($43.4 \text{ \AA}$) the rocking curves exhibit a much sharper feature around the origin (figure 5 (b)), which has a FWHM of 0.76° only. It is most likely that this feature represents the first layers of $Gd(0002)$, which

Figure 4. Typical XRD patterns for 15ML Gd samples as prepared (a) and annealed (b), and for 200 Å Gd film (c). For comparison, magnified sections of (b) and (c) around the Gd(0002) reflection are displayed in (d). The samples are of similar geometrical structure: $MgO(001)/15 \text{ ML } ^{nat}Fe/3.5 \text{ ML } ^{57}Fe/5 \text{ ML } Cr/Gd(t)$, with $t=43.4 \text{ Å}$ (15ML) or 200 Å. Annealing was performed in UHV at different temperatures and times, the maximum temperature was 210 °C. The position of the reflections for bulk Gd are shown as vertical bars in (d). (Cu-K_α radiation).

Figure 5. Rocking curve scan of the (0002)-reflection of a thick Gd-film (200 Å) (a) and of a thin Gd-film (43.4 Å) (b), both inside the structure $MgO(001)/15 \text{ ML } ^{nat}Fe/3.5 \text{ ML } ^{57}Fe/5 \text{ ML } Cr/x \text{ Å } Gd$ and annealed.

elastically distort their unit cell in order to adapt to the in-plane epitaxial condition with $Cr(001)$. The broad rocking curve can be assigned to a mosaic spread, probably induced by misfit dislocations within a relaxed structure. It can also originate from the reduced lateral coherence length related to the small lateral size of Gd grains. A broad rocking curve was also measured for the Fe layer (not shown).

CEM spectra at RT for samples with different Cr thicknesses are shown in figure 6. While the Mössbauer spectrum of pure bcc Fe shows the well-known Zeeman sextet with sharp Lorentzian lines [22], the present spectra exhibit asymmetric line broadening and distinct shoulders. Therefore, the CEM spectra were least-squares fitted with two blocks of distributions of hyperfine magnetic fields $P(B_{hf})$ [plus a central single line for the annealed sample with a 5 ML Cr interlayer (figure 6 (b))] in the range of 0-18 T (low-field region, distribution 1) and 18-36 T (high-field region, distribution 2), which are characteristic for ^{57}Fe atoms at the Fe/Cr interface [23]. A linear correlation between the hyperfine field B_{hf} and the isomer shift δ had to be assumed in order to achieve satisfying fits. This well known correlation [24] is based on the fact that the electronegativity of Fe is larger than that of Cr. Consequently, the s-electron density of Fe is expected to increase with a higher number of Cr neighbours, leading to a more negative isomer shift.

At the same time the higher number of Cr neighboring atoms reduces the magnitude of the hyperfine magnetic field B_{hf} . The line intensity ratios of the sextets, which contribute to the distribution, were fixed at values of 3:4:1:1:4:3, which implies an in-plane orientation of the Fe-spins. Distribution 2 exhibits five maxima, which are located

Figure 6. Typical RT-CEM spectra of as-prepared samples with 4 ML Cr (a), and with 5 ML Cr after annealing at 210 °C in UHV (b). (a) was least-squares fitted with two blocks of magnetic hyperfine-field distributions $P(B_{hf})$ (0-18 T (blue), 18-36 T (green)). (b) was least-squares fitted with two similar blocks of hyperfine-field distributions and a central single line (dark blue). The corresponding hyperfine field distributions, $P(B_{hf})$, are inserted below the respective CEM spectrum.

at 19.2 T, 22.4 T, 25.6 T, 28.4 T and 32.8 T (figure 6, inserts). They correspond to different atomic surroundings of the ^{57}Fe atoms at the Fe/Cr interface. Lower hyperfine fields indicate an increased number of Cr neighbours. Very smooth interfaces should also exhibit an enhanced hyperfine field (≈ 34.5 T) originating from the second Fe subsurface [23], but this is not the case for our samples since a mixing of Fe and Cr on the atomic scale was unavoidable. The diffusion of Fe and Cr in the first three samples (table 1) cannot be severe since no paramagnetic component (central single line) with $B_{hf} = 0$ T is observable. One can conclude that the quality of the Fe/Cr interface is sufficient to produce closed Cr layers, which safely separate the Fe and Gd layers from each other, starting from 3 ML Cr (the lowest thickness which we examined). The low-field distributions contribute only $\sim 10.5\%$ to the total spectral area (total integrated

Table 1. Spectral Mössbauer parameters for samples with different Cr thickness. $\langle\delta\rangle$: average isomer shift(relative to α -Fe at RT; only δ for single line), $\langle B_{hf}\rangle$: average hyperfine field, Γ : linewidth (FWHM). Hyperfine-field distribution 1 corresponds to the low-field region (0-18 T), distribution 2 corresponds to the high-field region (18-36 T).

	$\langle\delta\rangle$ (mm/s)	$\langle B_{hf}\rangle$ (T)	Γ (mm/s)	rel. spectral area (%)
3 ML Cr (as prepared)				
Distribution 1	+0.02(5)	7.0	0.35	10
Distribtuion 2	-0.01(2)	29.0	0.32	90
4 ML Cr (as prepared)				
Distribution 1	+0.12(5)	6.7	0.35	10
Distribtuion 2	-0.01(1)	28.9	0.32	90
5 ML Cr (as prepared)				
Distribution 1	+0.22(5)	7.1	0.35	11
Distribtuion 2	-0.01(1)	29.9	0.32	89
5 ML Cr (annealed)				
Distribution 1	+0.12(5)	6.7	0.35	10
Distribution 2	-0.01(1)	28.9	0.32	86
Single line	-0.10(2)	-	0.35	4

intensity) in all samples (table 1). The spectrum of the annealed sample with 5 ML Cr had to be fitted with an additional narrow single line with $\delta=-0.10(2)$ mm/s and a relative spectral area of 4%. From this finding one can conclude that the annealing procedure created a small amount of paramagnetic ^{57}Fe impurities, which diffused into the Cr layer during annealing and which only sense Cr nearest neighbours. Since the structure of Cr is cubic, it produces a single line with negative isomer shift in the CEM spectrum. The negative isomer shift of the single line is typical for ^{57}Fe impurities in a Cr matrix [25, 26]. Interestingly, the spectral intensity of 4% stems only from the high-field region (distribution 2), which is reduced from 90% to 86% (table 1). This means that those ^{57}Fe atoms which have a relatively large number of Fe neighboring atoms, diffuse easier into the Cr layer than Fe atoms with more Cr neighbors.

4. Theoretical results

We have performed first principles calculations based on density functional theory to study the $Gd/Cr/Fe(001)$ system. The computational unit cell consisted of 1 ML Gd, 1 ML Cr and 5 MLs of Fe. Plane wave projector augmented wave basis was used in the generalized gradient approximation for the exchange correlation potential as implemented in the VASP code [27, 28]. Gd 4f states were kept in the core. The plane wave cut off energy used was 400 eV. A $6 \times 6 \times 2$ Monkhorst Pack k-points set was used for the integration in Brillouin zone. Atoms were relaxed until the Hellman

Figure 7. (left) Interplanar separations from surface to bulk. $i=1, 2, \dots$ denote Gd, Cr layer respectively as indicated in the right panel. (right) Layer projected magnetic moments from surface to bulk.

Feynman forces were minimized up to $0.01 \text{ eV}/\text{\AA}$. The optimized interplanar separations are shown in the left panel of figure 7. As Gd is a bigger atom, the separation between Gd and Cr (next layer) is rather large. The distance between Fe and Cr layers is reduced compared to Fe-Fe separations in the next layers. It is observed that the bulk Fe-Fe interlayer distance is achieved after 4th Fe layer. The right panel of figure 7 shows the layer projected spin moments. As expected, Gd has $7 \mu_B$ moment coming from half-filled 4f shell. The small fractional moment ($\sim 0.1\mu_B$) arises from the 5d shell. The Cr moment is antiparallel to Gd and Fe moments. The interface Fe atom (Fe₁) has a reduced moment whereas the moments on the next Fe layers increase until they reach the bulk value. Figure 8 shows the local DOSs projected on the d-orbitals of Gd, Cr

Figure 8. Density of states (DOS) projected on the d-orbitals of interface Fe, Cr and Gd atoms.

and the interface Fe (Fe₁) atoms. As 4f states of Gd are kept in the core, they are not seen here. The spin-polarized Gd 5d-orbital is seen with a small exchange splitting. Exchange splittings of Cr and Fe d states are much higher, as seen in the figure. As

Cr is antiparallel to Gd and Fe, the majority and minority spin states are reversed. A considerable hybridization between the Cr and Gd states is observed close to the Fermi level. The reminiscence of bcc Fe electronic structure is observed for the interface Fe atom. The spin-up d-states (upper half, figure 8) are nearly full whereas the Fermi level cuts through a pseudogap in the spin-down DOS.

5. Conclusions

Trilayer systems of the type Fe/Cr/Gd have been grown on clean MgO(001) substrates by MBE. Tracer layers of 3.5 ML thick $^{57}\text{Fe}(001)$ on top of 11.5ML ^{nat}Fe were inserted, in order to perform ^{57}Fe CEM measurements and to probe the structural quality of the Fe(001)/Cr(001) interface. The Fe layers were grown on MgO(001) at 350 °C, the other two layers near RT. The growth of Fe and Gd followed the Volmer-Weber growth mode, as indicated by RHEED. The Fe and Cr films exhibit well-ordered surfaces, whereas the Gd layer had a rough surface. The in-plane lattice parameters of Fe and Cr were -1.58% and -1.8% lower than their bulk values. The Gd/Cr epitaxial relationship is unusual and was found to be $Gd(0001)\parallel Cr(001)$ with otherwise random orientation in the sample plane. An average in-plane expansion of the Gd lattice of +4% was found from comparison with a simulated RHEED pattern for random in-plane orientation of tiny Gd(0001) crystallites with their c-axes perpendicular to the sample plane. X-Ray rocking curve scans around the Gd(0002) reflection indicate a transition from an elastically distorted Gd film at lower thickness, which adapts to the Cr(001) surface, to a relaxed structure for thicker layers. Annealing at 210 °C led to an improvement of the crystalline quality of the Gd layers and a smoother Gd surface structure. However, the appearance of a weak central single line in the CEM spectrum points to a small fraction of paramagnetic ^{57}Fe impurities, which diffused into the Cr layer during annealing. First principles calculations for the density of states, the interplanar separations and the layer projected magnetic moments were presented. The Fe/Cr/Gd system studied here has a great potential for sensor applications, since the parallel coupling of Fe and Gd moments combined with the huge Gd moment (observable at RT due to the strongly enhanced Gd Curie temperature [9]) may result in a huge magnetization of this trilayer.

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