X-ray resonant magnetic scattering study of $[\text{Co}_2\text{MnGe}/\text{Au}]_n$ and $[\text{Co}_2\text{MnGe}/\text{V}]_n$ multilayers

A. Bergmann, J. Grabis, A. Nefedov, K. Westerholt and H. Zabel

Ruhr-Universität Bochum, 44780 Bochum, Germany

E-mail: kurt.westerholt@ruhr-uni-bochum.de

Abstract. We study the structure and magnetism of the ferromagnetic half metallic Heusler compound Co_2MnGe in high-quality $[\text{Co}_2\text{MnGe}/\text{Au}]_n$ - and $[\text{Co}_2\text{MnGe}/\text{V}]_n$ - multilayers by hard x-ray scattering and soft x-ray resonant magnetic scattering (XRMS). The diffuse hard x-ray scattering reveals that in $[\text{Co}_2\text{MnGe}/\text{Au}]_n$ at the interfaces correlated roughness dominates and interdiffusion is negligible, whereas in $[\text{Co}_2\text{MnGe}/\text{V}]_n$ the roughness is uncorrelated and dominated by interdiffusion. An analysis of energy-dependent scans in the soft x-ray regime at the superlattice Bragg peaks allows a determination of the element specific magnetic moment density profile within the Co_2MnGe layers. We find that the magnetic moment density profile determined for Co and Mn is definitely different, moreover, it is narrower than the chemical density profile and asymmetric with respect to the growth direction. For $[\text{Co}_2\text{MnGe}/\text{Au}]_n$ at room temperature a non-ferromagnetic interface layer with a thickness of about 0.6 nm at the bottom and 0.45 nm at the top of the Co_2MnGe layers exist, for $[\text{Co}_2\text{MnGe}/\text{V}]_n$ at the bottom and the top the corresponding thicknesses are 0.5 nm and 0.35 nm, respectively.

PACS numbers: 75.70.Cn, 85.75.-d, 78.70.Dm, 81.15.Cd

Keywords: XRMS, diffuse scattering, Heusler compounds, half-metallic metals, magnetization depth profile, magneto-optics

1. Introduction

In the current literature one notes an upsurge of interest in ferromagnetic Heusler compounds with half metallic character i.e. with the Fermi energy lying in a gap in the minority spin band [1]. Heusler compounds are ternary intermetallic alloys with the chemical formula A_2BX , where A and B are by atoms from the 3d and 4d transition metal group and X denotes atoms from 4th and 5th group of the periodic system. For several of these compounds theoretical electronic energy band structure calculations predicted half metallic character [2, 3, 4, 5, 6, 7, 8, 9, 10] which make them highly interesting for the rapidly evolving field of spin electronics (spintronics) [11, 12, 13]. The most popular half metallic Heusler compounds under current investigation are PtMnSb, Co_2MnSi , Co_2FeSi and Co_2MnGe . The main issue in the experimental literature at the moment is the design and the optimization of magnetic tunneling junctions using these Heusler half metals as electrode material with the aim to eventually obtain huge values for the tunneling magnetoresistance (TMR). This turned out to be quite difficult and only recently encouraging progress has been achieved [14, 15].

We have started systematic investigations on metallic multilayers combined of the half metallic Heusler compound Co_2MnGe and nonmagnetic metals with the original intention to study the Giant Magnetoresistance (GMR) effect on antiferromagnetically coupled multilayers or trilayer spin valves [16]. However, the GMR-values obtained in antiferromagnetically coupled $[\text{Co}_2\text{MnGe}/\text{V}]_n$ multilayers and in $\text{Co}_2\text{MnGe}/\text{Au}/\text{Co}_2\text{MnGe}$ spin valve systems were very small, typically of the order of 1% or lower [16]. From the thickness dependence of the magnetic order in these Heusler multilayers we hypothesized that at the interface with other metals the Heusler compound might loose its half metallic character or even its ferromagnetic order [17]. This scenario seems realistic, because the half metallic character and the strong ferromagnetism of the Heusler compounds is related to perfect chemical order of L_{21} type, which might be lost at interfaces and surfaces by interdiffusion and/or segregation of one of the constituents of the Heusler alloy. Actually the systematic analysis of surfaces of Heusler compounds revealed that deviations from the bulk stoichiometry frequently occur [18]. The same mechanism could also be responsible for the loss of half metallicity and full spin polarization at the Heusler/insulator interface in TMR junctions. Thus it would be valuable to have a method available which can resolve the magnetization profile or the magnetic moment density profile of thin Heusler layers interleaved between other metallic or insulating layers.

For this purpose we have started a systematic investigation of x-ray resonant magnetic scattering (XRMS) on Heusler-multilayers using synchrotron radiation at the Co and Mn $\text{L}_{2,3}$ edge [19]. The technique is related to the more familiar x-ray magnetic circular dichroism (XMCD) in the sense that both methods sensitively probe the exchange splitting of the 3d-conduction band states and give element specific magnetic information. The use of high quality multilayers provides the possibility to study the reflectivity at different order Bragg peaks of the multilayer superstructure. Only this

yields the necessary sensitivity which allows an unambiguous derivation of the magnetic moment density profile inside the Heusler layer.

The complete analysis of XRMS on a $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ multilayer has been published recently [19]. In the experimental section below we will review these results shortly and compare them to new XRMS results obtained on $[\text{Co}_2\text{MnGe}/\text{V}]_{20}$ multilayers. The $[\text{Co}_2\text{MnGe}/\text{V}]_{20}$ multilayer system is interesting, as it represents the only example of antiferromagnetic interlayer magnetic order in a Heusler/metal multilayer observed until now [20]. The magnetic ordering in this system is related to a granular magnetic structure and superparamagnetic behavior at high temperatures [20]. The determination of the magnetic moment density profile for the Heusler layers should elucidate the peculiar magnetic properties of this system.

2. Sample preparation and experimental

The samples used in the present study were grown by dual source rf-sputtering at a pressure of 5×10^{-3} mbar Ar and a substrate temperature of 300°C on Al_2O_3 a-plane, as described in detail elsewhere [17]. The multilayers for the present study had the nominal composition $[\text{Co}_2\text{MnGe}(3\text{nm})/\text{Au}(2.2\text{nm})]_{50}$ and $[\text{Co}_2\text{MnGe}(3\text{nm})/\text{V}(1.5\text{nm})]_{20}$.

The structural characterization was carried out using non-resonant hard x-ray scattering ($E = 8$ keV) at the wiggler beamline W1 at the HASYLAB (Hamburg, Germany). Two types of scans were performed as schematically depicted in Fig. 1. In the specular reflectivity (a) the scattering vector $\vec{q}$ is perpendicular to the sample surface. From these measurements information on layer thicknesses and the electron density gradient perpendicular to the surface, i.e. the structural roughness, can be obtained. In a transverse scan, q_z is kept constant and q_x is varied. The scattering vector contains an in-plane component and then yields information about the in-plane correlation lengths.

The soft XRMS experiments were performed with the diffractometer ALICE [21] at the undulator beamlines UE56/1-PGM and UE56/2-PGM2 at BESSY II (Berlin, Germany). The diffractometer comprises a two-circle goniometer and works in horizontal scattering geometry. The vertical entrance and detector slits were set to $300 \mu\text{m}$ each, resulting in an instrument resolution of 0.14° . Circularly polarized light in the energy range of 600 eV - 900 eV was used with an energy resolution of approximately $\Delta E/E = 1 \cdot 10^{-4}$. A magnetic field can be applied in the scattering plane along the sample surface either parallel or antiparallel to the photon helicity, which corresponds to the longitudinal magneto-optical Kerr effect (L-MOKE) geometry. The maximum field was ± 0.11 T, high enough to fully saturate the ferromagnetic Co_2MnGe -layers. The magnetic contribution to the scattered intensity was measured by reversing the magnetic field while keeping the photon helicity fixed.

Photon energies were tuned to the range of the Mn and Co $L_{2,3}$ absorption edges in order to determine the element-specific magnetic structure. The resonant magnetic scattering

length is given by [22]

$$f = (\vec{\epsilon}_f^* \cdot \vec{\epsilon}_i)F^c + i(\vec{\epsilon}_f^* \times \vec{\epsilon}_i) \cdot \vec{m}F^{(1)} + (\vec{\epsilon}_f^* \cdot \vec{m})(\vec{\epsilon}_i \cdot \vec{m})F^{(2)}, \quad (1)$$

where $\vec{\epsilon}_i$ and $\vec{\epsilon}_f$ are the polarization vectors of the incident and scattered x-rays and $\vec{m}$ is a unit vector pointing in the magnetization direction. The scattering amplitude splits in three terms with distinct polarization dependence, where $F^c = -r_e Z + F^{(0)}$ describes the non-resonant (Thomson) and resonant charge scattering and $F^{(1)}$ and $F^{(2)}$ denote the first-order and second-order magnetic amplitudes. In the L-MOKE geometry using circularly polarized light the leading magnetic contribution to scattering arises from the $F^c F^{(1)}$ interference term. Since $F^{(2)}$ is generally small compared to $F^{(1)}$ and second-order contributions do not change upon magnetization reversal, these contributions are neglected in the data analysis.

As in hard x-ray scattering, both, the specular reflectivity and diffuse scattering were measured simultaneously. In order to separate the structural and magnetic contribution to the scattered intensity it is appropriate to measure the energy-dependent intensity at a fixed scattering angle 2Θ as well. All hard and soft x-ray measurements shown below have been taken at room temperature.

3. Results and discussion

3.1. Hard x-ray reflectivity

In Fig. 2 x-ray specular reflectivity data measured at a photon energy of 8048 eV of the $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ and the $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ multilayer is shown. Due to the large difference in the electron density of Au and Co_2MnGe , the x-ray scattering contrast between both sublayers is large even in non-resonant scattering. For the $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ sample superlattice peaks up to the 9th order are visible, indicative for smooth interfaces. In contrast, the difference of the electron density of V and Co_2MnGe is small and superlattice peaks for the case of the $[\text{Co}_2\text{MnGe}/\text{V}]_{20}$ sample are less intense (see Fig. 2b). A theoretical fit to the data by the Parratt formalism [23] yields thicknesses of 2.29 nm and 2.93 nm for the Au and Co_2MnGe layers in the $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ sample. For the case of the $[\text{Co}_2\text{MnGe}/\text{V}]_{20}$ multilayer we get 1.45 nm and 2.93 nm for the V and Co_2MnGe layers, respectively. The rms interface roughnesses σ of the Au and the Co_2MnGe layer in the $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ sample are $\sigma_{\text{Au}} = 0.4 \pm 0.1$ nm and $\sigma_{\text{Heusler}} = 0.3 \pm 0.1$ nm, respectively. For the $[\text{Co}_2\text{MnGe}/\text{V}]_{50}$ multilayer one has comparable values, namely $\sigma_{\text{V}} = 0.4 \pm 0.1$ nm and $\sigma_{\text{Heusler}} = 0.3 \pm 0.1$ nm.

Additional information on the in-plane structure of the interfaces and their correlations can be obtained by analyzing the diffuse scattering. One important parameter, which can be derived, is the in-plane correlation length ξ [24, 25]. In Fig. 3 we show 2D maps of $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ and $[\text{Co}_2\text{MnGe}/\text{V}]_{50}$ multilayers with the logarithm of the reflectivity contours plotted as a function of x-ray incident (α_i) and exit angles (α_f). The diagonal ridge at $\alpha_i = \alpha_f$ is the specularly reflected intensity. If the interfacial

roughness is perfectly correlated in the vertical direction, the diffuse intensity along Q_z would be peaked at the Bragg conditions, visible as so-called Bragg sheets. For random perpendicular roughness, the diffuse intensity will be spread out uniformly in q_z [24, 25]. In the case of the $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ multilayer Bragg sheets up to the fourth order can easily be identified (Fig. 3a). Thus the rms roughness is mainly caused by topological height fluctuations. For the $[\text{Co}_2\text{MnGe}/\text{V}]_{50}$ sample the perpendicular roughness correlation exists too, but the intensity of the corresponding Bragg sheets is low, indicating that random roughness due to interdiffusion is predominant.

In Fig. 4 single transverse q_x scans for both multilayers are shown. The intensity of the diffuse scattering is more than two orders of magnitude smaller than the specular intensity. Besides the Yoneda wings other optical features arising from the multilayer periodicity are visible. For the simulations (solid lines in Fig. 4) we used the Mingh model [26], which describes an intermediate case between uncorrelated and correlated roughness and assumes that vertical correlations do not depend on the lateral scale of the roughness. The parameters used for this model are the vertical correlation length L_v , the horizontal correlation length L_h and the "jaggedness" parameter h . The vertical correlation was taken from the out-of-plane coherence length obtained from large angle diffraction (see below). The jaggedness and the in-plane correlation length are left as the only free parameters, h being a value between 0.1 and 1. For small h values the surface is extremely jagged, if $h = 1$, the surface has smooth hills and valleys [25]. The best fit to the experimental data was obtained for a lateral roughness correlation length of $\xi_c^l = 18$ nm and $\xi_c^l = 14$ nm for the $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ and $[\text{Co}_2\text{MnGe}/\text{V}]_{20}$ multilayer, respectively, with a hurst parameter $h = 1$ [25]. The lateral correlation length can be assigned to the Co_2MnGe crystallite size. An additional component of diffuse scattering can be seen at small q_x values close to the specular peak. Since this q position is far apart from the critical angles, it can be fitted within the kinematic approximation by a Lorentzian curve (corresponding to $h = 0.5$). From the width we deduce a correlation length of $0.5 \mu\text{m}$ and $0.4 \mu\text{m}$, respectively, which corresponds to the typical terrace length of the Al_2O_3 substrate surface.

3.2. High angle Bragg scattering

The $[\text{Co}_2\text{MnGe}/\text{Au}]_n$ multilayers grow with perfect $\text{Co}_2\text{MnGe}(110)/\text{Au}(111)$ texture out-of-plane, whereas the $[\text{Co}_2\text{MnGe}/\text{V}]_n$ samples grow with $\text{Co}_2\text{MnGe}(110)/\text{V}(110)$ texture. Within the plane both are polycrystalline [27]. In Fig. 5 we show Bragg scans across the $\text{Co}_2\text{MnGe}(220)/\text{Au}(111)$ and $\text{Co}_2\text{MnGe}(110)/\text{V}(110)$ Bragg peaks. Satellite peaks up to the fourth and third order, respectively, can be resolved, indicative of a coherently grown superstructure in the growth direction. The vertical coherence length derived from the width of the satellite peaks is $\xi_v = 30$ nm for the $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ multilayer and $\xi_v = 15$ nm for the $[\text{Co}_2\text{MnGe}/\text{V}]_{20}$ multilayer. The positions of the satellite peaks yield the same superlattice period as the small-angle reflectivity.

3.3. X-ray resonant magnetic reflectivity

If the exact structural and magnetic sample composition is known, the dispersive and absorptive corrections to the refractive index can be measured from the energy-dependent peak position and width, as it has been demonstrated by Mertins et al. for an $[\text{Fe/C}]_n$ superlattice [28]. We have chosen the opposite approach here, i.e. with the knowledge of the magneto-optical constants and the precise knowledge of the chemical multilayer structure we determine an element-specific magnetization depth profile.

We have measured the reflected intensity of circularly polarized x-rays after magnetic saturation in the directions parallel (I_+) and antiparallel (I_-) to the photon helicity at the angular position of the Bragg peaks. The position is indicated by the arrows in Fig. 6, where the specular reflectivity of the $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ multilayer up to the third-order Bragg peak, measured by hard x-rays and by circularly polarized soft x-rays at the Co and Mn L_3 edge are compared. The reflectivity spectra of both $[\text{Co}_2\text{MnGe}/\text{Au}]_n$ and $[\text{Co}_2\text{MnGe}/\text{V}]_n$ multilayers are shown in Figs. 7 and 8 for the Co and Mn $L_{2,3}$ edges. The scanned q_z range is indicated by two vertical lines for each scan in Fig. 6.

The sum of the intensities $(I_+ + I_-)/2$ reflects the charge scattering and is independent of the magnetization of the sample. Superimposed on this line shape are the strong intensity variations due to absorption, when the energy is passing the L_3 and L_2 absorption edges of Co and Mn.

The magnetic contribution to the resonant scattering can best be visualized by taking the asymmetry ratio $(I_+ - I_-)/(I_+ + I_-)$ (second row in Figs. 7 and 8). In order to evaluate a magnetization depth profile for the multilayers from the magnetic part of the reflectivity spectra in Figs. 7 and 8, the energy-dependent intensities and asymmetries have been modelled within a magneto-optical matrix formalism developed by Zak et al. using the classical dielectric tensor [29, 30]. Within this formalism it is possible to calculate the reflectivity for electromagnetic radiation of arbitrary incidence angle and polarization on layered structures having an arbitrary magnetization depth profile. The formalism is not limited to Bragg reflections and has been used to model magneto-optical effects at soft x-ray energies in a number of publications before [31, 32, 33].

The analysis following Ref. [29] needs the knowledge of the energy dependence of the refractive index $n = 1 - (\delta_c + \delta_m) + i(\beta_c + \beta_m)$ with the charge contributions δ_c and β_c and the magnetic contributions δ_m and β_m (Fig. 9). This has been determined for a Co_2MnGe film in a separate x-ray absorption experiment [19]. The imaginary part of the refractive index is directly proportional to the absorption coefficient. The real part is then calculated using the Kramers-Kronig relations [34, 35].

Furthermore, from the previous analysis by hard x-ray small angle reflectivity we already have a set of well defined parameters characterizing the chemical structure, i.e. the thickness and roughness parameters, which we keep fixed in the fit of the spectra in Figs. 7 and 8.

In the upper panels of Figs. 7 and 8 we compare the measured and the calculated

Table 1. Parameters defining the magnetic moment density profile with the top and bottom non-ferromagnetic layer thickness d_t and d_b and the magnetic roughness parameter σ_{mag} .

	Co $L_{2,3}$ edge			Mn $L_{2,3}$ edge		
	d_t [nm]	d_b [nm]	σ_{mag} [nm]	d_t [nm]	d_b [nm]	σ_{mag} [nm]
$[\text{Co}_2\text{MnGe}/\text{Au}]_n$	0.3	0.45	0.3	0.6	1.1	0.3
$[\text{Co}_2\text{MnGe}/\text{V}]_n$	0.3	0.4	0.3	0.4	0.6	0.3

charge scattering intensity $(I_+ + I_-)/2$ taking all parameters from the hard x-ray measurements and the optical constants as just explained. One finds overall good agreement of the measured and calculated spectra.

The next and in the present context most essential step is to fit the asymmetry given in the lower panels in Figs. 7 and 8 with the same set of fixed structural and optical parameters. The only free parameter is the profile for the depth dependence of the ferromagnetic magnetization, in particular its shape, as described in detail below.

Assuming that the magnetic moment density profile is exactly identical to the chemical one, even qualitative features of the asymmetry spectra cannot be reproduced. Only if non-ferromagnetic interlayers at the interface of $\text{Co}_2\text{MnGe}/\text{Au}$ or $\text{Co}_2\text{MnGe}/\text{V}$ are allowed, the complex features of the experimental spectra can be modelled. Thus in the modelling we assume a magnetic moment density profile for Co and Mn which is narrower than the chemical density profile and may be asymmetric with respect to the chemical profile, i.e. the top non-ferromagnetic layer thickness d_t can be different from the bottom non-ferromagnetic layer thickness d_b . The best fits we obtained are shown as solid lines in the lower panels of Figs. 7 and 8 and reproduce the experimental spectra quite well. The corresponding magnetic moment density profiles of Co and Mn for the $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ and $[\text{Co}_2\text{MnGe}/\text{V}]_{20}$ multilayers are depicted in Fig. 10.

For a better comparison of charge and magnetic profiles in Fig. 10 the refractive indices are normalized according to

$$\rho_c(z) = \frac{|\delta_c(z) - \delta_{c,\text{Au}}|}{|\delta_{c,\text{Co}_2\text{MnGe}} - \delta_{c,\text{Au}}|}, \quad \rho_m(z) = \frac{\delta_m(z)}{\delta_{m,\text{Co}_2\text{MnGe}}}, \quad (2)$$

so that $\rho(z) = 1$ ($\rho(z) = 0$) if the refractive index corresponds to the bulk Co_2MnGe (Au/V) value. The corresponding imaginary part $\beta_{c,m}$ has the same z dependence as the real part. The parameters describing the magnetic density profile are summarized in Tab. 1. The profile is clearly asymmetric with the bottom non-ferromagnetic layer always thicker than the top non-ferromagnetic layer. One should note that the non-magnetic layer thickness derived for Mn is definitely larger than for Co. For Co_2MnGe grown on Au the bottom non-ferromagnetic layer thickness is largest, namely $d_b = 1.1$ nm.

The shape of the asymmetry at the Bragg peaks of different order is very sensitive to the magnetization profile assumed. In order to demonstrate this sensitivity we show a model calculation of the sample $[\text{Co}_2\text{MnGe}/\text{Au}]_{50}$ for the second-order Bragg peak of Mn

assuming a constant total non-ferromagnetic layer thickness $d_{nm} = d_t + d_b = 1.63$ nm and a variable d_b/d_t ratio in Fig. 11. Only the distribution with $d_t = 0.58$ nm and $d_b = 1.08$ nm can reproduce the experimental spectrum. It should be stressed that this asymmetric distribution yields the best fit in all orders of the Bragg peaks.

3.4. Microscopic origin of the magnetic moment density profile

What remains to be explained is the microscopic origin for the magnetization profile inside the Heusler layers, and especially the origin of the very different Co and Mn profile. Principally XRMS cannot resolve this question, it only proves its existence. In Fig. 12 we propose a qualitative model as an explanation, which is based on the intimate relationship between the chemical structure and the ferromagnetism of a thin Co_2MnGe layer.

Starting from the bottom of the Heusler layer growing on an Au or V film (see Fig. 12), the first few Heusler monolayers grow as a bcc-type random mixture of the Ge, Mn and Co atoms. The magnetic order for this layer is of spin glass type with a low saturation magnetization and appears essentially non magnetic in the XRMS experiments at room temperature. We have clearly observed spin glass type of magnetic order in multilayers with very thin Heusler layers [36]. Then, after the deposition of the first few monolayers, the Heusler film starts developing chemical short range order with each of the Heusler constituents beginning to occupy its own L2_1 type sublattice. However there is still substantial site disorder between the Co and Mn positions. Theoretical model calculations [37] have shown that in this case there is an essential difference between the magnetic behavior of an antisite Co and an antisite Mn atom: Mn sitting on a regular Co position has its moment oriented antiparallel to the Co-nearest neighbours moments, whereas Co on a Mn position keeps its parallel moment direction. Thus in XRMS, which measures the average Mn moment density, the Mn moment is not yet visible, whereas the Co moment is detected. This explains why the magnetization profile for Mn is narrower than the Co profile. Then, in the core of the Heusler layer, the chemical order approaches the ideal L2_1 superstructure and the Mn moments are seen in the XRMS signal.

Moving further towards the top of the Heusler film in Fig. 12 one finds the same sequence of magnetic phases in reversed order however definitely thinner than at the bottom of the Heusler film. This indicates that upon the deposition of the top Au or V layer a few monolayers of the ordered L2_1 type Heusler layer become disordered again. Thus it seems that interactions at the interface destroy the chemical ordering of the Heusler phase, or in other terms, at the interfaces in thermodynamic equilibrium the Heusler L2_1 type order is unstable.

3.5. Magnetic diffuse scattering

Similar to the case of the non-magnetic off-specular scattering, one also can study the off-specular magnetic scattering and derive information about the correlation of the

Table 2. Parameters of the transverse scans with the in-plane coherence lengths ξ_1 and ξ_2 and the hurst parameter h (see main text) as derived from Fig. 13.

	[Co ₂ MnGe/Au] ₅₀				[Co ₂ MnGe/V] ₂₀			
	ξ_1 [μm]	h_1	ξ_2 [nm]	h_2	ξ_1 [μm]	h_1	ξ_2 [nm]	h_2
Co, charge	0.6	0.5	24.5	1.0	0.65	0.5	9.0	1.0
Co, charge-magnetic	1.0	0.7	27.5	1.0	0.55	0.5	9.0	1.0
Mn, charge	0.6	0.5	22.5	1.0	0.5	0.5	9.0	1.0
Mn, charge-magnetic	0.7	0.5	22.0	1.0	0.6	0.4	9.0	1.0

magnetic roughness [38, 39, 40, 41]. Fig. 13 shows charge $(I_+ + I_-)/2$ and magnetic $(I_+ - I_-)$ transverse scans at the q_z position of the first-order superlattice peak for the studied samples at the Co and Mn edge, respectively. Both charge and magnetic scans exhibit the same three components as the hard x-ray transverse scan in Fig. 4: the specular peak at $q_x = 0$, a narrow component due to the substrate roughness (ξ_1, h_1) , and a broad diffuse component corresponding to a short-range in-plane correlation (ξ_2, h_2) . The experimental data do not show any indication of multiple reflections like Yoneda wings. Therefore the Born approximation is sufficient to describe the diffuse scattering [39, 40]. The parameters for the best fits of the transverse scans are listed in Tab. 2.

For simplicity the vertical correlation of the interfaces is assumed to be perfect. This assumption is justified by the fact that the vertical correlation length as determined from the hard x-ray data is larger than the penetration depth of the soft x-rays at these energies and incidence angles. The roughness parameters for the charge and the magnetization are taken from the simulation of the reflectivity.

Since the intensity difference $(I_+ - I_-)$ is dominated by the charge-magnetic interference term, the existence of magnetic diffuse scattering at the Bragg peaks already indicates that the chemical and magnetic interfaces are correlated. Within the experimental error bars the magnetic interface morphology follows exactly the chemical one (see Tab. 2). This observation confirms that the presence of non-ferromagnetic layers is intrinsically correlated to chemical disorder in the sample. Both chemical and magnetic interfaces have a correlated roughness on the scale of the in-plane crystallite size.

4. Summary and conclusions

In summary, we have demonstrated that XRMS is a powerful technique for the determination of the magnetic moment density profiles in Heusler multilayers. However, the procedure takes some efforts: First, one needs high quality multilayers and second, a complete set of fixed input parameters from the analysis of hard x-ray scattering and optical constants determined by x-ray absorption. Only then the magnetic moment density profile is left as the only free parameter in the fitting procedure and an unambiguous determination of the profile becomes possible.

For the multilayer systems we have studied here the analysis of the XRMS spectra revealed that at room temperature the Co_2MnGe layers interleaved between V and Au possess non-ferromagnetic or weakly ferromagnetic layers at the interface with a thickness of about 0.5 nm at the bottom and 0.3 nm at the top. The loss of Mn moments, indicative of massive structural disorder, holds for even thicker interlayers so that for a 3 nm Co_2MnGe layer typically only the inner core of about 1.5 nm thickness develops the full magnetization of the chemically ordered bulk Heusler compound. XRMS does not reveal the microscopic origin for the loss of magnetic moments as can be segregation of one of the Heusler atomic species at the interface, interdiffusion of atoms from the Au or V layer, structural disorder or a combination of these effects. For the multilayers under study here we think that with Au interlayers the chemical disorder is most important, in the case of V interlayers additionally the diffusion of V into the Heusler surface layer probably contributes to disorder and loss of moments.

The non ferromagnetic interface layers offer a plausible explanation for several peculiar magnetic features we have observed in the $[\text{Co}_2\text{MnGe}/\text{V}]_n$ and $[\text{Co}_2\text{MnGe}/\text{Au}]_n$ multilayers. The small GMR amplitude [16] e.g. finds a natural explanation, since the main contribution to the GMR originates from an asymmetric spin dependent scattering at the interfaces. The superparamagnetic behaviour observed at high temperatures for $[\text{Co}_2\text{MnGe}/\text{V}]_n$ multilayers with the thickness of the Heusler layer below 3 nm is more plausible, since the effective ferromagnetic layer thickness is much smaller than the nominal thickness. In the $[\text{Co}_2\text{MnGe}/\text{Au}]_n$ multilayer system we have observed an exchange bias phenomenon at low temperatures [36] and speculated that it might be due to a spin glass formation in the Au/ Co_2MnGe interface layer. This hypothesis is supported here by the finding of non-ferromagnetic interface layers by XRMS at room temperature.

More generally, it is feasible that in thin film heterostructures with Heusler compounds weakly ferromagnetic interface layers might be a common phenomenon. For the fabrication of tunnel junctions with an Al_2O_3 barrier e.g. one usually starts with the preparation of a metallic Al layer on the top of the Heusler film [42]. In a second step the Al film is oxidized thermally or by plasma oxidation. If during the deposition of the Al layer on top of the Heusler film the ferromagnetic order of a Heusler surface layer is weakened and concomitantly the full spin polarization is lost, one could easily explain the difficulty to observe the predicted 100% spin polarization experimentally in TMR junctions using the Heusler half metals [14, 15].

Acknowledgments

We would like to thank S. Erdt-Böhm for sample preparation and O. Seeck (HASYLAB), H.-C. Mertins, W. Mahler and B. Zada (BESSY) for their help with beamline operation. We thank D. Lott for the helpful discussions regarding the simulation of reflectivities. This project is funded by BMBF O3ZA6BC2 and SFB 491.

5. References

- [1] P.H. Dederichs and J. Galanakis, editors. *Half-metallic Alloys - Fundamentals and Applications*. Springer, Berlin-Heidelberg-New York, 1 edition, 2005.
- [2] S. Ishida, S. Fujii, S. Kashiwagi, and S. Asano. *J. Phys. Soc. Jpn.*, 64:2154, 1995.
- [3] S. Ishida, S. Kashiwagi, S. Fujii, and S. Asano. *Physica B*, 210:140, 1995.
- [4] S. Ishida, T. Masaki, S. Fujii, and S. Asano. *Physica B*, 245:1, 1998.
- [5] I. Galanakis, S. Ostanin, M. Alouani, H. Dreyssé, and J. M. Wills. *Phys. Rev. B*, 61:4093, 2000.
- [6] I. Galanakis, P. H. Dederichs, and N. Papnikolaou. *Phys. Rev. B*, 66:134428, 2002.
- [7] I. Galanakis, P. H. Dederichs, and N. Papanikolaou. *Phys. Rev. B*, 66:174429, 2002.
- [8] S. Picozzi, A. Continenza, and A. J. Freeman. *Phys. Rev. B*, 66:094421, 2002.
- [9] S. Picozzi, A. Continenza, and A. J. Freeman. *IEEE Trans. Mag.*, 38:2895, 2002.
- [10] C. Felser, B. Heitkamp, F. Kronast, D. Schmitz, S. Cramm, H. A. Dürr, H.-J. Elmers, G. H. Fecher, S. Wurmehl, T. Block, D. Valdaitsev, S. A. Nepijko, A. Gloskovskii, G. Jakob, G. Schönhense, and W. Eberhardt. *J. Phys.: Condens. Matter*, 15:7019, 2003.
- [11] G.A. Prinz. *Science*, 282:1660, 1998.
- [12] D. Awschalom and J. Kikkawa. *Physics Today*, 52:33, 1999.
- [13] J.F. Gregg, I. Petey, E. Jougelet, and C. Dennis. *J. Phys. D: Appl. Phys.*, 35:R121, 2002.
- [14] J. Schmalhorst, S. Kämmerer, M. Sacher, G. Reiss, A. Hütten, and A. Scholl. *Phys. Rev. B*, 70:024426, 2004.
- [15] M. Oogane, J. Nakata, H. Kubota, Y. Ando, A. Sakuma, and T. Miyazaki. *Jap. J. Appl. Phys. Part 2*, 44:L760, 2005.
- [16] K. Westerholt, A. Bergmann, J. Grabis, A. Nefedov, and H. Zabel. Magnetism and structure of multilayers based on the fully spin polarized heusler alloys Co_2MnGe and Co_2MnSi . In P.H. Dederichs and J. Galanakis, editors, *Half-metallic Alloys - Fundamentals and Applications*, Lecture Notes in Physics. Springer, 2005.
- [17] U. Geiersbach, A. Bergmann, and K. Westerholt. *Thin Sol. Films*, 425:226, 2003.
- [18] H.-K. Jeong, A. Caruso, and C.N. Borca. Surface segregation and compositional instability at the surface of half-metal ferromagnets and related compounds. In P.H. Dederichs and J. Galanakis, editors, *Half-metallic Alloys - Fundamentals and Applications*, Lecture Notes in Physics. Springer, 2005.
- [19] J. Grabis, A. Bergmann, A. Nefedov, K. Westerholt, and H. Zabel. *Phys. Rev. B*, 72:024438, 2005.
- [20] A. Bergmann, J. Grabis, B.P. Toperverg, V. Leiner, M. Wolff, H. Zabel, and K. Westerholt. *Phys. Rev. B*, 72:in press, 2005.
- [21] J. Grabis, A. Nefedov, and H. Zabel. *Rev. Sci. Instr.*, 74:4048, 2003.
- [22] J. P. Hannon, G. T. Trammel, M. Blume, and D. Gibbs. *Phys. Rev. Lett.*, 61:1245, 1988.
- [23] L. G. Parratt. *Phys. Rev.*, 95:359, 1954.
- [24] D. E. Savage, J. Kleiner, N. Schimke, Y.-H. Phang, T. Jankowski, J. Jacobs, R. Kariotis, and M. G. Lagally. *J. Appl. Phys.*, 69(3):1411, 1991.
- [25] S. K. Sinha, E. B. Sirota, S. Garoff, and H. B. Stanley. *Phys. Rev. B*, 38:2297, 1988.
- [26] Z. H. Ming, A. Krol, Y. L. Soo, Y. H. Kao, J. S. Park, and K. L. Wang. *Phys. Rev. B*, 47:16373, 1993.
- [27] U. Geiersbach, A. Bergmann, and K. Westerholt. *J. Magn. Magn. Mater.*, 240:546, 2002.
- [28] H.-C. Mertins, O. Zaharko, A. Gaupp, F. Schäfers, D. Abramsohn, and H. Grimmer. *J. Magn. Magn. Mater.*, 240:451, 2002.
- [29] J. Zak, E. R. Moog, C. Liu, and S. D. Bader. *Phys. Rev. B*, 43:6423, 1991.
- [30] J. Zak, E. R. Moog, C. Liu, and S. D. Bader. *Phys. Rev. B*, 46:5883(E), 1992.
- [31] J. B. Kortright and S.-K. Kim. *Phys. Rev. B*, 62:12216, 2000.
- [32] D. Lott. *Magnetic X-ray Reflectivity*. PhD thesis, Ludwig-Maximilians-Universität München, 2001.
- [33] H.-C. Mertins, S. Valencia, D. Abramsohn, A. Gaupp, W. Gudat, and P. M. Oppeneer. *Phys.*

- Rev. B*, 69:064407, 2004.
- [34] J. E. Prieto, F. Heigl, O. Krupin, G. Kaindl, and K. Starke. *Phys. Rev. B*, 68:134453, 2003.
 - [35] K.-E. Peiponen, E. M. Vartiainen, and T. Asakura. *Dispersion, Complex Analysis and Optical Spectroscopy*, volume 147 of *Springer Tracts in Modern Physics*. Springer, 1999.
 - [36] K. Westerholt, U. Geiersbach, and A. Bergmann. *J. Magn. Magn. Mat.*, 257:239, 2003.
 - [37] S. Picozzi, A. Continenza, and A. J. Freeman. *Phys. Rev. B*, 69:094423, 2004.
 - [38] J. F. MacKay, C. Teichert, D. E. Savage, and M. G. Lagally. *Phys. Rev. Lett.*, 77:3925, 1996.
 - [39] R. M. Osgood III, S. K. Sinha, J. W. Freeland, Y. U. Idzerda, and S. D. Bader. *J. Magn. Magn. Mat.*, 198-199:698, 1999.
 - [40] C. S. Nelson, G. Srajer, J. C. Lang, C. T. Venkataraman, S. K. Sinha, H. Hashizume, N. Ishimatsu, and N. Hosoi. *Phys. Rev. B*, 60:12234, 1999.
 - [41] D. R. Lee, S. K. Sinha, C. S. Nelson, J. C. Lang, C. T. Venkataraman, G. Srajer, and R. M. Osgood III. *Phys. Rev. B*, 68:224410, 2003.
 - [42] J. Moodera, R. Kinder, L. T. Wong, and R. Meservey. *Phys. Rev. Lett.*, 74:3273, 1998.
 - [43] B. L. Henke, E. M. Gullikson, and J. C. Davis. *At. Data Nucl. Data Tables*, 54:180, 1993.

6. Figures

Figure 1. Scattering geometry in reciprocal space for (a) a specular reflectivity ($\Theta-2\Theta$ scan, $q_x=0$) and (b) diffuse scattering (q_x scan, q_z constant). Bragg peaks in the specular reflectivity and diffuse Bragg sheets are schematically shown as dots and dotted lines, respectively.

Figure 2. Reflectivity of the $[\text{Co}_2\text{MnGe}/\text{Au}]$ (a) and $[\text{Co}_2\text{MnGe}/\text{V}]$ (b) multilayer measured with linearly σ polarized hard x-rays ($E = 8048$ eV) at wiggler beamline W1 at HASYLAB and simulation (black solid line).

Figure 3. Two-dimensional (2D) maps of the x-ray intensity scattered from the $[\text{Co}_2\text{MnGe}]/\text{Au}_n$ (a) and $[\text{Co}_2\text{MnGe}]/\text{V}_n$ multilayer (b) as a function of the angle of incidence α_i and scattering α_f . The logarithmic intensity color scale is shown on the right side.

Figure 4. Transverse q_x scans at the position of the Bragg peak (dots) for the $[\text{Co}_2\text{MnGe}]/\text{Au}_n$ (a) and $[\text{Co}_2\text{MnGe}]/\text{V}_n$ multilayer (b) theoretical fits (solid line).

Figure 5. Longitudinal high-angle scans of the $\text{Co}_2\text{MnGe}(220)/\text{Au}(111)$ (a) and $\text{Co}_2\text{MnGe}(220)/\text{V}(110)$ Bragg peak (b).

Figure 6. Specular reflectivity measured with hard x-rays (top curve) and soft x-rays at the Co (middle) and Mn (bottom) L_3 edges for the $[\text{Co}_2\text{MnGe}]/\text{Au}_n$ sample.

Figure 7. Charge intensity $(I_+ + I_-)/2$ (top) and asymmetry $(I_+ - I_-)/(I_+ + I_-)$ at the first and second order Bragg peak (BP) at the Co $L_{2,3}$ absorption edges. The dots represent measured data, the lines are model calculations as described in the main text.

Figure 8. Charge intensity (top) and asymmetry at the first and second order Bragg peak (BP) at the Mn $L_{2,3}$ absorption edges. The dots represent measured data, the lines are model calculations as described in the main text.

Figure 9. Magneto-optical constants at the $L_{2,3}$ edges of Mn and Co and a comparison to the tabulated refractive index (open symbols) taken from Ref. [43].

Figure 10. Structural and magnetic moment density profiles of Co and Mn for the samples $[\text{Co}_2\text{MnGe})/\text{Au}]_n$ (a) and $[\text{Co}_2\text{MnGe})/\text{V}]_n$ (b) as determined from model calculations (see main text). z denotes an axis perpendicular to the film surface.

Figure 11. Modell calculations of the second order BP compared to the experiment. The ratio of the bottom non-ferromagnetic layer thickness d_b and the top non-ferromagnetic layer thickness d_t is varied while the sum $d_b + d_t = 1.66$ nm is kept fixed.

Figure 12. Schematic picture of the sequence of structural phases in a 3 nm thick Co_2MnGe film between two Au-layers. The vertical scale gives the distance from the bottom of the Co_2MnGe -film.

Figure 13. Transverse q_x scans at the Co (red) and Mn edge (blue) for the $[\text{Co}_2\text{MnGe}]/\text{Au}]_n$ (a) and $[\text{Co}_2\text{MnGe}]/\text{V}]_n$ multilayer (b). The measured charge (circles) and magnetic (triangles) intensity is modelled within the framework of Born approximation (lines) as described in the main text.