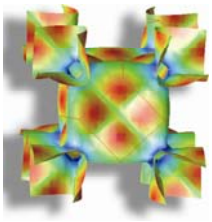

MATERIALS IN MAINZ SCIENCE

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“New materials for spintronics,

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Abstracts Poster

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Preparation of thin films of the Heusler compound Co_2FeAl

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Heusler compounds are potential candidates for showing half metallic properties (100% spin polarization) with a large band gap at the Fermi energy and a high Curie temperature above room temperature.

A study of the crystallographic structure, surface morphology and magnetization of the Heusler compound Co_2FeAl has been carried out.

The Co_2FeAl thin films are deposited on MgO buffer layers which are deposited on MgO substrates. The MgO buffer layer is deposited in a molecular beam epitaxial chamber by electron beam evaporation. The Co_2FeAl thin film is deposited by rf magnetron sputtering. RHEED and STM are used to analyze the morphology of the Heusler compound. The images show a smooth and well ordered film surface after an annealing process at 550°C.

The Heusler compounds have a X_2YZ composition in a $L2_1$ crystallographic structure. The crystallographic study is made by a two and a four circle X-ray diffractometer in order to determine the structure, the lattice parameter and the order of the atoms in the crystallographic structure. A simple cubic unit cell with 5.73 Å as lattice parameter is the result from these measurements. A small tetragonal distortion due to thermal expansion is deduced. No evidence of $L2_1$ order is found. A B2 structure (completely mix Fe-Al atom positions) with a 12% of disorder in the Co sites is determined.

Magnetization measurements are made by a Quantum Design SQUID magnetometer with a magnetic field parallel to the surface plane and by XMCD. The magnetic moment of the film is important for comparing with the theoretical magnetic moment expected from the Slater-Pauling rule for half metals. The magnetic moment using the SQUID is 4.86μB/f.u. which is only 2.8% less than the value predicted theoretically (5.0μB/f.u.) pointing to a good quality of the film for obtaining a high spin polarization.

The characterization of thin films of Heusler compounds is important for the preparation of good magnetic tunneling junctions in order to measure their spin polarization.

The first ternary intermetallic Heusler nanoparticles: Co_2FeGa

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Synthesis of materials with controlled particle size in nanometer regime is an active area in the field of materials research. With the control over particle size the electronic and magnetic properties of material can be tuned. To study the effect of nanometer dimensions on the properties of Heusler alloys, a first example of Nano-Heusler is presented. Co_2FeGa Heusler nanoparticles were produced by reducing methanol impregnated mixture of $CoCl_2.6H_2O$, $Fe(NO_3)_3.9H_2O$ and $Ga(NO_3)_3 .xH_2O$ after loading on fumed silica. The dried samples were heated under pure H_2 gas at 900°C. The synthesized Co_2FeGa Heusler nanoparticles were characterized by HRTEM, XRD and Mossbauer. All peaks of XRD patterns can be attributed to a $L2_1$ Heusler structure with the lattice constant a_0=0.537 Å. The size of the particles, as determined by transmission electron microscopy, is between 16-20 nm. Ferromagnetic behaviour of the particles as determined by the SQUID is presented and compared with the bulk Co_2FeGa Heusler alloy.

Investigation of Li compounds with $C1_b$ und $L2_1$ structure

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We investigated Li containing compounds of the $L2_1$ and $C1_b$ structure types.
The compounds of the $C1_b$ – type, also referred to as Half-Heusler compounds, have the formula *XYZ* and the compounds of the $L2_1$ type are called Heusler compounds and have the general formula X_2YZ. $C1_b$ compounds crystallize in the space group F-43m and $L2_1$ compounds crystallize in the space group Fm-3m. *X*, *Y* are transition metals; *Z* is from III, IV, and V main group. In the case of LiAlSi the compound consists of a I, III, and IV main group element. Some Heusler alloys are predicted to be half metallic ferromagnets and are candidates for application in spintronic. Li containing $C1_b$ compounds with 18 valence electrons (VE) are supposed to be good anode materials.
We investigated LiAlSi by X-Ray diffraction, Li-NMR, and DSC measurements. We did band structure calculations for $LiCo_2Ge$, Li_2CuSi, $LiNi_2In$ and LiAlSi.

Fabrication of highly ordered Co_2MnSi single crystals

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Co_2YZ Heusler compounds are an interesting class of materials mainly because of their magnetic properties. In particular, Co_2MnSi is predicted to be a half-metallic ferromagnet. Consequently, Co_2MnSi shows quite high TMR- ratios at low temperatures. In order to study the magnetic properties and the conductivity of Co_2MnSi with respect to the crystallographic axis, single crystals of high purity and with a high degree of order are essential.
Therefore, Co_2MnSi singlecrystals were synthesised by a floating zone technique in a Gero mirror furnance.
Rods of polycrystalline Co_2MnSi (precursor) are placed in the shared focus of two doublehemispherical mirrors, which are equipped with two 1000 Watt lamps.
These lamps provide the energy to melt the rod of the polycrystalline Co_2MnSi.
The rod is molten at a small area of ca 3-5mm length. Then the rod is moved through the focus. Due to the slow crystallisation, guaranteed by this technique, single crystalline rods are obtained.
These rods are cut perpendicular to the growth direction and precharacterised by metallographic methods. These methods revealed comparable large single crystalline areas of several mm length and of the whole width of the rod.
Promising pieces of the rods are selected and their singlecrystallinity is proved by X-ray diffraction using a Bruker GADDS.
After the successful growth of big Co_2MnSi single crystals these can be cut with respect to the crystallographic axis, resulting in samples, which can be used to measure the anisotropic properties of the Heusler compound Co_2MnSi, such as conductivity or magnetic properties.

Interlayer exchange coupling in chemically disordered Co-Mn-Si based epitaxial trilayer structures

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Theoretical predictions of 100% spin polarization in half-metallic full-Heusler alloys have attracted much interest in recent years for their promising applications in future

spintronic devices. We previously reported the enhancement of GMR values using Co_2MnSi (CMS) as electrode [1]. The knowledge of interlayer exchange coupling (IEC) in half-metallic ferromagnet based structure is very important in both fundamental physics and further development of GMR devices. In our previous study, we reported unusual oscillatory 90º coupling (3.3-3.5 nm) with no sign for any contribution of 180º coupling in epitaxial CMS/Cr/CMS trilayer structures [2]. The present research is focused on one question; is this IEC behavior related with half-metallicity, i.e., spin polarization of Heusler alloy? Band structure calculations in full-Heusler alloy CMS predicted that half-metallic electronic structure is destroyed by its chemical disordering, especially by Co antisites [3]. In this study, we have fabricated Co enriched CMS i.e., $Co_{2+X}MnSi$ and investigated the change of coupling behavior with the Co composition in $Co_{2+X}MnSi$(20 nm)/Cr(1.2 nm)/$Co_{2+X}MnSi$(7 nm) trilayers, systematically. The ratio of two fundamental peak intensities I(002)/I(004) measured from XRD, i.e., the degree of B2 ordering decreases with the Co composition and disappears for very high Co compositions over 75 at.%. Likewise, the 90º coupling strength $-J_2$ decreases in a similar fashion with the Co composition and shows a minimum at a Co content about 70 at.%. Afterwards, the contribution of $-J_1$, i.e., 180º coupling appears for CMS layers with highly Co antisite defective (A2) structures. This suggests a clear relationship between the B2 ordering and IEC.

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New quarternary LiMgPdSb-type half metallic materials

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A lot of half metallic materials have been found in Heusler alloys. Heusler alloy is ternary X_2YZ compounds with $L2_1$ structure. Recently, we find a good method to develop new materials with half metallicity is to combine two Heusler alloys which have half metallic properties. The new materials are quaternary LiMgPdSb-type compounds contained all atoms in the two parents Heusler alloys. Based on the first principle calculations, CoMnTiAl and CoFeMnSi have been investigated in detailed.
The electronic structure of the compounds was calculated by means of the full potential linearized augmented plane wave (FLAPW) method as implemented in Wien2k. The exchange-correlation functional was taken within the generalized gradient approximation (GGA) in the parameterization of Perdew *et al*.

Giant magnetoresistance in rare earth compounds

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Ternary intermetallic rare earth compounds *REXY* (*RE* = lanthanide element, *Y* = transition metal, *Z* = sp element), with 18 valence electrons have been investigated by the means of magnetic, resistance and magnetoresistance measurements. All results are in good agreement with band structure calculations. Interestingly many of the compounds with MgAgAs structure are semiconducting although they are made out of metal elements [1, 2], while compounds with other structures are metallic. Additionally for some of these compounds a metal-insulator transition was found. The metal - insulator transition temperature depends strongly on the preparation conditions.
Some of these compounds show a negative giant magnetoresistance (GMR) above the magnetic ordering temperature in the paramagnetic temperature regime. This magnetoresistance scales roughly with the square of the magnetization in the paramagnetic state, and is related to the metal-insulator transition.
The nonmagnetic semiconducting LuNiBi compound shows a large postitve MR effect of 25% at room temperature (figure 1). The positive MR may be due to metallic bismuth impurities in the sample that cause an extraordinary magnetoresistance (EMR) [3].
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Investigation of $Co_2Y_{(1-x)}Ti_xGe$ (Y = Mn, Fe) Heusler compounds with 27.8 valence electrons

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Half-metallic ferromagnets have been proposed as ideal candidates for spin injection devices because they have been predicted to exhibit 100% spin polarization at the Fermi energy. From the applications point of view, a high Curie temperature for a half-metallic ferromagnet may be an important condition. The finger print of compounds showing a giant magneto resistance consists of three parts: a spin density wave, a saddle point and a

local magnetic moment. Heusler compounds with 27.8 valence electrons were predicted to show instabilities at the Fermi energy (spin density wave and saddle point). $Co_2Cr_{0.6}Fe_{0.4}Al$ has attracted great interest as a potential material for magneto-electronics. The drawback of is material is that it is hard to be stabilized in the $L2_1$ structure; the weak hybridization of Co and Al leads to an anti-site disorder between Al and Fe/Cr positions. Calculations also show that anti-side disorder will destroy the high spin polarization implying that precise control of the atomic structure of the Heusler alloys is also required. Here we present the investigation of Heusler compounds with 27.8 valence electrons exhibiting the above mentioned favorable properties. The compounds were synthesized by arc-melting; the order of the samples was improved by annealing at elevated temperatures. The structure of the compounds was examined using XRD, EDX, REM and Mössbauer methods. The magnetic properties were investigated by SQUID measurements. In addition, DSC was carried out to study the temperature dependent behavior. Here the results obtained for $Co_2Y_{(1-x)}Ti_xGe$ (Y=Fe, Mn) are displayed.

Physics of new magnetoresistance devices: Heusler Interfaces

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Magnetoresistance is the property of a material or composite to change its resistance in an applied magnetic field. This property is essential for various applications like magnetic memory (MRAM) or hard disk drives in which information is stored in magnetic bits. The magnitude of the magnetoresistance effect depends on the electronic band structure of the employed materials. The largest effects can be obtained using magnetic tunneling junctions (TMR). Conventional ferromagnets like CoFe have a maximum spin polarization of ≈ 60%. However, Heusler compounds (e.g. $Co_2Cr_{0.6}Fe_{0.4}Al$) are theoretically predicted to be 100% spin polarized. In the semi classical model the conductivity of a metal – insulator - metal tunnel junction depends only on the density of states at the Fermi energy. Since tunneling is spin conserving the relative alignment of the magnetization of the ferromagnetic tunnel electrodes determines the junction conductivity and results in a magnetoresistance. The effect becomes larger if the spin polarization of the electrodes is increased.

We are preparing epitaxial thin films and multilayers of the Heusler compounds $Co_2Cr_{0.6}Fe_{0.4}Al$ and Co_2FeAl and investigate the interface and tunneling properties.
A planar tunneling junction requires that the current is send perpendicular through the ferromagnet – insulator - ferromagnet stack. Thus little “towers” (mesas) are prepared by photolithography and ion beam etching.
Tunneling processes are sensitive to the electronic properties of the electrodes in the interface region, which can be very different from the bulk characteristics. We investigate

the structural and magnetic interface properties by tunneling microscopy (STM), Transmission Electron Microscopy (TEM), diffraction experiments (X-ray, RHEED, LEED, neutrons) and XMCD (with H.-J. Elmers).

The tunneling magnetoresistance can be directly related to the spin polarization of the electrodes, if a rough and amorphous barrier is assumed. Within this model the observed magnetoresistance corresponds to ≈ 60% spin polarization of the $Co_2Cr_{0.6}Fe_{0.4}Al$ electrode.

Ni_2MnGa and Mn_2NiGa: Heusler shape memory compounds as thin films

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The ternary intermetallic nickel—manganese—gallium has been known for over a decade as a ferromagnetic shape memory compound. In other words, this material both undergoes a martensitic transition and the magnetocrystalline anisotropy in the low-temperature phase couples the magnetic easy axis to the axis of tetragonal distortion strongly enough that the martensitic variants can be changed by the application of a magnetic field. The theoretically achievable strain between the cubic (high temperature) and orthorhombic or modulated tetragonal (low temperature) phases is around 10%. Depending on the relative orientation of the crystallographic plane between the martensitic variants and the surface of the crystal, the mode of actuation can be lengthening, kink propagation, or bending. In thin film form, released cantilevers of sputtered shape memory material have been shown to exhibit a response similar to that of bulk single crystals.
With a precise control of the deposition conditions, the martensitic transition in off-stoichiometric films can be tailored to be above room temperature. This makes the topographic changes associated with the lowering in symmetry from Fm-3m to I4/mmm available to both optical and atomic force microscopes (AFM), and extensive AFM imaging is therefore undertaken during this effort.

Long-distance magnetic interaction between transition metals und radicals

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Photosynthesis is one of the oldest and most important processes on Earth, transforming light to chemical energy. One step in this process is the oxidation of water to molecular oxygen, which occurs in the “oxygen evolving complex” of photosystem II in green plants and algae. The active site of this protein contains a manganese tetramer, which interacts with a tyrosine radical. The radical is directly involved in electron transport and also feels a weak magnetic interaction as a result of long-distance spin-polarization effects.
Our recent research focuses on the nature of these effects. Therefore we synthesize stable radicals as paramagnetic organic compounds and combine them with transition metal ions. Thus we are building up a new organic-inorganic hybrid material with interesting magnetic properties.

Mössbauer spectroscopy of $Co_{2-x}Fe_{1+x}Si$

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This work reports about the properties of the solid solutions of $Co_{2-x}Fe_{1+x}Si$ Heusler alloys. Generally the X_2YZ Heusler compounds crystallise in the cubic $L2_1$ structure (space group no. 225: Fm-3m). The cubic X_2YZ compounds are not only found with the $AlCu_2Mn$ type structure but also with the $CuHg_2Ti$ type structure. This formal XYXZ-type structure exhibits T_d symmetry (space group no. 216: F-43m). In that structure the two X atoms occupy non equivalent positions in contrast to the $L2_1$structure. This structure is frequently observed if the nuclear charge of the Y element is larger than the one of the X element from the same period, that is Z(Y)>Z(X) for two 3d transition metals. However, the two structures may be hardly distinguishable by X-ray diffraction as both have the general fcc-like symmetry. Therefore, ^{57}Fe Mössbauer spectroscopy was performed to determine the local environment and hyperfine magnetic fields of the iron atoms. Two different hyperfine magnetic fields were clearly detected due to the two different local environments of the Fe atoms in $Co_{2-x}Fe_{1+x}Si$ Heusler alloys crystallising in the $CuHg_2Ti$ type structure.

Interface magnetic properties of Al/Heusler films investigated by XAS and XMCD

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Ni_2MnGa is a shape memory material that shows a magnetically induced length change of up to 10%. This large effect makes it a promising material for applications as actuators and magnetocaloric devives. A precondition for its implementation in nanoscopic devices is the understanding of interface properties of this complex Heusler compound. Previous studies,i. e., have claimed that the martensitic phase transition is suppressed at the surface.

In order to clarify this point, we investigated epitaxial Ni_2MnGa (110) films capped with Al, using X-ray absorption spectroscopy to find pronounced differences in the absorption signals of the surface and the bulk. We measured the total electron yield (TEY) which provides a surface sensitive signal with a typical information depth of about 2-3 nm. Simultaneously, we measured the lumininescence yield from the substrate. This signal integrates along the surface normal of the film and provides bulk-like information.

We find a remarkable change of the Ni X-ray absorption spectra in the bulk occurring at the temperature of the phase transition (T_m) which indicates specific changes of the electronic structure in agreement with theoretical predictions. The main change of the spectra is an emerging satellite peak at 3.8 eV above the L_3 absorption maximum. This peak is suppressed at the surface. Furthermore, the magnetic moments of Ni_2MnGa are strongly reduced at the surface. The differences between surface and bulk properties are caused by a decreased Mn content near the surface according to a quantitative evaluation of X-ray absorption spectra.

In addition Al interdiffuses at the interface from the capping layer into the Heusler compound at elevated deposition temperatures. Photoemission microscopy reveals an inhomogeneous interdiffusion. The interdiffusion could also explain difficulties in the preparation of devices containing half-metallic Heusler films.

Perpendicularly magnetized tunnel junctions with $L1_o$-CoPt epitaxial films

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Tunneling magnetoresistance (TMR) effect in magnetic tunnel junctions (MTJs) is one of the typical phenomena studied in the spintronics research filed. Recent rapid enhancement of TMR ratio gives us a great possibility to develop a high performance spintronics device such as high density magnetic random access memory (MRAM) [1]. A remained critical issue for high density MRAM is reduction of thermal stability caused by miniaturization of the device below a few tens nanometers. In order to achieve enough thermal stability though decreased cell volume, MTJs using high perpendicular magnetic anisotropic ferromagnets (pMTJs) is required. In comparison with MTJs using conventional ferromagnets having the magnetic easy-axis in film plane, pMTJs not only can satisfy the thermal stability requirement but also have no limit of cell aspect ratio. Therefore, to explore the pMTJs is strongly desired.

We report on tunnel magnetoresistance effect in pMTJs with $L1_0$-CoPt epitaxial films. We adopt $L1_0$-CoPt film as ferromagnetic electrodes in the pMTJ because CoPt has very large magnetic anisotropy of 4.9×10^7 erg/cm^3. The pMTJ were prepared on a MgO(001) substrate by using magnetron sputtering. The stacking structure was MgO(001)/Cr(40 nm)/Pt(3 nm)/CoPt(20 nm)/MgO(3 nm)/CoPt(30 nm)/capping layer. The Cr/Pt buffer layer was inserted to improve the surface morphology, crystal structure and the magnetic properties of the bottom CoPt electrode. After optimization of the thickness, annealing temperature and Ar pressure during sputtering of the buffer layers, we obtained well-ordered perpendicularly magnetized CoPt films. The XRD pattern of the film showed sharp (001) and (002) peaks. Calculating from the peak intensity ratio of these peaks with considering the film thickness correction, we obtained the long-range ordering parameter S of >0.8. In order to achieve the different coercive force between the both electrodes in a pMTJ structure, we altered the post-annealing temperature (T_s) and the Ar pressure (P_{Ar}) during the fabrication for each electrode. The conditions were CoPt (T_s= 600°C, P_{Ar}= 0.6 Pa)/MgO/CoPt (T_s= 400°C, P_{Ar}= 1.2 Pa). Eventually, we obtained clear difference of the coercive force in the out-of-plane magnetization curve.

The pMTJ showed the TMR ratio of 6% at RT and 13% at 10 K under the magnetic field normal to the film plane[2]. This result is a remarkable advance for the application of perpendicularly magnetized pMTJ to the next generation high density MRAM.

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Brillouin Light Scattering Investigations of $Co_2MnAl_xSi_{1-x}$ Heusler Thin Films

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Co-based full-Heusler alloys are quite focused compounds to be Half-metallic ferromagnets (HMFs). Among the compounds, Co_2MnSi and related alloys are expected ones because of both theoretical predictions [See Ref. 1] and experimental reports [2]. Thinking of such Heusler system, fundamental magnetic properties like magnetic anisotoropy and exchange stiffness constant are attractive topics as well as exploring half-metallicity of Heusler alloys. Here, we investigated exchange and anisotropic properties of $Co_2MnAl_xSi_{1-x}$ (CMAS) epitaxial thin films by using of Brillouin light scattering (BLS) spectroscopy [3].
On single crystalline MgO (001) substrates, epitaxially grown 40 nm Cr / 30 nm $Co_2MnAl_xSi_{1-x}$ / 2 nm Ta structures, where the values of x are raging 0 - 0.4 and 1.0 were prepared by magnetron sputtering system. All the BLS spectra were measured at room temperature at a transferred wave vector of q// = 1.67 cm-1 using laser light with a wave length of λ = 532 nm. The magnetization vector was oriented parallel to an in-plane easy axis direction of the CMAS samples and perpendicular to the wave vector of the incident light. We confirmed epitaxial (100) growth and B2 ordering of CMAS films which value of x is from 0 to 0.2 and 1.0 by means of x-ray diffraction. Two magnonic peaks originating from the Damon-Eshbach (DE) and perpendicular standing spin-wave (PSSW) modes are visible in the measured BLS spectra. Both peaks shift upon the variation of CMAS film composition, meaning systematical variation of saturation magnetization and exchange stiffness constant.
Obtained values of exchange stiffness constants are 0.56 and 0.44 for Co_2MnSi and Co_2MnAl respectively. Those values agree well those obtained from ab initio calculations. The amplitude of exchange stiffness constants of CMAS films are small compared to the values for conventional 3d transition metals.

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Spinpolarised Electron Spectroscopy Through Tunneling Barriers

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The polarisation of electrons with very low energies tunnelling from a ferromagnet through a barrier is an important information for the design and use of such barriers between two ferromagnetic layers in spin valves or other spintronic devices. Spin polarization measurements require a spectroscopic technique that can discriminate between the spin-up and spin-down electrons near the Fermi energy. One of the well established methods is the spin-resolved photoelectron spectroscopy technique. It permits insight into both electronic ground-state properties and the dynamics of the photoexcitation within a solid. The addition of spin analysis to the photoemission technique allows the investigation of the spin character of electronic bands and the magnetic properties of clean and adsorbate-covered surfaces, thin films, and multilayers.

Heusler compounds exploited by high energy photoemission

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The electronic structure of Heusler compounds - Co_2TiZ, Ni_2MnGa, Co_2MnSi - was exploited by means of hard X-ray photoemission spectroscopy (HAXPES).
The HAXPES experiments have been performed at the beamline BL15XU and Bl47XU of the Japanese electron storage ring SPring-8 with fixed photon energies of 5.946 keV or 7.894 keV, respectively. The overall energy resolution (monochromator plus analyzer) has been set to 250 meV at BL15XU and 150 meV at BL47XU. Additionally, spectra close to the Fermi energy have been taken with a resolution of 150 meV or better. The angle between electron spectrometer and photon propagation is fixed at 90°. For variable

escape depth of the electrons, the sample is rotated in the plane of incidence. Detection angles from near normal emission (θ=2°) to 60° have been used.
Measurements were performed at polycrystalline Co_2TiZ (*Z*=Al, Si, Ge, Sn, and Sb). It turned out that the Sb compound exhibits a remarkable deficiency of Co resulting in $Co_{1+x}TiSb$ with x about 0.4, as extracted from the core level spectra. For the remaining compounds, the valence band spectra exhibit systematic changes if going from Al to Sn. Ni_2MnGa was investigated as single crystal. Changes of the emission from the valence band were observed being caused by the structural phase transition from cubic to tetragonal. Further measurements were performed on so called "half" tunnel junctions that are thin films of Co_2MnSi underneath MgO. Starting from the substrate, the structure of the samples is: MgO(buffer) - Co_2MnSi - MgO(t) - AlO_x with a thickness t of the upper MgO layer of 2 nm and 20nm. The valence band spectra have been used to estimate the mean free path of the electrons through the MgO layer to be 17 nm at kinetic energies of about 6 keV. In particular it is shown that the buried Co_2MnSi films exhibit the same valence density of states as in bulk samples.

1D vs. 3D – Phosphonates as Versatile Ligands in Building Magnetic Extended Systems

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In the field of molecular magnetism, there is much current interest in the slow relaxation in magnetic nanosystems such as single-molecule magnets (SMMs) and single-chain magnets (SCMs). This is because they show unusual physical properties, such as quantum tunneling of the magnetization and quantum phase interference that are not observed in bulk magnets. Just a few examples of single chain magnets are currently known and among them homospin SCMs are extremely rare. One reason is that the one-dimensional chain compounds have to be completely isolated magnetically in the solid-state. This is only possible if the used ligands are really bulky or if there are bulky counterions which separate the chains from each other.
So, very often instead of having a single-chain magnet a three-dimensional ordering occurs. The compound presented here, $[Co(HOOCC_6H_4PO_3H)_2(H_2O)]_n$ is a homospin one-dimensional chain compound that exhibit a magnetic phase transition at $T_N = 3.5K$. An intrachain spin canting is assumed, which leads to a net intrachain magnetic moment that orders antiferromagnetically in three dimensions. Both AC-measurements and a specific heat measurement prove the phase transition at $T_N = 3.5K$.

Ab initio calculations of exchange interactions of ferromagnetic metals and alloys with SPR-KKR

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We have calculated the Heisenberg exchange energies of ferromagnetic metals and Heusler alloys with the SPR-KKR program developed by Ebert *et al*. The itinerant electron system was mapped on an effective Heisenberg Hamiltonian. The exchange energies were obtained directly from the ground state potential using the local force theorem to calculate the total energy changes associated with a local rotation of the magnetisation direction. From the exchange energies various other properties like Curie temperatures and magnon dispersions can be calculated. The Curie temperatures were obtained within the mean field approximation (MFA) and the results show good agreement with the experimental values. Nonstoechiometric alloys can be treated within the coherent potential approximation (CPA). The CPA treatment seems to underestimate the exchange coupling of sites which are partially occupied by an element with a large magnetic moment and one with no magnetic moment and the obtained Curie temperatures a thus too low. The calculated spin wave dispersions are in good agreement with previous calculations using the frozen magnon approach.

Amorphous iron oxide: Magnetism and Structure

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In this poster, it will be shown that amorphous iron oxide can be prepared using a simple photochemical approach capable of lithographic deposition. The magnetic properties of this amorphous iron oxide were studied by SQUID magnetometry, and it will be shown that this material exhibits room-temperature ferromagnetic properties. To the best of our knowledge, this is the first report of room-temperature ferromagnetism in amorphous iron oxide. The composition and local structure of this amorphous material were also studied by x-ray absorption spectroscopy (XANES + EXAFS).

Spin polarization and dynamic properties of $Co_2Cr_xFe_{1-x}Al$ (CCFA) Heusler compounds.

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Half metallic Heusler compounds such as CCFA are promising candidates for spintronics applications due to their predicted minority spin gap at the Fermi energy. This leads e.g. to better TMR device performance as compared to transition metal based structures.
In this contribution we present data obtained by surface sensitive methods such as LEED, Auger and spin polarized photoemission spectroscopy (SPES). The preparation procedure leading to well ordered surfaces is monitored step by step for different substrates and annealing temperatures for CCFA samples with x=0,6. The spin resolved spectra show a characteristic peak in the minority spin density of states, which is shifting depending on the iron content of the sample. This structure vanishes if we use spin- and time-resolved two photon photoemission. Here the spin filter effect of intermediate states above the Fermi energy leads to an increase of the total spin polarization. First time resolved measurements yield spin lifetimes of excited electrons which might be useful in hot electron spintronic devices.

Signal propagation in time-dependent spin transport

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The signal propagation in spin transport is analyzed theoretically by modulating the current passing through magnetic multilayers. We find that time-dependent spin transport possesses a wave character that leads to modifications of pure spin-diffusion. The wave-like characteristics allow us to extract a finite spin signal-propagation velocity. The extension to non-collinear magnetic system is also studied.