phases associated with intriguing solid-solid phase transformations), the atomistics of interfacial structure and growth mechanisms of many precipitate phases remains poorly understood.

Here we present a structural study by aberration-corrected scanning transmission electron microscopy (STEM) of Al-Cu precipitate phases in several model aluminium alloys. These phases, Guinier-Preston (GP) I zones, theta" (Al_3Cu) and theta' (Al_2Cu) phases, are classic crystalline precipitates of the simplest age-hardened alloys [1], [2]. Using a combination of experimental and simulated high-angle annular-dark-field STEM imaging, we demonstrate that these well-known phases in fact exhibit structural features hitherto unreported. Atomic-scale models of interfacial structures are provided. Furthermore, trace additions of Sn are shown to result in precipitate nanoscale thicknesses exhibiting "magic" values. These findings resolve a long-standing mystery [3] and provide new insights into the atomistic mechanisms of precipitate growth in these systems.

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Keywords: aluminium, precipitate interface, TEM.

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A simultaneous multiple angle-wavelength dispersive X-Ray reflectometer

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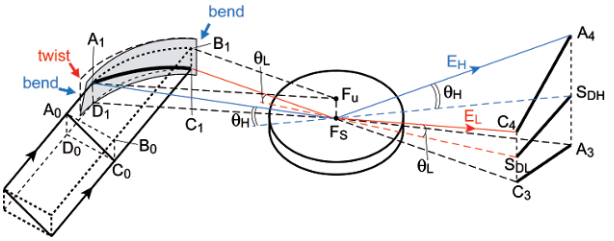
In previous studies[1], [2], [3], we reported a method of measuring specular X-ray reflectivity curves with no need of angle scanning of the sample, detector and monochromator crystal during the measurement. In this method, the reflectivity curve is measured with a position sensitive detector as a function of X-ray energy using a convergent X-ray beam which has a one-to-one correspondence between direction and energy. Because the practically covered energy range was limited, the measured range of the momentum transfer (q=4πsinθ/λ: θ and λ being the glancing angle and wavelength of the X-ray beam) was not wide enough for quantitative analysis.

In the present study, we report improvements of the method for widening the simultaneously covered rang of the momentum transfer by realizing a convergent X-ray beam with which the wavelength (energy) and the glancing angle to the specimen surface of the X-ray beam change continuously at the same time as a function of direction. For realizing such a convergent beam, we used a bent and twisted crystal. An inclined slit is placed upstream of the crystal, so that the foot print of an X-ray beam is along a line from the upper left to lower right corners of the crystal. The crystal is elliptically bent in the horizontal plane and furthermore twisted around the cross line of the crystal surface and the horizontal plane. The beam reflected at the upper left corner is slightly deflected downward, while that at the lower right keep the same vertical direction. Another big improvement is the use of a pixel array detector (PILATUS 100K) instead of an X-ray CCD.

Reflectivity curve profiles from a silicon wafer were simultaneously recorded covering a q range from 0.05 to 0.5 $Å^{-1}$. Measured minimum reflectivities were 1×10^{-8} and 1×10^{-6} with data collection times of 100 s and 1 s, respectively.

We will report results of a performance test experiment and discuss means to further improve the performance of the reflectometer including the time resolution.



Geometry of simultaneous multiple angle-wavelength dispersive X-ray reflectometer

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Key words: X-ray_reflectivity_curve, simultanous_measurement, multiple_angle-wavelength_dispersive

MS21.P08

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Long-range order and interface stability in Co_2FeSi/GaAs hybrid structures

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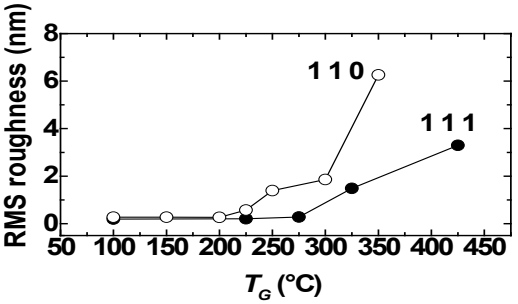
Ferromagnet/semiconductor hybrid structures are well suited for spin injection as a first step towards the design of spintronic devices. The half-metallic and ferromagnetic Heusler alloy Co_2FeSi exhibits a high degree of spin polarization as well as a large Curie temperature of about 1,100 K and is perfectly lattice matched to the semiconductors GaAs and Ge. Spin injection has already been demonstrated. The properties of the ferromagnet/semiconductor interface and long-range order in the Heusler alloy are important for an improvement of the spin injection efficiency. The Co_2FeSi structures on GaAs are grown by solid source molecular beam epitaxy. The long-range order and the interface stability of the structures are investigated by transmission electron microscopy (TEM), x-ray diffraction, atomic force microscopy (AFM) and secondary ion mass spectrometry. At high substrate temperatures T_S during growth, a precipitation process near the Co_2FeSi/GaAs interface is observed, which is connected to an enhanced diffusion of Co, Fe, and Si into GaAs. We use the value of T_S at which precipitation begins as the limit of the interface stability. The critical value of T_S depends on the crystallographic orientation of the interface. For (001) and (110) interfaces, these temperatures are near T_S= 250°C and T_S= 200°C, respectively, whereas for the (111) interface this temperature limit is considerably higher: T_S= 325°C. As a result, the (111) interface is the most stable interface, and an overgrowth of the ferromagnetic film with Ge could be possible for this orientation [1]. The figure demonstrates the surface roughness of the Co_2FeSi film measured by AFM for two orientations of the interface (110 and 111) and several growth temperatures T_G.

For a quantitative characterization of long-range order we determine the average order parameters in Co_2FeSi using x-ray diffracttion and image the lateral inhomogeneities of the compositonal order in the films on the nanometer scale using the dark-field mode of TEM with superlattice reflections. A fundamental reflection is insensitive to long-range order, and the dark-field image of that reflection is usually almost homogeneous. A superlattice reflection images the distribution of long-

range order [2]. Different types of superlattice reflections are sensitive to different types of disorder. The image of the (222) reflection is more homogeneous than the one of the (111) reflection, indicating that the *B*2 order is more widespread compared to $L2_1$ order in the film. In the Co_2FeSi /GaAs system, an almost perfect interface can be prepared. However, the films still exhibit lateral fluctuations of the compositional order, which may be connected to the formation of magnetic domains.



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Keywords: magnetic material, semiconductor, MBE

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The Surface Structure of Nano-Materials: Combining In-situ PDF Analysis and IR Spectroscopy

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Interfaces are important for the functionality of catalysts, sensors and materials for separations and sequestration. Understanding the structure of the interface, at an atomic scale, is key to controlling the functional behavior of these systems. The reactivity of catalysts, for example, can be directly derived from the structure catalytic centers at the surface of the material. Further, functional properties can be strongly dependent on the size and morphology of the particles; the surface structure of nano-particles may vary significantly from the structure of bulk materials.

What is surface structure of a nano-particle? How does it interact with molecular species? These are the questions we aim to answer by simultaneously combining the pair distribution function (PDF) method with infra-red spectroscopy. The structural characterization of nano-particle surfaces and the resulting interfaces they form can be challenging to probe, as the structures can deviate from that of the bulk; coordinately unsaturated metals, and defects are common. The surface structure may also change with the size of particles. The pair distribution function (PDF) method has shown great promise for providing quantitative insight into the structure of nano-materials. Recent advances in experimental methods have improved the sensitivity of X-ray PDF measurements allowing the correlations of molecules bound to nano-particle surfaces to be selectively recovered. We have developed an approach that allows simultaneous measurement of a secondary probe, namely infrared (IR)spectroscopy. IR enables the differentiation between molecular binding sites and brings molecular restrains to the PDF modeling. The structural insights from the combined PDF and IR data allow the surface structure and binding sites on nano-materials to be quantitatively determined.

Keywords: PDF, infra-red, surface

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Hysteresis effects of weak *E* fields on the domain structure in thin $PbTiO_3$ films

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Thin films of $PbTiO_3$ (PTO) of thickness ranging from 2.4 to 41.5 nm deposited by RF magnetron sputtering on $SrTiO_3$ (STO) single crystal (0 0 1) faces have been studied by X-ray scattering to explore the impact of weak electric fields on domain structure. In this thickness range *c*-oriented 180º domains of very high perfection are formed in the PTO film, *i.e.* with the polar *c*-axis aligned in the growth direction. Electric fields of varying magnitude and either direction (up and down) were applied along the polar *c*-axis employing a new sample holder [1]. To a film of thickness 50 unit cells (uc) or 20.7 nm was applied potential differences of magnitude up to 1200 V. This corresponds to a nominal field strength of ~ 100 V/cm over the film, < 0.05% of the estimated coercive field.

Bragg reflections 1 0 3 and 0 0 3 were examined by scans in ù with step length 0.01º using SR of energy 12.763 keV. Images were recorded for steps of 200 V in applied voltage within the range +1200 to -1200 V. Reciprocal space reconstructions show diffuse scattering in the shape of an annular ring or cylinder centred on the Bragg truncation rod (BTR). This is consistent with domain 'stripes' in a nearly random in-plane orientation. Very similar patterns, in some cases developing into square patterns of diffuse intensity reflecting stripes being arranged with increasing perfection along the tetragonal axes *a* and *b*, have been reported by several groups, *e.g.* [2], [3], [4], [5].

In the present study we have found in addition 1) Increasing positive fields (***E*** direction from substrate into film) instigate an increase in the diffuse intensity of the ring with a concomitant decrease in intensity of the BTR. The process reaches a maximum at ~ +1000 V. A reduction in magnitude and subsequent change in polarity of ***E*** initiates a reversal of this process. With increasing negative fields, the annular ring gradually vanishes with a parallel increase in intensity of the BTR. There is a hysteretic relationship between the development of these intensities and changes in ***E***. 2) An offset in *c** between the centres of the annular ring and of the film Bragg reflection relays a contracted *c* for the material that gives rise to the diffuse scattering. A small hysteretic variation in Ä *c** with ***E*** is mainly due to small changes, of the order 0.1%, in *c* for PTO. 3) At the present level of accuracy the domain period Ë that can be retrieved from the diameter of the annular ring seems to be dependent on ***E***, increasing slightly with increasing positive field. These results appear to be novel, not previously discussed in the literature.

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Keywords: synchrotron X-ray scattering, perovskite oxides, thin ferroelectric films

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The pyrite (100) surface structure in dry and aqueous ambient conditions