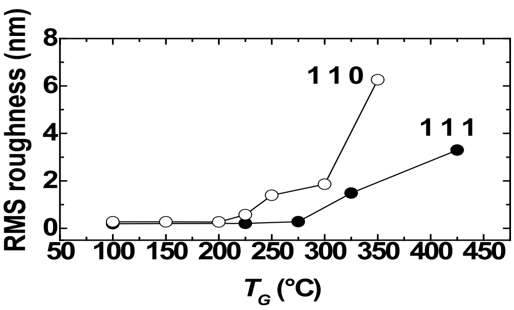
range order [2]. Different types of superlattice reflections are sensitive to different types of disorder. The image of the (222) reflection is more homogeneous than the one of the (111) reflection, indicating that the *B*2 order is more widespread compared to $L2_1$ order in the film. In the Co_2FeSi /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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The pyrite (100) surface structure in dry and aqueous ambient conditions