angle was 0.7 or 0.9 times the critical angle for total reflection. Thus, a depth of 2 and 3 nm, respectively, of the top-layers was probed.

For the bulk microstructure, no long-range order has been experimentally established in Pt-Rh owing to small interactions and sluggish kinetics. Only recently, weak diffuse maxima were found at 1 ½ 0 positions. For the near-surface microstructure, typically 600 positions were measured, with about 500 counts in 200 s. After calibration and subtraction of the inelastic scattering contributions, the remaining elastic scattering was decomposed into short-range order scattering, size-effect scattering, and Huang scattering. Local order was revealed for both surfaces, but there were differences, too. For the (110) surface, the diffuse maxima were located at 1 ½ 0 positions as for the bulk microstructure, for the (111) surface they were at ½ ½ ½ positions. In the evaluation, surface segregation was considered negligible, an assumption that seemed justified in view of the measured and calculated segregation profiles.

Keywords: grazing incidence diffraction, alloys, short-range order

P.12.10.1

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Shape, Polydispersity and Aggregation Number of Alkyl Sulphate Micelles

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Based on the thermodynamic consideration that the micellar cores are compact and consist entirely of portions of the hydrocarbon chains, the length of the latter should limit at least one micellar dimension. Due to the fluctuations in the local electrostatic field, the hydrocarbon chains in ionic micelles with realistic aggregation numbers can fit the above spatial constraints only if the micellar shape is a prolate or oblate ellipsoid.

The recent methods of interpreting experimental data are ambiguous in this respect in that the results they provide may be compatible with each of the above given types of micellar shape. One of the reasons for this is that the scattering pattern from monodisperse spheroids can be fitted e.g. by a set of polydisperse spheres. The present work is devoted to demonstrate that the scattering patterns from alkyl sulphate micelles can be well fitted by assuming either monodisperse prolate- or polydisperse oblate ellipsoidal micelles. Because the two types of micelle have significantly different mean aggregation numbers, the decision on the shape and polydispersity may be based on independent information of the mean aggregation number stemming e.g. from thermodynamic theories.

Keywords: micelles, interfaces, scattering

P.12.11.1

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Evolution of Nanocrystallinity in Periodic Mesoporous Anatase Thin Films

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Within the last few years, many periodic mesostructured forms of titania denoted meso-TiO_2 have been produced based upon the self-assembly method. Besides the usual benefits of the self-assembly method including high surface area and uniform pore size and shape, the crystallinity and crystallite size of the anatase composing the channel walls of meso-TiO_2 are an equally important factor since potential applications rely upon the intrinsic properties of titania governed by the extent and nature of its crystalline phase. Although crystallite growth, during the film calcination step, within the mesostructured titania framework should be considered the critical step in the formation of meso-TiO_2 thin films, the issue of crystallite growth has yet to be identified as a major determining factor with respect to the properties of meso-TiO_2 thin films and their applicability to electroactive and photoactive devices.

Herein we report the first kinetic study of the intrachannel wall phase-transition of amorphous titania to nanocrystalline anatase for periodic mesoporous titania thin films, monitored by time-resolved *in-situ* high temperature X-ray diffraction (HTXRD).[1] Structural transformations associated with the phase transition are further probed by high-resolution scanning electron microscopy (HRSEM) and transmission electron microscopy (HRTEM). The model found to be most consistent with the kinetic data involves 1-D diffusion controlled growth of nanocrystalline anatase within the spatial confines of the channel walls of the mesostructure. The observation of anisotropic, rod-shaped anatase nanocrystals preferentially aligned along the channel axis implies that the framework of the liquid crystal templated mesostructure guides the crystal growth.

[1] Choi S.Y., Mamak M., Speakman S., Chopra N., Ozin G.A., S*mall*, 2005, **1**, 226.

Keywords: crystal growth, *in situ* temperature diffraction, thin-film material

P.12.11.2

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Sol-gel Synthesis and Study of $LaPO_4$ Doped with Cerium(III) and Ytterbium(III) Thin Films

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In this research nanocrystalline thin films of Lanthanium phosphate doped with cerium(III) and ytterbium(III) were prepared.

Lanthanium oxide reacted with hexa hydrated cerium nitrate or ytterbium oxide dissolved in nitric acid and mixed with chelating agent for the metal ions (i.e. water-ethanol solution containing citric acid). The required amount of Poly ethylene glycole (PEG) as cross-linking agent and diamonium hydrogen phosphate were also added using a sol-gel method. The product was then dried on silica glass substrate. Heating on dried films for 5 hours in the temperature range of 800-1000°C results in formation of Lanthanium phosphate doped with cerium(III) and ytterbium(III). X-ray diffraction (XRD) and FT-IR spectroscopy, SEM and Fluorimetrie of doped lantanium phosphates were presented.

[1] Robertson J.M., et al., *Appl. Phys. Lett.*, 1980, **37**, 471. [2] Alemi A.A., Shirazi S., *Iranian J. of Cryst. and Mineralogy*, 1994, **2**, 109. [3] Lin L., Saenger D.U., et al., *Thin Solid Films*, 2000, **360**, 39. [4] Yu M., Lin J., Fu L., Wang S., *J. Mater. Chem.*, 2002, **12**, 86. [5] Meng Q., Lin J., Fu L., Zhang H., *J. Mater. Chem.*, 2001, **11**, 3382. [6]Rao R.P., *Solid State Commun.*, 1996, **99**, 439.

Keywords: sol-gel, lanthanium phosphate, cerium and ytterbium

P.12.11.3

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Pulsed Laser Deposition Growth of thin Hydroxyapatite Layers on Titanium Substrates

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Hydroxyapatite-based ceramics are largely applied as coatings on metallic components of prostheses for inducing osteoblasts apposition and subsequent regrowth. However the ceramics-metal interfaces are often the seat of residual stresses with amplitude primarily depending on the deposition technique and the coating conditions. The amplitude of this stress can be very high causing a failure mechanism at the interface. Our aim is to validate new methods of laser ablation deposition (PLD), making it possible to control the residual stresses in ceramic layers and adherence to titanium substrates. We present a

study of the growth of the layers of Hydroxyapatite obtained by PLD.
Keywords: laser ablation, thin films, hydroxyapatite

P.12.11.4
Acta Cryst. (2005). A**61**, C414
Strain-mediated Phase Coexistence at Phase Transitions in Epitaxial Films
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We show that the first-order structural phase transitions in heteroepitaxial films proceed in a way qualitatively different from the same transitions in bulk crystals. Instead of an abrupt transition with a temperature hysteresis inherent to the first-order transition in bulk crystals, the two phases coexist in the film in a large temperature interval with the fraction of the low-temperature phase linearly increasing on cooling and linearly decreasing on heating. The phase coexistence is explained by the restriction on lateral expansion of the film imposed by the substrate. The coexistence is a result of the balance between the free energy released at the phase transformation and the emerging elastic energy.

We study the MnAs epitaxial films on GaAs(001) and (111) and find the phase coexistence in the temperature interval as large as 20°C. We obtain, in detailed x-ray diffraction studies [1-5], the phase fractions, the domain sizes, and their periodicity in the whole coexistence range. We demonstrate, by comparing the observed domain structure with the energy-minimizing one, that the film is close to the equilibrium. We reveal the periodic surface corrugations due to difference in lattice spacings of the two phases.

[1] Kaganer V.M., et al., *Phys. Rev. Lett.*, 2000, **85**, 341. [2] Kaganer V.M., et al., *Phys. Rev. B*, 2002, **66**, 045305. [3] Plake T., et al., *Appl. Phys. Lett.*, 2002, **80**, 2523. [4] Jenichen B, et al., *Phys. Rev. B*, 2003, **68**, 132301. [5] Jenichen B., et al., *Z. Kristallogr.*, 2004, **219**, 201.
Keywords: phase transitions, phase equilibria, epitaxial layers

P.12.11.5
Acta Cryst. (2005). A**61**, C414
Structural Properties of Ferromagnetic GaMnAs Layers
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Thin layers of ferromagnetic GaMnAs, prepared by MBE under various conditions, were examined by X-ray diffraction and reflection. Preparation of samples was performed by low temperature (LT) growth (200-250°C) using both As_4 and As_2 molecular beams at various As/Ga ratios. Subsequently, samples were annealed in order to optimize their transport properties and to enhance their Curie temperature.

To determine the structural parameters high resolution X-ray diffraction measurements and reciprocal space mapping close to the symmetrical (002), (004) and asymmetrical (224) Bragg reflections as well as specular and diffuse scattering measurements close to the (000) reflection were performed. The combination of different X-ray scattering techniques allows more complete characterization of the samples.

Structural and compositional parameters of the samples (strain, lattice constant, Mn concentration, As nonstoichiometry, defects, inhomogeneity) were evaluated and discussed in relation with their galvanomagnetic properties and preparation conditions.

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Keywords: magnetic semiconductors, high resolution X-ray diffraction, epitaxial thin layers

P.12.11.6
Acta Cryst. (2005). A**61**, C414
Estimation of Lattice Structure of Strained-Si Wafers Using Highly Parallel X-ray Microbeam (I)
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We demonstrate the estimation of lattice structure of commercially available strained-Si wafers by high-resolution X-ray diffractometry using a highly parallel X-ray microbeam [1].
A strained-Si wafer has 3 layers of strained-Si, constant composition of SiGe (CC) and graded composition of SiGe being epitaxially grown on a [001]-oriented Si substrate. The thicknesses of these layers are 17.5 nm, 3.2ìm and 2.4 ìm, respectively.

Diffracted X-rays from extremely thin strained-Si layer could be detected by use of the X-ray microbeam. The intensity distribution maps in reciprocal lattice space show that the lattices in strained-Si, and CC layers are greatly misarranged to the Si substrate. However, the equi-tilt maps, which are intensity distribution measured under fixed rotation angles of the sample and an analyzer crystal, reveal that the lattice tilt variation of these layers is not random but roughly aligned in mainly its crystallographic orientation parallel to one of the two <110> directions. Furthermore, it would be considered that the crystallographic orientation of lattices in the strained-Si layer matches to that of the underlying CC layer.

[1] Matsui J., et al., *proceeding of the 4th international symposium on advanced science and technology of Si Materials*, 2004, 237.
Keywords: silicon technology, synchrotron X-ray diffraction, X-ray microanalysis of thin specimens

P.12.11.7
Acta Cryst. (2005). A**61**, C414
Estimation of Lattice Structure of Strained-Si Wafers Using Highly Parallel X-ray Microbeam (II)
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Strained-Si (s-Si) wafers are expected as the next generation high-speed electronic devices. In order to estimate the crystallinity of s-Si wafers, we developed a high flux X-ray microbeam with a small angular divergence and a narrow energy bandwidth. The X-ray microbeam is formed at SPring-8 by combining the Si single crystals and an X-ray mirror.

We estimated two commercially available s-Si wafers. One is a s-Si/SiGe/Si wafer and the other is a s-Si/SiO2/Si wafer. The thicknesses of s-Si layers of two samples are 17 nm and 15 nm, respectively. The high flux X-ray microbeam enable us to obtain the reciprocal lattice maps of these extremely thin s-Si layers.

The intensity distributions in reciprocal lattice space maps reveal that the lattice parameters of s-Si layers are almost the same as expected values. However, the crystallographic directions normal to s-Si lattice planes greatly distribute about 500 micro radian.

[1] Matsui J., et al., *proceeding of the 4th international symposium on advanced science and technology of Si Materials*, 2004, 237.
Keywords: silicon technology, synchrotron X-ray diffraction, X-ray microanalysis of thin specimens

P.12.11.8
Acta Cryst. (2005). A**61**, C414
Study of Te Diffusion into Structure GaSb-n/GaSb-p on GaSb-n Substrate
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The study of the influence about Te diffusion in structural properties of thin layers GaSb-p with the high resolution X-ray