instead 264. The minimal energy surface was accordingly mapped by changing the values of those none (twelve) factors. Consequently, atoms are allowed to move in particular directions dictated by the symmetry relations between groups.

[1] R. Caputo, A.Tekin, W. Sikora, A. Zuttel, *Chemical Physics Letters* **2009**, *480,* 203-209. [2]. W. Sikora, L. Pytlik, Copyright @ **2010** by Nova Science Publishers, NY in *Group Theory: Classes, Representations and Connections, and Applications.* **2010**, *1*, 1-40.

Keywords: complex borohydrides, symmetry analysis, first-principles crystal structure prediction

MS20.P06

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Local instability above t_c in abo_3 perovskites with discontinuous phase transitions

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One of the direct proofs for local lattice instability above T_C in ferroelectric perovskites ABO_3 is a weak birefringence [1]. Its temperature dependence characterizes local maximum on $\Delta n(T)$ run, with large thermal hysteresis. This is due to a specific co-existence above T_C of the local lattice instability and non-polar matrix. Bussmann-Holder *et al* [2] have theoretically considered temperature range of this co-existence as polar micro/nano-regions. However, such instability has not been verified yet for antiferroelectric phase transition. That is why for model antiferroelectric material lead zirconate $PbZrO_3$, in which transition from the paraelectric to aniferroelectric phase is realized directly or through an intermediate ferroelectric phase, the investigations of the optical, dielectric, electrostrictive properties and local electric conductivity measured in nano-scale by means of LC-AFM method have been carried out. The goal of these experiments was to check if locally breaking symmetry is a common feature for discontinuous phase transitions regardless of whether transition is realized as the transition to a polar (ferroelectric) phase or to a non-polar (antiferroelectric) phase. Similar experiments have been performed for solid solutions based on the antiferroelectric $PbZrO_3$. The temperature range of the pre-transitional local instability has been verified for different phase transformations appearing in these solutions.

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Keyword: perovskites, phase transitions, local breaking symmetry

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A quinquethiophene based self-assembled monolayer for organic electronic applications

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In organic electronics the use of self-assembly is one promising approach to high yield and reproducibility in device fabrication. Thin film transistors have been built from a quinquethiophene self assembled monolayer with a yield of one and accordingly integrated circuits like bit generators could be realized [*E.C.P. Smits et al., "Bottom-up organic integrated circuits", Nature 455, 956-959 (2008)*]. Three elements of the molecule are crucial for the monolayer formation and the electronic properties. First the monofunctional anchoring group which avoids uncontrolled polymerization, second the flexible dodecyl part and third the rod-like quinquethiophene units. The flexible spacer groups allow the semiconducting quinquethiophene units to form two-dimensional crystallographic order. It is the first system reported with a long range ordered self-assembled monolayer formed on silicon oxide. The formation of monolayers has been followed by atomic force microscopy and x-ray reflectivity. The in-plane order of the monolayer has been investigated by grazing incidence in-plane diffraction which reveals three nicely pronounced Bragg rods already in the submonolayer state. Two-dimensional crystals with a rectangular unit cell are deduced with up-right standing molecules which are packed in a herringbone pattern. Several irreversible effects are observed by heat treatment: i) a phase transition where the molecules are tilted 13° towards the b-axis of the unit cell is found after a heat treatment at 400K and ii) a gradual increase of the tilt angle with increasing temperature of heat treatment. In-situ experiments reveal that the expansion of the unit cell is not fully reversible, that the crystallographic order is lost above 520K and that the monolayer remains in an amorphous state until 620K. Above that temperature, desorption of the self-assembled monolayer is clearly detectable by a reduction of the monolayer thickness. No detectable monolayer is present above 880K.

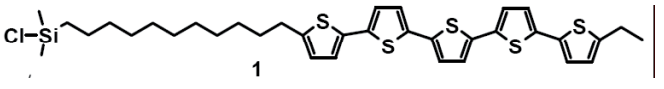

Figure: Chemical structure of the quinquethiophene based molecule used to prepare self-assembled monolayers on silicon oxide surfaces

Keyword: monolayer, organic semiconductor

MS21.P02

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Quick measurement of crystal truncation rod in multi-wavelength dispersive mode

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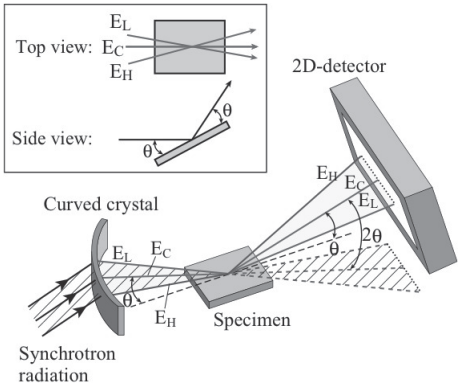
To observe structural dynamic behaviors at surfaces and interfaces, we developed a new method of simultaneously measuring X-ray crystal truncation rod (CTR) scattering profile without mechanical motion of the specimen, detector and X-ray optics during the measurement, using a geometry shown in the figure. A curved crystal polychromator produces a horizontally convergent X-ray beam having a one-to-one correlation between energy and direction. The convergent X-ray beam components of different energies are diffracted within corresponding vertical scattering planes by a specimen placed at the focus. In the specular geometry, although the glancing and exit angles, θ, are the same for all the directions, the momentum transfer continuously varies because the X-ray energy (wavelength) changes as a function of direction. The normalized horizontal intensity distribution behind the specimen represents the CTR scattering profile.

A convergent X-ray beam covering an energy range of 16 to 22 keV was produced by a curved crystal (Si 111 reflection). Scattering intensity was detected by a two-dimensional pixel array detector, PILATUS-100K. For 00L reflection (specular geometry) of a GaAs/AlAs superlattice on GaAs(001) substrate, reflected intensity was simultaneously measured in the range 1.6<L<2.4 around the GaAs 002 Bragg reflection. The CTR profile down to reflectivity of 1×10^{-10} was measured with a sufficient data collection time 1000-7000 s. The CTR profile was well reproduced by that measured by the conventional step-by-step angle scan method with a monochromatic X-ray beam.

Its potential for time-resolved measurement was demonstrated by measuring CTR profile in short data collection time. With an exposure time of 10 ms, CTR profiles down to reflectivity of 1×10^{-7} could be measured. Changes in CTR profile during rotation of the specimen were successfully measured with time resolution of 1.0 and 0.1 s. The present method can be a powerful tool to study irreversible structural changes at surface and interface such as material growth and reactions.



The simultaneous multi-wavelength dispersive diffractometry.

Keywords: surface_x-ray_diffraction, synchrotron_radiation, time_resolved_measurement

MS21.P03

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Ordering of pores in InP (001) subsurface multilayers: formation and structural characterization

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Porous single- and multilayed semiconductors are of significant interest both as an object with advanced physical properties and a material for different applications. Typically these layers with meso- and nanopores are formed by anodization technique. Etching under passing of electrical charge produces the confused morphology of pores and architecture of porous multilayers. The structural characterization of porous layers is a main task.

In the present study we show an application of high-resolution X-ray diffraction and scanning electron microscopy methods for determination of structural parameters and space configuration of pores. The porous structures (≈6mkm) with single- or four bilayers were formed by anodic oxidation of n-type InP(001) substrates in aqueous HCl solution. The structural parameters of the sublayers were varied by changing the electrochemical etching mode (potentiostatic/galvanostatic). The X-ray diffraction experiment was performed on the E2 Station of Hasylab with radiation energy of 10 keV. To collect data one dimensional MYTHEN detector was used. The reciprocal space intensity maps (RSM) near the InP 004 reflection were obtained at different azimuth angle (φ=0,90) (Fig). The map's features demonstrate two completely different types of pores in InP oriented particularly along <111>B and <001> directions. To extraction features of pore a model for scattering from such systems is proposed based on the statistical dynamical diffraction theory. Theoretical scattering maps have been fitted to the experimental ones. It is shown that a mathematical analysis of the scattering intensity maps makes it possible to determine the structural parameters of sublayers. The reconstructed parameters (thickness, strain, porosity of sublayers and the shape and space arrangement of pores) are in satisfactory agreement with the scanning electron microscopy data.

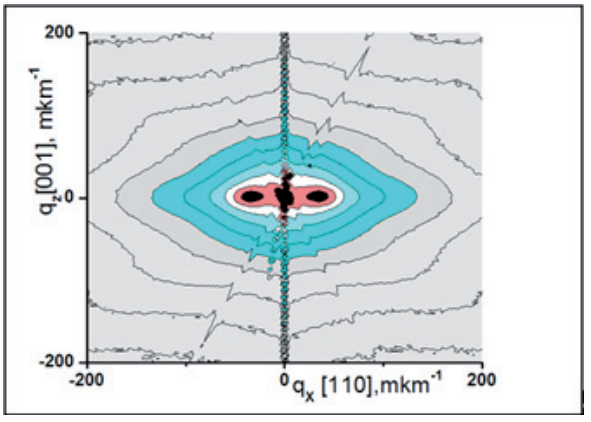

Figure. X-ray RSM from InP porous multilayers obtained in the vicinity of 004 reflection at φ=0. Two black sports demonstrate presence in the structure a middle ordering with correlation length 170nm.

Keywords: characterization, porous, multilayer

MS21.P04

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GISAXS study of interfaces in high-performance La/B_4C multilayer mirrors

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