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

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Strain-mediated Phase Coexistence at Phase Transitions in Epitaxial Films
Vladimir M. Kaganer, Bernd Jenichen, Wolfgang Braun, Lutz Däweritz, Klaus H. Ploog, *Paul-Drude-Institut für Festkörper-elektronik, Berlin, Germany*. E-mail: kaganer@pdi-berlin.de

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

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Structural Properties of Ferromagnetic GaMnAs Layers
Zbynek Šourek, O. Pacherová, M. Cukr, V. Novák, J. Kub, *Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic*. E-mail: sourek@fzu.cz

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

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Acta Cryst. (2005). A**61**, C414
Estimation of Lattice Structure of Strained-Si Wafers Using Highly Parallel X-ray Microbeam (I)
Kazunori Fukuda[a], N. Tomita[a], K. Hayashi[a], Y. Tsusaka[a], Y. Kagoshima[a], J. Matsui[a], A. Ogura[b], [a]*Graduate School of Material Science, University of Hyogo. Hyogo, Japan.* [b]*School of Science and Technology, Meiji University. Kanagawa, Japan.* E-mail: K_fukuda@sci.u-hyogo.ac.jp

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)
Yoshiyuki Tsusaka[a], K. Fukuda[a], N. Tomita[a], K. Hayashi[a], Y. Kagoshima[a], J. Matsui[a], A. Ogura[b], [a]*Graduate School of Material Science, University of Hyogo., Hyogo, Japan.* [b]*School of Science and Technology, Meiji University., Kanagawa, Japan.* E-mail: tsusaka@sci.u-hyogo.ac.jp

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
Enrique Rosendo[a], R.Vargas-Sanabria[b], J. Martínez[a], T. Díaz[a], H. Juárez[a], F. De Anda[c], M. A. Vidal[c], [a]*CIDS-ICUAP 14 Sur y San Claudio, Col San Manuel, Puebla, México C. P. 72570.* [b]*Facultad de Ciencias UAEMex. Instituto Literario 100 Centro, Toluca, México C. P. 50000.* [c]*IICO-UASLP. Ave. Karakorum 1470, Lomas Cuarta Sección, SLP, México. C. p. 78210.* E-mail: erosendo@siu.buap.mx

The study of the influence about Te diffusion in structural properties of thin layers GaSb-p with the high resolution X-ray

diffraction technique, having like Te source a layer type-n is presented in this work. The samples were grown with structure GaSb-n/GaSb-p on GaSb-n substrate by LPE technique. The diffusion process was done through heat treatment to different temperatures and times. The results obtained with X-ray diffraction are in agreement with the photoluminescence measurement.

Keywords: diffusion, high resolution X-ray diffraction, LPE

P.12.11.9

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Density and Mobility of Carriers in AlGaSb and InGaAsSb Alloys Obtained by LPE

Hector Juárez[a], E. Rosendo[a], R. Romano[a], T. Díaz[a], G. García[a], J. Martínez[a], M. Rubin[b], H. Navarro[c], [a]*CIDS-ICUAP, BUAP.* [b]*Facultad de Ciencias de la Computación, BUAP, 14 Sur y San Claudio, Col. San Manuel, Puebla, México. C. p. 72570.* [c]*IICO-UASLP. Ave. Karakorum 1470, Lomas Cuarta Sección SLP, México. C. p. 78210.* E-mail: cs001062@siu.buap.mx

The density of carriers and its mobility of AlGaSb and InGaAsSb alloys have been obtained by simulation. The Berreman technique was used in this work, which allows simulating the spectra of reflectivity in the far-infrared region. Liquid Phase Epitaxy (LPE) technique was used to growth several AlGaSb thin layers in the range of temperatures of 250 to 450 °C. The reflectivity spectra in the far infrared region show to bands, the first one near to 230 cm^{-1} which corresponds to TO and LO GaSb-like modes and other one near to 318 cm^{-1} which corresponds to TO AlSb-like mode and it confirms the presence of the ternary alloy. In the quaternary alloy case, the temperature of growth was 410 °CThe reflectivity spectra show the TO and LO modes in the region of 180 to 250 cm^{-1} and correspond to the binary combinations of the four present elements.

Keywords: liquid phase epitaxy, reflectivity spectra, ternary alloy

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XRD Study of Strongly Textured and Stressed Thin Films

Radomír Kužel[b], Daniel Šimek[a], [a]*Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic.* [b]*Faculty of Mathematics and Physics, Charles University, Praha, Czech Republic.* E-mail: kuzel@karlov.mff.cuni.cz

Determination of the residual stress in highly oriented thin films can be rather difficult. Since only certain grain orientations are present, conventional X-ray methods of stress evaluation cannot be applied. In some cases, the problem can be solved by the so-called crystallite group method [e.g. 1]. However, for investigation of microstructure the scan of significant part of reciprocal space is necessary. The method of reciprocal space mapping and Rietveld-type refinement of the maps was developed and tested on strongly textured TiB_2 coatings deposited on steel substrates. The maps were measured with modified conventional two-axis goniometer in parallel beam arrangement and some measurements were also performed with Eulerian cradle and polycapillary. The method is particularly useful for simultaneous analysis of stress and texture especially in non-cubic materials. It could also be used for the estimation of other parameters like film thickness, microstrain and domain size. Both the extreme elastic models (Voigt/Reuss) have been adopted for the case of fibre texture, often present in thin films. Residual stress could be estimated even for the strongest 001-texture with angular halfwidth of a few degrees. In the maps, the presence of stress is indicated by the inclination of elliptical spots. Expected increase of the residual compressive stress with substrate bias was observed and analyzed.

[1] Kužel R. Jr., Černý R., Valvoda V., Blomberg M., Merisalo M., *Thin Solid Films*, 1994, **247**, 64-78.

Keywords: powder diffraction, reciprocal space mapping, thin films

P.12.11.11

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Residual Stress in Tungsten Thin Films for Photon Counting Applications

Davor Balzar[a,b], L. M. Kaatz[a], A. Lita[b], D. Rosenberg[b], S. Nam[b], A. J. Miller[b], R. E. Schwall[b], [a]*Department of Physics and Astronomy, University of Denver, Colorado, U.S.A.* [b]*National Institute of Standards and Technology, Boulder, Colorado, U.S.A.* E-mail: balzar@du.edu

We report on tungsten thin films used for superconducting transition-edge-sensors (TES) that are capable of accurately counting the number of photons, which can be exploited in astronomical and quantum-information applications.

The superconducting transition temperature (*Tc*) of tungsten films was found to strongly depend on the deposition conditions and the existence of an underlayer or coating. For instance, a film with *Tc* of about 100 mK is under tensile stress when grown on bare Si wafers, whereas another film with *Tc* of 200 mK is under compressive stress when grown on in-situ sputtered amorphous Si. Furthermore, coating tungsten films with SiO_2 suppressed *Tc* below 60 mK. Sputtered tungsten thin films usually contain two crystallographic phases: α-W (bcc) with *Tc* of 15 mK, and β-W (A15) with *Tc* between 1 to 4 K. Thus, *Tc* might be influenced by both phase composition and stress associated with the deposition and neighboring layers.

We used laboratory and synchrotron (APS high-energy 6-ID-MU beamline) X-ray diffraction to assess both the phase composition and residual stress state in tungsten films at room and low (8 K) temperatures. Results indicate no significant changes in phase composition in this temperature range. Residual stress at room temperature did not strongly vary among the films, indicating that the changes in *Tc* are likely due to additional thermal stress induced by cooling to cryogenic temperatures.

Keywords: residual stress, thin films, tungsten

P.12.11.12

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Ordered SAMS of Peptide Nucleic Acids on Surfaces with DNA Recognition Capability

José A. Martín-Gago[a,b],Carlos Briones[a], Eva Mateo-Martí[b], [a]*Centro de Astrobiología. INTA. Torrejón de Ardoz. 28850 Madrid.* [b]*Instituto de Ciencia de Materiales de Madrid. Cantoblanco, 28049-Madrid, Spain*. E-mail: gago@icmm.csic.es

Self-organisation of molecules have inspired new trends in nanotechnology based on a bottom-up approach. Self-assembled monolayers (SAMs) of alkanethiols were widely studied due to their relevant technological properties. Based on such knowledge, thiolated DNA has been immobilised on surfaces, although it forms disordered formless globular structures with reduced bioactivity.

We report on the formation and structural characterization of ordered SAMs of peptide nucleic acid (PNA) on mono- and polycrystalline gold surfaces. PNA is an achiral and uncharged DNA mimic of high biochemical stability which allows different applications in biotechnology. We show that, in spite of their length of up to 7 nm, cysteine-modified single-stranded (ss) PNA oligomers assemble by themselves standing-up on gold surfaces similarly to the SAMs of short alkanethiols. They stabilize on the surface by chain-chain interaction trough non-complementary H-bonding. BioSAMs of ssPNAs maintain their capability for recognizing ssDNA, and discriminate even a point mutation in target ssDNA. These structural and functional results have been obtained using label-free techniques for surface characterization such as synchrotron radiation based X-ray photoemission spectroscopy, X-ray absorption near-edge spectroscopy, atomic force microscopy and infra red spectroscopy.

Keywords: self-assembled monolayers, peptide nucleic acids, biosensors