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such that icosahedral nano-clusters occur in fcc crystal. At the same time, the transformation of a cuboctahedron to a regular icosahedron induces strong distortion fields in the crystal. Using the diffraction data, we could establish that such fields are able to cause the x-ray interbranch resonance [2], observed as the fine structure effect. Assuming elastic distortions, we calculate the resonance splitting of rocking curve, which equals to inverse length of the x-ray interbranch extinction and is in line with the experimental results.

The approach presented in the work can be also useful for high-energy electrons. As was reported [3], the similar fine structure of Bragg's peak appears in the case of electron diffraction with strained nano-clusters.

[1] Chmelevskaya V.S., et. al., *Russian Surface*, 1998, **N6**, 95. [2] Shevchenko M.B., *Acta Cryst*., 2003, **A59**, 481. [3] Reinhard D., et. al., *Phys. Rev. B*, 1997, **55**, 7868.
Keywords: X-rays, dynamical diffraction, nano-cluster

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Application of Particular X-ray Standing Wave for Accurate Determination of Electron Density

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Study of electron density in crystals is of great interest for understanding a host of their useful properties. We present the new approach for simulation of atomic electron density. The particular standing waves previously predicted for low energy electrons [1], are applied for it. It should be noted, atomic size effects influence position of the nodes of these waves such that the nodes coincide with the atomic planes in the case of 's' scattering. Moreover, formation of such waves leads to minima of intensity of the non-specular reflex. This dynamical effect is similar to multi-beam ones, which happens in the cases of x-ray and high energy electron diffraction [2,3].

In this work, we propose the special scheme for four-beam x-ray Bragg's diffraction, which provides for excitation of the particular standing wavefields. Assuming spherically symmetric model of atomic electron density, it is shown that the sharp changes of intensity of reflected asymmetrically wave, are caused by small varying radius of electron shell. Thus, the particular x-ray standing waves are helpful tool for accurate determination of atomic electron density, whereas the ordinary x-ray standing states are effective for precious determination of interplanar spacing. The particular standing wave effect can be also used to study multilayers and superlattices. In doing so, it is possible to obtain the detailed information about their chemical composition by registering the x-ray diffracted intensity only.

[1] Shevchenko M.B., *NATO ARW 4-8.08.2002, Kyiv, Ukraine. Abstracts*, 59. [2] Chang S., *Multiple Diffraction of X-rays in Crystals.*, Springer-Verlag, 1984. [3] Matsuhata H., Gjonnes J., *Acta Cryst*., 1994, **A50**, 107.
Keywords: electron density, X-rays, dynamical diffraction

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Some Features of X-ray Diffraction in Monocrystals in Presence of the Temperature Gradient

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At defined external parameters of the influences (temperature gradient (TG), acoustic vibrations) and for reflecting atomic planes(10 $\bar{1}$1) of the quartz, the X-ray complete pumping process occurs from transmission to the diffraction direction [1]. In work [2] it is also shown that the change of the crystal-medium heat exchange the complete pumping conditions is varying.

For prove the obtained experimental results, the heat conductivity equation with boundary conditions of the experiment was solved. The obtained temperature field in the crystal gives picture about distortion field inside the crystal. Afterward the Takagi equations were solved for given distortion field. It is obtained that with TG growth the intensity of the diffracted reflected radiation is increasing up to the saturation (intensity of the diffracted transmitted radiation decreased until zero). With the further TG growth the intensity is decreasing and the rocking curve is continuing monotonically expand. From the theoretical analysis obtained that in case increase of the crystal-medium heat transfer the corresponding TG which is satisfying to the X-ray complete pumping condition is decreases. The obtained theoretical results are in good agreement with the experimental results.

[1] Mkrtchyan A.R., Navasardyan M.A., Mirzoyan V.K., *Pisma w ZhTF*, 1982, **8**, 677. [2] Kocharyan V.R., Movsisyan A.E., *"X-Ray Optics-2004"*, Annual Workshop, N.Novgorod, 2-6 May 2004.
Keywords: dynamical X-ray diffraction theory, heat transfer, crystal lattice distortion

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Parametric Down Conversion of X-rays under the Dynamical Diffraction Condition

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Parametric down conversion[1] is known as phenomena that an X-ray photon is converted into two photons satisfying the conservation laws of energy and momentum. The refractive index of materials for X-rays is isotropic and has a simple dependence on the wavelength. Thus the reciprocal lattice vector is inevitable to satisfy those conservation laws, that is, the phase matching condition. Hitherto most works are done under the kinematical diffraction condition, and the coincidence technique is used to detect those two photons emitted in different directions[2].

In this work parametric down conversion of X-rays is studied under the dynamical diffraction of a perfect crystal to satisfy the phase matching condition. The process that a photon with an energy of 20.6 keV is converted into two photons with almost the same energies of 10.3 keV is observed under the asymmetric diffraction condition of Ge 800 reflection. One of paired photons is detected by a combination of a channel-cut crystal analyzer and a solid-state detector, and photons with a half of incident energy are observed only when the phase matching conditions are satisfied.

[1] Eisenberger P., McCall S.L., *Phys. Rev. Lett*., 1971, **26** , 684. [2] Yoda Y.,et al., *J. Synchrotron Rad.*, 1998, **5**, 81.
Keywords: parametric down conversion, X-ray dynamical diffraction, non-linear phenomena

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Dynamics from Diffraction

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A model-independent approach for the extraction of detailed lattice dynamical information from neutron powder diffraction data is described. The technique is based on a statistical analysis of atomistic configurations generated using reverse Monte Carlo structural refinement.

Phonon dispersion curves extracted in this way are shown to reproduce many of the important features found in those determined independently using neutron triple-axis spectroscopy. The extent to which diffraction data are sensitive to lattice dynamics is explored in a range of materials.

The prospect that such detailed dynamical information might be accessible using comparatively facile experiments such as neutron powder diffraction is incredibly valuable when studying systems for which established spectroscopic methods are prohibitive or inappropriate.

[1] Goodwin A.L., et al., *Phys. Rev. Lett*., 2004, **93**, 075502. [2] Goodwin A.L., et al., *Phys. Rev. B*, *manuscript submitted.*

Keywords: dynamical properties, diffraction theory, reverse Monte Carlo

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Space Shift between Relaxed Si and Strain-compensated SiGeC Epitaxial Layers

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Investigation method based on the high-resolution and non-destructive Grazing-Angle Incidence X-ray Backdiffraction (GIXB) technique [1, 2] is extremely sensitive for the measurements of the longitudinal space phase shifts stipulated by the misfit dislocations in interface planes of the epitaxial layers. Diffracting net planes of the epitaxial layers considered in presented theoretical paper have the same lattice constant, though there exist a longitudinal space shift between space periods of these layers. Carbon introduction into the SiGe films suppresses outdiffusion of boron, by which the parasitic barriers would be created, so the performance features of HBTs with SiGeC base layer practically do not change after the high temperature processing. Reflectivity coefficient of specular vacuum X-ray wave field is investigated depending on the values of the phase shift between space periods of the layers of Si/SiGeC heterostructure and of the Bragg angle in the case of GIXB technique.

[1] Bezirganyan H.P., Bezirganyan P.H., *Phys. Stat. Sol. (a)*, 1988, **105**, 345. [2] Bezirganyan H.P., *Phys. Stat. Sol. (a)*, 1988, **109**, 101.

Keywords: epitaxial semiconductor layers, grazing incidence x-ray diffraction, x-ray backscatter diffraction

P.15.11.2

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Crystal Relief Investigation under the X-ray Diffraction on Surface Acoustic Wave in Bragg-Laue Grazing Geometry

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The intensity of X-ray radiation diffracted from a monocrystal in Bragg-Laue grazing geometry when the reflecting planes slightly differ from surface normal, allows to carry out the topographical observation of crystalline defects in near-surface superfine layers [1]. In the case of crystal surface modulation by acoustic wave the sensitivity of the method may become much better. In the ordinary Bragg geometry Rayleigh surface acoustic waves (SAW) can focus the incident X-ray wave [2]. In the case of the standing SAW there is no need of a stroboscopic technique of synchronization.

In the present paper the influence of crystal relief on focused image forming under the diffraction of X-ray radiation in Bragg-Laue grazing geometry is studied. The analysis of the intensity distribution in the diffracted wave averaged by time for the standing SAW shows that in the nearest zone of diffraction a focusing from the SAW concave parts occurs. It is shown that separate regions of the crystal relief which are characterized by local sizes and curvature radius, essentially change the registered image in local part of the topogram. The sensitivity of he method is about nanometer. At the same time the focal image of SAW serves as a scale reference point for the crystal relief characteristics determination.

[1] Aleksandrov P.A., Afanasiev A.M., Stepanov S.A.. *Phys. Stat. Sol.(a)*, 1984, **86**, 143. [2] Cerva H., Graeff W., *Phys. Stat. Sol. (a)*, 1984, **82**, 35.

Keywords: X-ray glancing-angle scattering, crystal surfaces, ultrasonics

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X-ray Diffraction Image under the Grazing Angles of Incidence on a Surface Acoustic Wave

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The X-ray diffraction in noncomplanar symmetric Laue geometry under the total external reflection is characterized by the formation of both the specularly reflected and specular reflected diffracted waves [1]. The character of the intensity distribution of these beams depends on the value of the grazing angle of incidence which in the case of crystal surface modulation by surface acoustic wave (SAW) will locally change.

In the present paper the process of diffraction of X-ray radiation on the planes perpendicular to the crystal surface modulated by Rayleigh SAW under the total external reflection has been studied. The character of the diffracted image essentially depends on the crystal-detector distance. In the nearest diffraction zone a focusing from the SAW concave parts occurs, which may be observed for the standing SAW, but in the case of the running SAW a synchronization technique is needed. With the increase of the crystal-detector distance the focused beams are covered and observed on the same pedestal. In the farthest diffraction zone diffraction satellites are formed both for the standing and for the running SAW. The dependence of the focal distance from the amplitude and length of SAW, the grazing angle of observation, the deviations from Bragg orientation, etc. are found. It is shown that the change of the crystal surface curvature may be controlled both by the focusing in the nearest diffraction zone and by the process of formation of diffraction satellites and their focusing.

[1] Afanas'ev A.M., Melkonyan M.K., *Acta.Cryst.*, 1983, **A39**, 207.

Keywords: X-ray glancing-angle scattering, ultrasonics, crystal diffraction

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New Method of Solid State Structural and Composition Analysis

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In the present paper, in contradistinction to Debye, Laue and Fudji grammas, new gramma based on the phenomena of parametric X-ray radiation (PXR) of the relativistic charge particle in single crystals is offered. On the analogue of X-Ray Laue gramma due to X-Ray "white" beam diffraction on crystalline lattice, the relativistic charge particle interacting with crystalline lattice originated grammas of PXR, consisting of variety of dynamic yields with specific angular and energy distributions. Actually it is an analogue of X-ray "white" beam diffraction with a slite difference, that in the case of PXR the X-ray radiation sources are disposed in crystal along the trajectory of relativistic charged particle passage.

Several experimental investigations of the PXR phenomena of electrons with energies 855MeV [1] and 20MeV [2] in quartz and niobate lithium single crystals were conducted. Appropriate grammas for observed targets-radiators were obtained.

Hereby, on the basis of obtained results new simple and express method to analyze solids composition and structure with accuracy not worse then by existing methods is offered.

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Keywords: crystallography, analysis, methods