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.

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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.

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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.

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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.

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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.

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