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The detailed simulations of forbidden reflections induced near the absorption edges by atomic motion are presented. The existence of such reflections, first predicted theoretically [1,2], is now well documented for Ge [3,4] and ZnO [5], see a detailed survey [6]. The reflections of this type can be also exited owing to the thermally independent dipole-quadrupole contribution [7]. The role of the temperature is to generate atomic displacements from the equilibrium sites and hence to provide the anisotropic terms of the tensorial atomic factor and to the structure factor. The numerical simulations were performed with the help of FDMNES, PARATEC and XKDQ codes, which allowed fitting the results both for Ge and for ZnO.

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Keywords: X-ray anisotropy, atomic factor, forbidden reflections

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MATHEMATICA Software for Anisotropic Resonant Scattering

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Forbidden reflections induced by atomic factor anisotropy appear in diffraction patterns of non-symmorphic crystals when the photon energy is tuned to an absorption edge resonance [1]. In order to simulate the properties of such reflections, the program package has been developed using Wolfram Research MATHEMATICA (version 4.0 and over). The package is now applicable for the crystals of cubic and hexagonal groups and it allows us to calculate the tensorial structure factor, hence the reflection intensity and polarization properties. Dipole-dipole, dipole-quadrupole and quadrupole-quadrupole contributions are included.

With this package the intensity azimuthal dependence was calculated for the 113 reflection in ZnO with wurtzite structure. This reflection forbidden by space group $P6_3mc$ was observed in [2]. The calculation results have shown to be in good accordance with synchrotron diffraction data.

The work was supported by INTAS grant 01-0822.

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Keywords: forbidden reflections, X-ray anisotropy, crystallographic software

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Universal X-ray Ellipsometer and X-ray Depolarizer

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We have developed an universal X-ray ellipsometer which consists of an X-ray polarizer, aberration-free multiple phase retarders[1] and an analyzer. It enables us to create an X-ray beam having a high degree (P > 0.98) of linear, circular or other polarization state in X-ray region. It also enables us to analyze precisely the polarization states of the beam transmitted or diffracted by the specimen. The available X-ray energy range is 6-18 keV. With this X-ray ellipsometer, we have successfully measured polarization-dependent DAFS (diffraction anomalous fine structure) spectra of an antiferromagnetic CoO single crystal at the cobalt K-absorption edge. The 111 reflection includes scattering from atoms having both up- and down-spin, while the 511 reflection includes scattering from atoms having either up- or down-spin. The difference in DAFS spectra for right- and left- circular polarization was observed in the 511 reflection (~5%), but not in the 111 reflection.

In addition, we propose an idea to generate non-polarized X-rays from polarized synchrotron X-ray radiation by using a transmission-type X-ray phase retarder as a depolarizer. The X-ray depolarizer is useful for experiments such as MAD where a specific polarization state is a nuisance for data analysis. The principle and performance of the depolarizer will be reported.

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Keywords: polarization optical technique, DAFS, MAD

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An Alternative Formation Theory of Beat Applied to the Pendelloesung Beat[1]

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An alternative theory of beat, in which a variation of the intensity of a composite wave is formed from definite distinct waves of which more than two have different frequencies is constructed. It is applied to Pendelloesung beat (hereafter, abbreviated as PB) as an apt example. PB has been observed only in some light elements (below atomic number 32) by using rather hard X-rays up to 60keV and above the room temperatures. These observations for the formation of PB support the view that the recoil energy loss plays essentially important role in beat production by the superposition of the photons with the reduction of the momentum.

The Bragg law for the reduction of the momentum is derived based upon the corpuscular character of the light and the principle of the equipartition of the recoil energy over all the atoms. The application of the Bragg law, to the superposition of the expected value of the even or odd time multi-reflex photons (taken by the binomial distribution as stochastic events) forms the two types of the transmitted or diffracted PB, respectively. The law predicts two types of the prominently positive projecting peaks at half wave at even times of π and the plus or minus projecting peaks at odd times of π, according to the multiplicity factor of the reflection, exist as pulsations of bare PB from AM by cosec $\Delta\omega t$ in the basic bare envelope curve. It turns out that the AM effect of the binomial distribution on bare PB makes all of the peaks contracted as if it is erased, and makes the intense collimated photon flux follow the Borrmann effect. This review can be confirmed by testing the prediction that the reflection intensity of PB fades into quantum PB near 0K by a reduction of the recoil reflections due to the enhancement of the crystal rigidity with decreasing temperature.

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Keywords: recoil diffraction, modified Bragg law, binomial distribution

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Fine Structure of Bragg's Peak as Dynamical Effect Specifying Nano-Clusters

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As is well known, x-ray and electron diffraction is commonly used to investigate the morphology of nano-clusters. It should be noted, one could increase diagnostic capabilities of these techniques by studying the fine features of diffraction phenomena. In this connection, we refer to effect resulting in the splitting of the x-ray Bragg's peak related to fcc lattice [1]. This happens after the plastic deformation of the lattice,

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

P.15.08.4

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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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