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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.

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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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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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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,