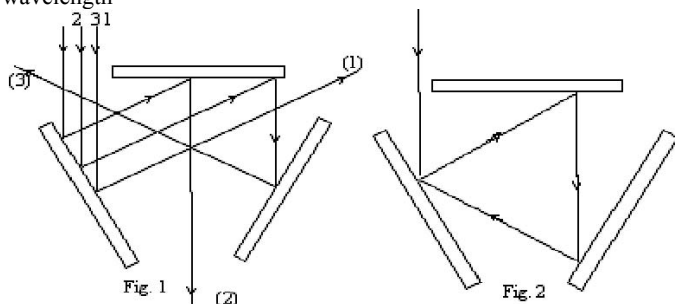


P.15.04.4*Acta Cryst.* (2005). **A61**, C432**A Three-block X-ray Monolite Resonator**

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An X-Ray Resonator for Silicon single crystal (440, 404) configuration's $\text{NiK}\alpha_2$ -radiation is offered and principally carried out. Asymmetric reflections (where reflecting planes consist 30° angle with block planes) were used. In contrast to [1], the incident beam enters the resonator and undergoes a closed cycle only through Bragg's reflections. The device was moving by a scanning mechanism perpendicular to the incident beam, and it made possible to take out of the resonator the beams reflected 1,2,3...times and detect them (Fig. 1). It is obvious that there exists a position in which the beam stays in the resonator, providing a closed cycle (Fig. 2). The device will give its best results in the case of synchrotron radiation, for in this case it is possible to choose a precise wavelength



[1] Deslattes R.D., *Appl. Phys. Letters*, 1968, **12**, 133.

Keywords: X-ray resonator, diffraction, monochromator

P.15.06.1*Acta Cryst.* (2005). **A61**, C432**ATS Scattering from Isomorphous and Polymorphic Crystals**

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The ATS scattering [1] is X-ray resonant scattering caused by the anisotropic terms of susceptibility. It can be observed in forbidden reflections near the absorption edge. It reveals the nature of empty electron-states of the atoms/ions in a crystal. We observed the scattering from pyrite structure, (FeS_2 , NiS_2 , CoS_2), spinel structure (Fe_3O_4 , ZnFe_2O_4 , NiFe_2O_4), corundum structure (Fe_2O_3 , Cr_2O_3), and polymorphic crystals of TiO_2 , rutil, anatase and brookite [2-5]. From experiments, we obtain following results. The scattering observed above the edges is caused by the dipole transition. The peaks in the pre-edge are caused by transitions through higher order terms. In the pyrite type, the energy spectra above the edges are similar to each other in spite of different ions. There are no peaks above the edges in a corundum type because the dipole transition is forbidden by the symmetry. In the pre-edge, hematite has a resonant peak, however eskolaite has a peak with a shoulder. The peaks show three (hematite) and six-fold (eskolaite) azimuthal dependence. They are explained by the quadrupole-dipole and the quadrupole transition. The ATS scattering in polymorphic crystals of TiO_2 shows their own properties determined by the site symmetry of them. The energy spectra are different from each other though the absorption curves are similar.

[1] Dmitrienko V.E., *Acta Cryst.*, 1983, **A39**, 29. [2] Nagano T., et al., *J. Phys. Soc. Jpn.*, 1996, **65**, 3060. [3] Hagiwara V., et al., *J. Phys. Soc. Jpn.*, 1999, **68**, 1592. [4] Kokubun J., et al., *J. Phys. Soc. Jpn.*, 1998, **67**, 3114. [5] Kanazawa M., et al., *J. Phys. Soc. Jpn.*, 2002, **71**, 1765.

Keywords: X-ray resonant scattering, forbidden reflection, quadrupole transition

P.15.06.2*Acta Cryst.* (2005). **A61**, C432**Anisotropic Resonant X-ray Scattering from Antiferromagnet Hematite, Fe_2O_3**

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Hematite has a corundum structure with antiferromagnetic moments perpendicular to rhombohedral [111] at room temperature. At the Morin temperature ($T_M = 250$ K) their directions change parallel. Anisotropic resonant scattering from hematite was first observed by Finkelstein et al.[1] We have investigated more detailed property of the resonant *forbidden* reflections 111 and 333.[2]

The experiment was carried out near the Fe K-absorption edge with synchrotron radiation source. We measured the energy spectra of the 111 and 333 forbidden reflections intensities. Both spectra show one peak in the pre-edge region and small non-resonant intensity. The azimuthal angle dependence of the forbidden reflections measured at the non-resonant energy shows twofold pattern, which can be explained by non-resonant magnetic scattering. At the resonant energy, however, the azimuth dependence of the 111 reflection shows threefold symmetry. This character is interpreted as a result of interference between electric dipole-quadrupole and quadrupole-quadrupole transition effect. The azimuth dependence of the 333 reflection at the resonant energy scarcely shows threefold symmetry in spite of manifest threefold pattern below the T_M . We conclude that the resonant 333 reflection is affected by resonant magnetic scattering.

[1] Finkelstein K.D., Shen Q., Shastri S., *Phys. Rev. Lett.*, 1992, **69**, 1612. [2] Kokubun J., Ishida K., *Photon Factory Act. Rep.*, 2002, **20A**, 21.

Keywords: X-ray resonant scattering, X-ray magnetic scattering, antiferromagnetism

P.15.06.3*Acta Cryst.* (2005). **A61**, C432**Near-Edge Forbidden Reflections in Resonant Diffraction by Modulated Crystals**

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High sensitivity of the atomic tensor factor near absorption edges to the displacements of both resonant and neighbouring atoms can provide additional reflections in resonant X-ray diffraction by incommensurately modulated crystals. In the presence of modulation the local symmetry of each resonant atom becomes lower than in the basic structure, hence additional tensor elements can appear. In this report, some calculations of the structure factors are presented for the Co-åkermanite taking into account what already known [1] about its two-dimensional modulation. Co atoms, in the corresponding basic structure, are in the (2a) sites with $\bar{4}m$ symmetry of the $P\bar{4}2_1m$ space group, which make it impossible to obtain any forbidden reflections near Co *K*-edge in the dipole-dipole approximation. However, the main reflections $h00$, $h=2n+1$ corresponding to the basic structure can appear near Co *K*-edge owing to the dipole-quadrupole contribution. We showed that the displacement terms in the anisotropic tensor factor could mainly contribute to the first order satellites, providing the forbidden reflections satellites near the Co *K*-edge with $hhl m0$, $m=2n+1$ or $h00 m$, $h=2n+1$.

This work was partly supported by INTAS grant 01-0822.

[1] Hagiya K., Kusaka K., Masaaki O., Iishi K., *Acta Cryst.*, 2001, **B57**, 271.

Keywords: X-ray anisotropy, incommensurate crystals, satellites

P.15.06.4*Acta Cryst.* (2005). **A61**, C432-C433**Thermal-motion-induced Forbidden Resonant Scattering: Experiment vs Theory**

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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 excited 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. This work was partly supported by INTAS grant 01-0822.

[1] Dmitrienko V.E., Ovchinnikova E.N., Ishida K., *JETP Letters*, 1999, **48**, 938. [2] Dmitrienko V.E., Ovchinnikova E.N., *Acta Cryst.*, 2000, **56**, 340. [3] Kokubun J., et al., *Phys. Rev. B*, 2001, **64**, 073203. [4] Kirfel A., et al., *Phys. Rev. B*, 2002, **66**, 165202. [5] Collins S.P., et al., *Phys. Rev. B*, 2003, **68**, 064110. [6] Dmitrienko V.E., Ovchinnikova E.N., *Cryst. Repts.*, 2000, **48**, S59. [7] Templeton D.H., Templeton L.K., *Phys. Rev. B*, 1994, **49**, 14850.

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

P.15.06.5

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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-symorphic 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.

[1] Dmitrienko V.E., Ovchinnikova E.N., *Cryst. Rep.*, 2000, **48**, S59. [2] Collins S.P., Laundry D., Dmitrienko V.E., Mannix D., Thompson P., *Phys. Rev. B*, 2003, **68**, 064110.

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

P.15.07.1

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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.

[1] Okitsu K., Ueji Y., Sato K., Amemiya Y., *Acta Cryst.*, 2002, **A58**, 146.

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.

[1] Nakajima T., *J. Low Temp. Phys.*, 2005, **138**, to be published.

Keywords: recoil diffraction, modified Bragg law, binomial distribution

P.15.08.2

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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,