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**Abstracts**

reflector. The transmission-type x-ray linear polarizer is well suited for spectroscopic measurements with polarized x-rays. Future applications of this polarization filter are presented.

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**M12.OE.006 X-RAY DIFFRACTION IN FINITE PERFECT CRYSTALS.** G. Thorkildsen, Department of Mathematics and Natural Science, Stavanger College, Ullandhaug, 4004 Stavanger, Norway.

The boundary-value Green function technique has been used along with the Takagi-Taupin equations [1] to investigate diffraction phenomena in finite perfect crystals subject to an incoming plane wave. This includes extinction, absorption and rocking curve calculations [2]. Starting from Maxwell's equations in a periodic dielectric medium, the differences and similarities between the present approach and the fundamental theory of dynamical scattering [3] are discussed. The geometrical region structures associated with point sources [4], the surface integrations necessary to calculate diffracted power and the concept of extended volumes [5] are explored. The displacement fields are handled either by series expansions or in the case of straight line boundaries by analytical functions provided by Uragami [6]. Anomalous scattering is included using a complex expansion parameter. Scattering planes with circular, rectangular and triangular shapes are studied. Examples of numerical results are related to silicon and germanium.

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**P12.OE.001 THE STANDING WAVE FORMED BY GRAZING-INCIDENCE X-RAYS IN A MULTILAYER WITH PLANES NORMAL TO SURFACE.** P.A. Bezirganyan (Jr.), Dep. of Computer Science, State Engineering University of Armenia, #6, Korjune St., Yerevan 375009, Armenia, and A.P. Bezirganyan and S.E. Bezirganyan, Dep. of Physics, Yerevan State University, #1, A. Manoogian St., Yerevan 375025, Armenia, and H.A. Bezirganyan (Jr.), Dep. of Informatics and Applied Mathematics, Yerevan State University, #1, A. Manoogian St., Yerevan 375025, Armenia.

X-ray standing waves (XSW) in multilayers have been observed (see the pioneer papers [1-3]) by fluorescence measurements similar to those using natural crystals. In the grazing angle incidence x-ray diffraction (GID) geometry the XSW technique uses the dynamical x-ray standing wave fields formed very close to sample entrance surface by the lattice planes perpendicular or nearly perpendicular to this surface. Above the sample surface the entire wave field intensity is periodical and is modulated along this surface (e.g. see [4]).

We consider X-ray GID by a periodical multilayer with layers' interface planes normal to vacuum-multilayer entrance surface, and assume that two types of amorphous layers have enough optical contrast to give a strong diffraction. The XSW technique in the GID case makes it possible to study atomic arrangement (correlation) and interfaces of multilayers very close to entrance surface. The mathematical model corresponding to the investigated amorphous multilayer is constructed. The description

of the standing wave formation is based on the method of construction of eigenvalues and eigenfunctions for this model.

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**P12.OE.002 OPTICAL COMPONENTS FOR POLARIZATION ANALYSIS OF SOFT X-RAY RADIATION.** H. Grimmer, M. Horisberger, S. Tixier, O. Zaharko, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, H.-Ch. Mertins and F. Schäfers, BESSY, D-14195 Berlin, Germany.

An instrument for measuring polarization typically consists of a phase shifter and a linear polarizer. Up to 600 eV, periodic structures can be used consisting of alternating layers of two materials, one of which has an absorption edge in the photon energy region of interest [1]. The phase shift of the transmitted beam and the intensity of the reflected beam show maxima at energies just below the edge. By means of DC magnetron sputtering, phase shifters have been deposited on 100 nm thick Si<sub>3</sub>N<sub>4</sub> films and linear polarizers on Si wafers. The latter were designed to work at the Brewster angle, where only s-polarized radiation is reflected. The corresponding multilayer period decreases from 8.5 nm at 100 eV to 1.4 nm at 600 eV. A reflectance of 6.8% was obtained at 512 eV for 150(V/Ni). It was shown that an Al coating reduces the oxidation of Ti/Ni multilayers.

In order to extend polarization measurements into the 1 keV region, the use of magnetic effects like magnetic circular dichroism (MCD) is being explored. This effect has been measured in 100(Fe/C) transmission multilayers close to the Fe L edge (700-750 eV). It is expected to be largest if the magnetic moments are aligned ferromagnetically and parallel or antiparallel to the beam direction, i.e. perpendicular to the layer surface. This can be realized at room temperature in periodic multilayers with 1 nm thick FeCoV layers separated by nonmagnetic layers, as shown for FeCoV/Ce by Moessbauer spectroscopy [2]. Presently, thin films of transition metal/rare earth metal alloys are being produced and investigated, in which perpendicular spin orientation at room temperature is also expected.

1. H.-Ch. Mertins et al., *Synchrotron Radiation News* **11** (1998) 42-46.
2. S. Tixier et al., *Physica B* **234-236** (1997) 473-474.

**P12.OE.003 RAY-TRACING STUDY OF A PARALLEL-BEAM TWO-AXIS DIFFRACTOMETER FOR POWDER AND THIN-FILM DIFFRACTION.** H. Toraya, H. Hibino and T. Ohnishi, Ceramics Research Laboratory, Nagoya Institute of Technology, Tajimi 507-0071, Japan

A two-axis diffractometer was built for versatile uses in powder and thin-film diffraction in x-ray laboratory. Its design is based on a parallel-beam optics using flat-specimen reflection geometry and capillary-specimen transmission geometry. The diffractometer consists of two rotary tables (Huber 410 and 420) for the  $\theta$  and  $2\theta$  axes and an encoder (Heidenhein, ROD 800) for reading the  $2\theta$  angle. Optical elements on the incident beam side were a parabolic multi-layer mirror, channel-cut crystal monochromators and slit systems. Horizontal parallel-slits or a flat analyzer crystal can be equipped on a detector arm together with a scintillation counter with a maximum count rate of 3M cps (Rigaku, SC300). These elements can be selectively combined in order to fit with experimental purposes, requiring narrow and strictly monochromatic beam or less parallel beam but with more flux. Ray-tracing was first conducted for analyzing the performance of each optical component. Its results were further

## 18. ELECTRON DIFFRACTION

**P05.18.001 KIKUCHI ELECTRON DOUBLE DIFFRACTION.** R.K. Karakhanyan and S.E. Bezirganyan, Department of Physics, Yerevan State University, #1, A. Manoogian St., Yerevan 375025, Armenia.

The purpose of the present work is to extend the phenomenon of the Electron Double Diffraction (EDD) to include the Kikuchi patterns. Kikuchi EDD means that once and twice diffracted electron beams as well as the primary electron beam can become sources of Kikuchi patterns, i.e. these diffracted beams are exposed to inelastic scattering process, which takes place for the primary electron beam [1]. The resulting Kikuchi pattern is a superposition of the primary pattern with the source in the incident beam and of secondary patterns with sources in once and twice diffracted beams. The single crystalline silicon films were used as specimens for investigations. Silicon Kikuchi transmission patterns were obtained when the incident beam is approximately parallel to [112], [110], [210], [310] and [111] axes.

Formation of forbidden and unindexed Kikuchi lines, enhancement of excess forbidden Kikuchi lines near spot reflexes with the same indices, mutual reversal contrast of excess and defect Kikuchi lines under passing of excess line near strong spot reflex with other indices, enhancement of excess line near spot reflex with other indices under passing of correspondent defect line near strong spot reflex are the direct consequence of Kikuchi EDD. It is shown [2,3], that under decrease of diffracted beams' intensity by means of crystal thickness, temperature, orientation variation and electron energy change all above mentioned manifestations of Kikuchi EDD grow weak, which confirms correctness of mechanism of their appearance proposed in present work.

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**P05.18.002 SIMULATION OF DIFFUSE SCATTERING FROM SHORT-RANGE-ORDERED  $\text{Cu}_3\text{Au}$  TYPE FACE-CENTRED CUBIC STRUCTURE.** X. J. Jiang, J. K. Bording and J. Taftø, Centre for Materials Science/Department of Physics, University of Oslo, Gaustadalleen 21, N-0371 Oslo, Norway.

It is well known that in some binary alloys, such as  $\text{Cu}_3\text{Au}$ , small domains of the ordered structure are present, separated by antiphase domain boundaries. The antiphase domains give rise to characteristic short-range-order diffuse scattering in the diffraction patterns. Several antiphase configurations and corresponding diffuse scattering have been proposed in the literature [1,2].

We have performed computer simulation using  $\text{Cu}_3\text{Au}$  as an example. In a wider perspective we intend to approach the more complex system Al-Zn-Mg that exhibits similar diffuse scattering. The atomic arrangement and resulting short-range-order scattering of  $\text{Cu}_3\text{Au}$  were simulated for different cooling rates. Special attention was focused on the antiphase domain boundary types and the accompanying diffuse scattering. The results of the simulation are in good agreement with the experimental observations of split spots presented in the literature.

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**P05.18.003 STRUCTURE DETERMINATION OF METAL-RICH COMPOUNDS FROM SELECTED AREA ELECTRON DIFFRACTION.** Th. E. Weirich, Mat. Science, Darmstadt Univ. of Technology, 64287 Darmstadt, Germany, X.D. Zou, S. Hovmöller, Structural Chemistry, Stockholm Univ., 10691 Stockholm, Sweden, A. Simon, Max-Planck-Inst. f. Festkörperforschung, 70506 Stuttgart, Germany, G. Cascarano, C. Giacobozzo, CNR-IRMEC Dip. Geomineralogico, Campus Univ. Via Orabona 4, 70125 Bari, Italy

Electron diffraction (ED) is due to the strong interaction of electrons with matter an excellent tool for studying the interior structure of small crystalline samples down to few nanometers in size. On the other hand the strong interaction gives rise to dynamical diffraction (multiple scattering) effects which often leads to diffracted intensities far away from the predicted by the kinematic theory. Although ED without any dynamical contribution can hardly be realised in practice, it is possible to find experimental conditions under which the dynamical effects can be kept at a low level. Such data can be treated in the first approximation as pseudo-kinematic, i.e. traditional strategies for solving crystal structures are expected to work. Here we show that quantified ED patterns can be used for solving crystal structures of non-light element compounds to high accuracy. Several known metal-rich structures  $\text{M}_x\text{X}_y$  ( $\text{M} = \text{Ti, Zr}; \text{X} = \text{S, Se}; x > y$ ) were investigated in a 300 kV Philips CM30ST microscope. Selected area ED patterns were recorded from prominent zone axis - in this series always along a short 3.5 Å crystal axis - and processed by ELD [1] for extracting integrated intensities. These 2D data sets were fed into SIR97 [2] modified with electron scattering factors and the most probable E-maps were calculated. The trial structures proposed by SIR97 revealed in all cases the complete structures. The projected atom positions agreed on average within 0.2 Å with those from the X-ray determination on single crystals. The obtained results show that dynamical effects can be controlled in a standard ED experiment so that direct methods can be applied for solving crystal structures in a quasi-automatic manner.

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- [2] SIR97: <http://www.ba.cnr.it/IRMEC/SirWare.html>

**P05.18.004 NEW METHOD OF ANALYSING ELECTRON DIFFRACTION DATA.** U. Wilke and W. Mader Institut für Anorganische Chemie der Universität Bonn, Römerstrasse 164, 53117 Bonn, Germany

Structure determination of small and defected crystals is the domain of electron diffraction. We present an application of a microdiffraction technique to inorganic crystal structure refinement. Our method is based on the program package ELSTRU by Jansen *et al.* [1]. We use convergent beam diffraction patterns taken with a spot size of  $\approx 8$  nm. Intensities for various beam directions are given by the corresponding position within the diffraction discs. This allows to obtain up to nine data sets for one specimen thickness. The discs obtained should not overlap because the background intensity around each diffraction disc needs to be subtracted which is performed by extrapolation. The intensities serve as input data for the program package ELSTRU. The method was tested on simulated [2] and on experimental diffraction patterns of corundum ( $\alpha\text{-Al}_2\text{O}_3$ ). The results calculated from different data sets of diffraction pattern (simulated as well as experimental) reproduced the same thickness and the known structural parameters. The different data sets corresponding to different directions of the incident beam yield shifts of the centers of Laue circles as expected. Experimental intensities are recorded on a 2kx2k CCD camera (Gatan Megascan) attached to a Philips CM300 UT FEG electron microscope.