Other

PS15.07.01 GEOMETRY OF SINGLE CRYSTAL-PLANE SCATTERING IN DYNAMICAL THEORY OF X-RAY DIFFRACTION. D.S. de Vasconcelos, W.A. Keller and Marek Urbanski, Instituto de Fisica, Universidade Federal da Bahia, Salvador, Brazil

X-ray diffraction from a crystal plane with zero thickness (two-dimensional problem) filled up by scattering electrical charge which can be treated as either a continuous or discrete distribution, has been calculated in analytical and numerical ways, respectively. The crystal plane scattering was regarded as due to radiation from classical dipoles activated in one case, only by the external electrical field, and in the second case, by the external field plus field due to other dipoles in the plane, determined self-consistently. In the first solution we consider the situation of a single plane wave, incident at the θ glancing angle, as the source of a field forcing the dipole oscillations. In the second, self-consistent solution, we also include fields of neighbouring radiating dipoles. It is then possible to show by using either analytical or numerical methods that the combined dipole radiation takes the form of two plane waves leaving symmetrically the crystal plane at θ angles which give rise to reflected and forward scattered waves. The resultant dipole waves calculated for the first mode of activation (external field only) have a phase shift equal to $+\pi/2$ in relation to the incident wave, a result which is known to violate conservation of energy. It is shown here that, the two methods of calculation (analytical and numerical) agree on the shift, they desagree on the minimum distance xP at which the resultant dipole waves are formed as plane waves. The analytical evaluation requires only xP>0, while the numerical one gives an approximate value xP=0.5-1.0λ, for distance between dipoles which are encountered in common diffraction experiments. In the self-consistent mode, once again the analytical and numerical methods yield the same values as above. More importantly, in this mode, which considers cooperative effects between scatterers, energy is conserved. The calculated phase shift is shown to be greater than $\pi/2$ by exactly the amount necessary to conserve energy.

PS15.07.02 THE EFFECT OF PENDELLÖSUNG OSCILLATIONS ON THREE-BEAM DIFFRACTION PROFILES. K. Hümmer and E. Weckert, Institut für Kristallographie, Universität Karlsruhe (TH), Kaiserstr. 12, D-76128 Karlsruhe, Germany

Three-beam diffraction provides a means of physical determination of triplet phases by interference of simultaneously excited waves inside a crystal. Recently triplet-phase determination of small protein crystals became feasible. Usually crystals of arbitrary shape with grown faces are used. Therefore, the diffracted beams will be simultaneously in Bragg as well as in Laue diffraction geometry. In the Bragg reflection case the interference profiles do not significantly depend on the thickness of the crystal. Theoretical calculations using plane wave dynamical theory taking into account the divergence and wavelength spread of the incident beam and experiments done at a high brilliance synchrotron source (ESRF, France) correlate nearly quantitatively. In the Laue transmission case, however, theoretical plane-wave calculations predict that interference effects will be affected by Pendellösung oscillations if crystal thickness exceeds the first maximum of the Pendellösung. Experiments performed with 'perfect' plate-shaped crystals of benzil at different wavelength confirm this theoretical predictions. However, the dependence of the interference effects on the thickness of the crystal is weaker than predicted theoretically. Two reasons may be considered for this behaviour: a. The divergence of about 2 arcsec used for the experiment is large compared to the extremely narrow dynamical reflection width of organic crystals and therefore the assumption of plane waves is a rough approximation. b. Small imperfection do already hinder the formation of Pendellösung interferences. Therefore, one can be sure, that in practice three-beam diffraction can be unambiguously exploited for triplet phase determination even of macromolecular structures.

PS15.07.03 THE STUDY OF THE BRILLOUIN ZONES BY MEANS OF THE KIKUCHI PATTERNS. R.K.Karakhanyan, P.L.Aleksanyan, S.E.Bezirganyan, Dep. of Solid State Physics, Faculty of Physics, Yerevan State University, No.1, A. Manoogian St., 375049 Yerevan-49, Armenia. Fax: +374-2-151087, gayane@arminco.com

In the present work on the basis of the correspondence of the Brillouin zones' boundaries to the Kikuchi lines [1,2] Brillouin zones of electronic states in crystal of silicon are investigated. It is shown, that the energy gap on the Brillouin zones' boundaries with the forbidden indices for structure of silicon is connected with the valent double diffraction on the crystalline planes, and these boundaries correspond to the forbidden Kikuchi lines [3]. It is found, that three-beams dynamical interactions transform the crossing of the boundaries of the bidimensional Brillouin zones into two branches of hiperbola, as well as the Kikuchi lines [4]. The obtained results are in acordance with the known data of theory of solids, concerning Brillouin zones [5]. The single crystalline silicon films were prepared by chemical etching, and the Kikuchi patterns were obtained at the accelerating voltage of 100 kV.

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PS15.07.04 ABSORPTION IN THE MODEL OF SELF-CONSISTENT X-RAY SCATTERING. W. A. Keller, D. S. de Vasconcelos, Instituto de Física, Universidade Federal da Bahia, Salvador, Brazil

Absorption is approached as a local and statistical event in contrast with a background of the global and strictly determined pattern of x- ray crystal scattering. While particular and detailed physical mechanism of the absorption phenomenon is here considered irrelevant, the main concern is given to the overall effects of absorption on the earlier developed self-consistent model of x-ray scattering. The above model substitutes a single dipole, used originally in Ewald's papers as the scattering unit, by the plane of dipoles, but at the same time taking advantage of the self-consistency principle as determining the scattering mode. The following points, diverging with the previous work, are: i) Absorption takes place exclusively at the electron sites arranged in a set of dipole planes. ii) The flux of photons incident in each dipole plane is divided into two branches. The first one, as suffering unknown a priori frequency changes, is considered redundant for the model. The second branch is that of the unchanged wavelength. It is scattered under exact satisfaction of the Ewald self-consistency principle and gives rise to the overall scattering pattern of a crystal. This principle, for a non-absorbing case, can guarantee that energy is conserved for each dipole plane separately and for the model as a whole. iii) Absorption is considered as a localized occurrence, with probability factor which can be proportional to the first or higher powers of intensity of the resulting stationary and local field. iv) The latter is calculated separately for both polarization states,

which for an non-absorbing crystal are quite independent of each other. The absorption is thus a unique link which interlaces these two states in the absorption effect. v) Absorption and refraction in this model of scattering are two distinct phenomena, which means that there is no necessity to introduce a complex index of refraction for absorbing crystals. The calculated absorption profiles reproduce the experimental results without the necessity of the corrections usually made by means of additional and arbitrary parameters.

PS15.07.05 ADVANTAGES OF X-RAY REFLECTOMETRY EXPERIMENTS USING GÖBEL MIRRORS. P.J. LaPuma, Siemens Analytical Instruments, Madison, WI

X-ray reflectometry is a very useful tool for characterizing thin films deposited on substrates. It provides highly accurate and nondestructive characterization of thin films and layer packages in the thickness range between 1 and 300nm. However, the sample properties determine the amount of information that can be obtained from the sample. High surface roughness and coatings with large electron densities will cause relevant information to become obscured soon after the total reflection plateau due to absorption and diffuse scatter. The only way to obtain information from these types of samples was to increase the measurement time in order to obtain better counting statistics, or make the measurement at a synchrotron light source. With Göbel Mirrors these measurements are now possible in the laboratory. Göbel Mirrors provide a higher flux and a parallel beam that is ideal for these measurements. Bragg peaks from repeating multilayers as well as oscillations from rough samples can now be seen at high angles.

PS15.07.06 CONTROL OF X-RAY DIFFRACTED AND X-RAY FLUORESCENCE BEAMS (TRANSMISSION OF SPEECH). Navasardian M.A., Gabrielian R. Ts., Mkrtchian V.P.; Physics Department of Yerevan State University, Al. Manoukian 1, Yerevan 375049, Armenia

The double modulation of X-ray beam for the purpose of transmission of signals [1] was a new step in X-ray diffraction studies. In investigations that followed two important results were obtained: under temperature gradient a pumping of primary beam energy into the direction of reflection [2] was observed, and a transmission (reception) of information, in particular of speech was realized by the Laue-diffracted beams [3].

In the present work the double modulation of X-rays at different values of wavelengths of X-rays, at different powers of X-ray tubes, and at different thickness of crystalline plate ($0.15 \leq \mu t \leq 10$) as well as the modulation of X-ray fluorescent radiation for different atoms has been investigated.

The following results were obtained:

1. At double modulation both by anomalous transmitting beams (Ga(220), $\mu t \geq 10$) and by diffracted beam in the direction of incidence (at $\mu t \leq 1$), the transmission of vocal signals (speech) is impossible. This is due to the fact that the intensity I of these beams decrease as the amplitude of electrical (acoustic) oscillations U applied to the modulator are increased. That is, I(U) is a decreasing function, while for proper operation of transmission systems I(U) should be an increasing function.

2. The double modulation of beams from low power sources (8W) will permit to use X-ray tubes without the cooling of anode.

3. Using the modulated X-ray beam we have obtained low-frequency (speech) echo from deep energy levels of the atom. At the excitation by Mo Kα radiation 30 atoms with different **Z** were used, the energies of K or L absorption edges were less than the energy of photons of Kα line of Molybdenum.

4. It will be submitted the improved scheme of the equipment for the transmission and reception of information by double modulated X-rays.

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