11.8–1 X-RAY AND NEUTRON SCATTERING BY QUASI-ONE-DIMENSIONAL AND QUASI-TWO-DIMENSIONAL REAL CRYSTALS AND INHOMOGENEOUS ALLOYS. By M.A.Krivoglaz, Institute of Metal Physics, Academy of Sciences of the Ukrainian SSR, Vernadsky 36, Kiev-142, USSR.

It is shown, that in order to determine static displacements around the defects in strongly anisotropic quasi-one-dimensional or quasi-two-dimensional crystals the generalized elasticity theory which takes into account the spatial dispersion and the discreteness of the lattice is needed. These effects manifest at middle distances which exceed considerably the interatomic distances and result in the unusual laws of decrease of the displacements with a distance (Krivoglaz, Zhurnal experimental'noi i teoreticheskoi fiziki (1981) 81, 277; Sov. Phys. JETP (1981) 54, 148).

As a consequence, the characteristic peculiarities of diffuse X-rays and neutron scattering by bounded defects in these crystals, for example, the new power-law dependences of the scattering intensity on the distances from reciprocal lattice points and anomalously pronounced angular dependences of intensity distributions must occur. The transformations of these distributions with the increase of the distortions near defects and their concentration are investigated, in particular, the establishment of power-law intensity dependence with a fractional exponent in the case of quasi-two-dimensional crystals and a formation of the bell-shaped quasi-Bragg-peak in the case of the quasi-one-dimensional or highly distorted quasi-two-dimensional crystals. The experimental data concerning the scattering by irradiated in a reactor graphite are explained by the developed theory (Krivoglaz, Fizika tverdogo tela (1981), 23, 2720; (1982) 24, 808).

It is shown, that there are physical factors leading to the formation of termodynamically equilibrium heterogeneous states in the alloys. They have the quantum nature, are connected with nonlocal long-range interaction due to the conductivity electrons and may be formed in the systems, in which the superstructure vectors of the reciprocal lattice are close to the diameters of the flattened parts of the Fermi surface. If ordering occurs as a phase transition of the first order the state is strongly modulated with respect to the amplitude of the order parameter and consists of the ordered regions in a disordered matrix. In the framework of a simple model the theory of such states is developed. The scattering by the heterogeneous structures is considered. The theory allows to describe the diffraction and electron microscopic data on inhomogeneous local order in some substitutional alloys and in the systems where omega-phases are formed (Krivoglaz, Zhurnal experimental'noi i teoreticheskoi fiziki (1983) 84, 355; Metallofizika (1984) 6, 3).

11.8–2 USING KATO'S THEORY OF SECONDARY EXTINCTION. By F.R. Thornley, Department of Applied Physics, University of Strathclyde, 107 Rottenrow, Glasgow, U.K.

Kato's theory has recently been extended to spherical crystals (Kawamura and Kato, Acta Cryst. (1983). A39, 305). The analytic approximation given for the extinction factor y is complicated, involving some 40 numerical coefficients. However, it has been found that, for non-absorbing crystals, a good fit to this was obtained with the simpler approximation of the familiar Becker and Coppens theory - i.e.

$$y = \left[1 + \frac{3X}{\sqrt{2}} + \frac{A(\Theta)X^2}{1+B(\Theta)X}\right]^{-1/2} \qquad (1)$$

where X is proportional to Kato's parameter $\beta = 2\tau_2(\sin\Theta/\lambda)QR$ for a sphere of radius R, τ_2 is the correlation length of the lattice phase factor, and $A(\Theta)$, $B(\Theta)$ are polynomials which represent the angular dependence. A match to the linear dependence for small β, $y = 1-4\beta/3$, is obtained by taking $X = 8/\sqrt{2}\ \beta/9$. Expressions found by least squares for the polynomials are $A(\Theta) = 1.317 + 0.625\cos 2\Theta$, $B(\Theta) = -0.027\cos 2\Theta$, for $0 < \Theta < 30°$; typical rms deviations between Kato's expression and (1) are 0.001 over the given range of $0 < \beta < 2$, corresponding to $1 \geq y \geq 0.23$.

The question of the relation of τ_2 to the defect structure of the crystal - e.g. τ_2 = constant for 'Type II' extinction - is a separate one, to be tested by trials of the universal function (1). The restriction to non-absorbing crystals is not a limitation, because Kato's expression separates into a product of absorption and extinction factors. The results of new analyses of existing data sets will be reported.

11.8–3 MEASUREMENT OF CRYSTAL STRUCTURE FACTORS BY DECOUPLING MULTIPLE DIFFRACTION REFLEXIONS. By Lisandro P. Cardoso and S.Caticha Ellis, Instituto de Física - UNICAMP - C.P.6165, 13100, Campinas, SP, BRAZIL.

In the intensity of an n-beam multiple diffraction (M-D) reflexion, n^2 structure factors are actually involved: those of the n RELP's simultaneously located on the Ewald sphere, plus the n(n-1) related to the vectors connecting any two of these RELP's. These structure factors can be recovered by means of a set of n^2 algebraic simultaneous equations (S.Caticha-Ellis,(1969), Acta Cryst.A25, 666). Usually, when trying to produce multiple reflexions by using Renninger's geometry (M. Renninger,(1937),Z.Phys.106,141) the experimenters choose rotation axes coinciding with a symmetry axis for the sake of experimental facility. This procedure leads inevitably to many beam cases, 8, 16 or even more so that the calculation becomes rather complicated and moreover several structure factors depend on the measurements of the intensity of a single M-D peak. By careful measurement of comparatively few M-D peaks one could get a rather high number of structure factors, so that the method can be envisage as experimentally feasible in the routine collection of data for determining crystal structures. It is to be noted that in this way obviously several independent measurements are obtained for each structure factor, so that the method carry in itself a measurement of its internal consistency. A small disadvantage is that the measurements are to be performed on a plate cut perpendicularly to the rotation axis; the experimental technique to do this has been

developed by Campos, Cardoso and Caticha-Ellis (1983), J. Appl. Cryst. 16, 360.
It must be noticed that the F's obtained by this method are automatically corrected for absorption, L.P. and extinction.
A further improvement which facilitates the calculation by decreasing n, consist in using as a rotation axis a crystallographic direction which does not coincide with any symmetry axis and corresponds to a forbidden reflexion. The effect is striking: 4 or higher order beam interactions are decoupled in 3-beam cases thus simplifying the calculations; secondary equivalent reflexions (which would lead to Bijvoet pairs in anomalous dispersion are clearly distinguished without the use of specially chosen wavelengths. "Absolute" indexing i.e. indexing with respect to the chosen axes is immediately possible.
The results applies independently of the presence of a center of symmetry in the structure. As examples the cases of rutile and silicon cut in the direction (201) will be shown.

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11.8–4 STRUCTURE FACTORS OF SOME "FORBIDDEN" REFLECTIONS OF SILICON CRYSTALS OBTAINED BY MULTIPLE DIFFRACTION OF X-RAYS. By S.Caticha-Ellis and Lisandro P.Cardoso. Instituto de Física- UNICAMP -C.P. 6165, 13100, Campinas,SP, BRASIL.

The space group forbidden reflection 222 of diamond-type structures, first detected by Sir W.H.Bragg in 1921, has been the subjected of many investigations and were measured for diamond, Si and Ge by many authors (for ex. Renninger (1937,60), Weiss (1964,66), Colella & Merlini (1966), Kohra and collab. (1971,74)).The importance of the measurements is of course the determination of the anti-symmetric part of the electron density, i.e., that of bonding electrons, whose geometry does not conform with atomic spherical scattering factors. Different experimental methods had been used, such as reflection profile, pendellösung fringes, integrated intensity with parallel and divergent beam, etc. Almost all the authors state that they tried to avoid measuring under conditions of multiple diffraction. Actual measurements of other forbidden reflections with $h+k+\ell=4n+2$, have been so far reported as negative; reflection 420 seems to have been observed by Wittels(1966) in doped Ge crystals but Colella & Merlini state that they could not observe it and conclude that it should be at least 20 times smaller than 222. Renninger was able to give upper limits for the 442 and 622.
By using the decoupled multiple diffraction method (Cardoso and Caticha-Ellis this meeting) with forbidden primary reflection of the type 4n+2 without symmetry it is possible in principle to measure several other "forbidden" reflections.
The experimental method used in our measurements involves very low intensities even when using a rotating anode generator. However it seems very promising in the determination of bonding electron distribution in covalent structures.The use of synchrotron radiation is envisaged for further, more precise measurements. Some preliminary results will be given.

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11.8–5 EXPERIMENTAL TEST OF Kawamura and Kato's SECONDARY EXTINCTION CORRECTION FORMULA By J. Harada, H. Miyatake and M. Sakata, Faculty of Engineering, Nagoya University, Chikusa-ku, Nagoya, Japan.

Recently, Kawamura and Kato (Acta Cryst. (1983) A39, 305) presented an analytical formula for extinction and absorption corrections to the integrated Bragg intensity data collected from a sphercal or cylindrical single crystal on the basis of Kato's new statistical dynamical diffraction theory. Though they have made a theoretical comparison with the widely accepted Becker and Coppens formula, any experimental test of the two theories so far seems to have not reported yet. Hence it is still not well understood the difference of the results when applying the two theories, particularly from the practical view point.
We have carried out such a comparison with the use of the data sets collected by both angle and energy dispersive neutron diffraction methods. It is revealed that both theories gave the same answer for the data by the conventional angle dispersive method, even though some reflections are noticed to be severely affected by extinction effect, while they gave a slightly different parameter sets for the data by energy dispersive method.