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