

14.1-7 ON THE THEORY OF N-BEAM LATTICE IMAGE FORMATION IN HREM ON THE BASIS OF THE BLOCH WAVE FORMALISM. By F.N.Chukhovskii and V.L. Vergasov, Institute of Crystallography, Academy of Sciences of the USSR, Moscow, USSR.

A lattice image in HREM is formed provided the N -beam symmetrical diffraction of fast electrons in crystal occurs, which is described by the dynamical matrix of the N -th rang ($N \gg 1$). It means that for determining proper wave vectors of electron Bloch waves the dispersion equation can be in general solved only numerically. In this report the analytical approach to the lattice image formation is developed by use of the Bloch wave function formalism. In practice of HREM the diffraction pattern and the dynamical matrix have the symmetry of one of the two-dimensional point groups, which allows to reduce the dispersion equation order essentially (Kogiso and Takahashi, J. Phys. Soc. Jap. (1977) 42, 223; Vergasov, Chukhovskii and Pinsker, Kristallografiya (1982) 27, 645). In the case under consideration the electron Bloch waves excited belong only to the identity irreducible representation of the diffraction pattern group symmetry and the corresponding dispersion equation has been obtained by the present authors (Izv. Akad. Nauk SSSR, ser. fiz. (1983) 47, 1174). In accordance with the group-theoretical method a complete set of N reflections is divided into two sets: first of ones consists of N_0 "strong" reflections and the second one is represented by a number of systems of N_K equal intensity reflections ($\sum N_K = N - N_0$). By taking into account the first set of reflections the electron Bloch wave functions can be constructed and they are an zero-order solution of the N -beam diffraction problem. Furthermore, the correct determination of the Bloch wave functions have been performed by the perturbation theory in powers of the values $(J(N_K)/J(N_0))^{1/2}$,

where $J(N_K)$ is the total intensity of N_K diffracted beams. Notice that each system of $N_K \neq 0$ beams corresponds to the single Bloch wave, for which the dispersion equation is the first order one.

As an example, the 37-beam diffraction problem (Si-crystal in orientation $\langle 111 \rangle$, electron energy $E=100$ keV) is studied analytically. The system of N_0 reflections of the zero-order approximation is shown in Fig.1. For the total intensity of these reflections $J(N_0)$ the results of analytical and numerical calculations (dashed and solid curves, respectively) are presented in Fig.2. It is seen that: (i) the main part of the intensity of the incident beam is concentrated in N_0 reflections drawn in Fig.1; (ii) analytical and numerical calculations are in a good agreement with an accuracy up to 3%.

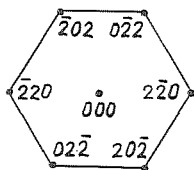


Fig.1

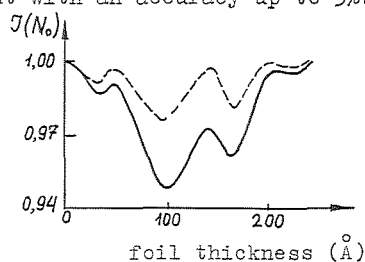


Fig.2

14.1-8 THE MULTIBEAM INTERACTION EFFECT ON ELECTRON DIFFRACTION IN POLYCRYSTALS WITH A DIFFERENT DEGREE OF ORIENTATION OF MICROCRYSTALS. By A.S.Avilov, Institute of Crystallography, Academy of Sciences of USSR, Moscow, USSR.

Electron diffraction analysis deals mainly with thin films which are, in fact, sets of microcrystals with a different degree of orientation (mosaic single crystals, textures and polycrystals) and angular and thickness distributions. The aim of this paper was to work out a method of calculation of reflection intensities in the case of multibeam reflections for mosaic single crystals and textures followed by thickness and orientation averaging.

The following model was used: a thin film represented a single layer of microcrystals, each of the microcrystals scattered electrons independently, and the scattering intensity in every direction was the sum of scattered intensities of single group of crystals, oriented likewise to the incident beam and having certain thickness distribution.

Fujimoto's matrix method was used (Fujimoto, J.Phys.Soc.Japan.(1959) 14, 1558). This method implies the obligatory calculation of diagonal elements of a "dynamic matrix" which depend on diffraction geometry. The paper suggests the ways of calculation of diagonal elements and intensity averaging. The $hk0$ -reflection intensities were determined for mosaic LiF single crystals and compared to the experimental data (Avilov, Crystallography (1979) 24, 178). Allowing for only 50-60 beams the divergence factor for intensities decreased from 32% (for kinematic approach) to 7%. An analogous result was obtained for texture PbSe samples (the texture axis $[001]$).

14.1-9 DYNAMICAL THEORY OF MANY-BEAM SCATTERING OF FAST ELECTRONS AND ITS APPLICATION TO STRUCTURE INVESTIGATION IN HIGH-RESOLUTION ELECTRON MICROSCOPY. By Z.G. Pinsker and F.N. Chukhovskii, Institute of Crystallography, Academy of Sciences of the USSR

By use of the group theory the many-wave problem of scattering of fast electrons in crystals is discussed. One finds that in the common case of the high-resolution electron microscopy when the electron beam is normally incident on the crystal surface in a crystallographic direction it is sufficient to solve the dispersion equation corresponding to a single irreducible representation of the symmetry group of the electron diffraction pattern. The main new results of the treatment developed are following:

1. the theorem establishing the connection of the highest degree of equation arising in factorization of the dispersion equation of the many-wave problem with the symmetry and structure of the electron diffraction pattern is proved;
2. the perturbation theory for finding electron Bloch waves is proposed.

Results of the analytical many-beam calculations for 100 keV to 1 MeV electrons incident of Au, Si, Ge crystals are given as examples. The correspondence between the results of the dynamical theory of diffraction and ones of the theory of electron channeling is considered.

References:

V.L. Vergasov, F.N. Chukhovskii and Z.G. Pinsker, Kristallografiya (1982) 27, 449-456; 27, 645-651