14.1—4   SYMMETRY ENHANCEMENT IN CONVERGENT BEAM ELECTRON DIFFRACTION. M. Tanaka, H. Sekii, O. Ueno and H. Takayoshi, Dept. of Physics, Faculty of Science, Tohoku University, Sendai, Japan.

Convergent-beam electron diffraction (CBED) patterns do not always show the true symmetries of a specimen crystal, but can show higher symmetries than those of the specimen (symmetry enhancement). If the phase of the structure factor can not be detected, a symmetry enhancement may take place. Lacking of an inversion center in a crystal can not be detected by X-ray diffraction, but can be unambiguously known by CBED.

When the structure factors at two reciprocal lattice points which are related by a twofold axis have the same amplitude but have different phases, we say that a pseudo twofold axis 2* is present. If a mirror plane is present, a pseudo twofold axis is accompanied perpendicularly to the mirror plane. In this case, two structure factors related by the pseudo twofold axis are complex conjugate each other. A pseudo mirror plane m* is defined in a similar manner.

A pseudo twofold axis and a pseudo mirror plane can cause a symmetry enhancement in the bright field pattern of CBED. However, the enhancement can not be observed, since the true mirror plane and the true twofold axis which give the same symmetries caused by the 2* and m* coexist in usual cases. In a general case, the symmetry enhancement can not be expected in the whole pattern and dark field pattern.

In a zincblende type crystal, whose space group is $F\bar{4}3m$, the approximate symmetry enhancement takes place in the 220 dark field pattern by 2* at [111] electron incidence, that is, HOLZ lines in the reflection shows the symmetry m_2. The reflections belonging to the 0-th Laue zone produce 2mm symmetry in the 220 dark-field pattern, since the phases of the reflections are zero. The imaginary part of the 220 reflection caused by two successive HOLZ reflections (Umweganregung) is proportional to $f_A^2 f_B^1 - f_A^1 f_B^2$, where f_X^i is the structure factor of X atom for the i-th reflection. When the scattering angle dependence of the structure factor for A atom is similar to that of B atom, the imaginary part and the resultant phase of the reflection becomes small, resulting a symmetry enhancement of m_2. The contribution of the Umweganregung via more than three reflections may be small. A 34 beam dynamical computation really shows m_2 symmetry in the 220 reflection.

The point group of 10H-SiC is 3m. However, it is known that the point group determined by X-ray diffraction is 6/mmm, which is Ramsdell type symmetry enhancement [L.S. Ramsdell and J.A. Kohn, Acta Cryst. 4 (1951) 111]. When the crystal is examined by CBED, the diffraction group and point group obtained at 0001 incidence were $3m1_R$ and 6m2, and those obtained at $1\bar{1}00$ incidence were $m1_R$ and 6mm. The symmetry enhancement occurs in the bright field pattern and the approximate symmetry enhancement occurs in the dark field patterns by m* in the (0001) and the ($11\bar{2}0$) planes and by 2* in the c axis and in the [$1\bar{1}00$] and the [$11\bar{2}0$] directions. It is noted that true twofold axes do not present perpendicularly to the pseudo mirror planes and that true mirror plane does not present in the ($1\bar{1}00$) plane. From the symmetries of the two set of the whole patterns and ±G dark field patterns, which do not exhibit the symmetry enhancement, true point group 3m can be deduced.

14.1—5   STRUCTURE FACTOR DETERMINATION FROM MULTIPLE BEAM SITUATIONS IN ELECTRON DIFFRACTION: By Jon Gjønnes and Erik Sørbrøden, Physics Department, University of Oslo.

Improvement of optics, vacuum condition, and measuring techniques is leading to increased accuracy and wider scope for structure factor measurements by electron diffraction methods.

We have reexamined theories pertaining to the methods which fall into the two categories:

Measurement relating to extinction distances or gap at the dispersion surface, e.g. thickness or convergent beam fringes, Kikuchi line splits (IKL method), whereby strong low order structure factors are obtained.

Measurement of intensity profiles from which structure factors (and phases) of weaker reflections can be obtained - the vanishing intensity at critical conditions being a special case.

The theoretical analysis of both types is based partly on three- and four-beam cases . (Gjønnes & Høier, Acta Cryst. (1971) A27, 313),(Hurley & Moodie, Acta Cryst. (1980) A36, 737).

Measurements of split lines, vanishing points and intensity profiles have been carried out in Kikuchi patterns and convergent beam patterns using photographic methods as well as intensities from a STEM detector. Applications are to silicon and a group of clinopyroxenes.

14.1—6   THREE-BEAM EFFECTS AND STRUCTURE FACTOR PHASE INFORMATION IN SACP PATTERNS. By K. Marthinsen and R. Høier, Institutt for røntgenteknikk, Universitetet i Trondheim-NTH, N-7034 Trondheim-NTH, Norway.

Selected-area channeling patterns (SACP) may be obtained from the individual grains in polycrystalline or mosaic crystals with grain sizes above some μm. As in the Kikuchi line case the two-beam line positions may be utilized to determine lattice parameters or electron wavelength/high tension with high accuracy. Information on the dynamic, non-systematic many-beam interactions on the other hand may be obtained from the intensity changes and line displacements frequently observed near line intersections. The present studies have been focused on the three-beam interactions which are observed near the intersection between two lines. Qualitatively a good agreement is obtained between the calculated and the observed intensity anomalies. The intensity in one of the lines, h, is found to depend on the size of the three structure factors involved, the deviation parameter of the coupled beam, s_g, and the invariant sum of the structure factor phase angles, $\alpha = \phi_{-h} + \phi_g + \phi_{h-g}$. In a centrosymmetric crystal α will for example be 0 or π and the line intensity will be larger or smaller than the two-beam value dependent on the sign of s_g. As in the Kikuchi line case the enhanced segments of several lines may combine to form ordinary or inverted envelopes dependent on the value of α. From the patterns a large number of the invariant quantity α may thus be determined experimentally. In a full structure determination these may then be used as a starting set in the standard treatment of the X-ray intensity data obtained from the same or a similar crystal. This possibility is at present being investigated. Compared with other electron diffraction techniques, where the same phase information may be obtained, the possible use of bulk specimens is a main advantage of the SACP method.