14.1-2 SPACE-GROUP DETERMINATION OF OSMIUM DISILICIDE BY CONVERGENT BEAM ELECTRON DIFFRACTION.

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This work is reported as an example of electron diffraction space-group determination using the tables published by Tanaka *et al.* (Acta Cryst. 1983, A39, 825-37) and Goodman (Acta Cryst. 1984, A40, 635-42) which, together with those of Buxton *et al.* (Phil. Trans. Roy. Soc. Lon. 1976, 281, 171-94) are to appear in unified form in International Tables for Crystallography Vol. B, (to be published).

Several crystals of a specimen of $OsSi_2$, prepared by arc melting and mounted in a tilt/rotate stage, on a Be grid, were examined in a Philips EM 430 (with EDS), using a 20 nm probe. Previous X-ray diffraction studies of the structure (Engström, Acta Chem. Scand. 1970, 24, 2117-25) revealed that it was isotypic with β-$FeSi_2$ with possible space groups $Cmca$ and $C2cb$ respectively, centro- and noncentro- symmetric. These two possible space groups were confirmed by the reflection conditions observed in CBED patterns taken at the [100], [110] and [010] zones. Further, the glide vector parallel to c was confirmed by GM lines along c^* in reflections 00ℓ, ℓ odd. The required mirror symmetries were perfect to the limit of observation and the reciprocity test (Goodman, Acta Cryst. 1975, A31, 804-10), using a pair of pictures, showed that the structure was centrosymmetric. The composition was checked by EDS and the orthorhombic unit cell (a = 10.14 Å, b = 8.15 Å and c = 8.22 Å) confirmed by measurement of the 3-dimensional diffraction pattern.

14.1-3 DYNAMICAL DIFFRACTION CALCULATIONS FOR RHEED AND REM. By L.-M. Peng and J.M. Cowley, Department of Physics, Arizona State University, Tempe, Arizona 85287, USA.

The calculation of dynamical electron diffraction amplitudes for the glancing-angle incidence of RHEED patterns and reflection electron microscopy (REM) is usually made by taking slices of crystal parallel to the crystal surface. This approach is satisfactory when there is perfect two-dimensional periodicty parallel to the surface, but does not allow a satisfactory treatment of diffraction by defects in the crystal surface such as surface steps. Use of a column approximation is not appropriate. The alternative approach of multi-slice calculations, taking slices perpendicular to the crystal surface has the advantages of involving only forward scattering and the use of standard multi-slice computer programs (Peng and Cowley, Acta Cryst. A42, 545 (1986)). By use of this method it is possible to follow the establishment of the wave-field of the electrons in the crystal surface layers and in the vacuum as the electron beam enters the crystal and reaches an equilibrium situation. Then the perturbation of the wave field by any type of defect can be observed and the resulting image and diffraction pattern can be calculated. By use of this method the effects of surface resonance diffraction conditions have been investigated. The requirements for accuracy in the calculations have been established. Applications have been made to the imaging of surface steps. An alternative approach based on the same formulation of dynamical diffraction is proposed as a means for calculating the perfect crystal case in reflection or for establishing the wave field as an input to calculations of perturbations due to defects.

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14.1-4 STRUCTURE DETERMINATION BY ELECTRON SCATTERING by A.F. Moodie and H.J. Whitfield, Division of Materials Science and Technology, CSIRO, Locked Bag 33, Clayton, Victoria, Australia, 3168.

Although electron scattering techniques are used routinely in structure determination, and although efficient numerical techniques have been available for many years the structure analytical content of the dynamical equations has not been made particularly explicit, and no systematic procedures, comparable to those devised for kinematical X-ray scattering exist.

Since trial structures are normally derived from images when electron scattering techniques are used, trial and error methods are often quite effective. Nevertheless it seems worthwile to attempt a more systematic approach, and a first step towards this is outlined.

With the standard notation the solution in the projection approximation is written $\Psi = \exp\{iHz\}\Psi_o$ in direct space and $|U\rangle = \exp\{iMz\}|0\rangle$ in reciprocal space. For simplicity in notation, suppose there is only one atomic species in the structure; then $M = \sum_n M_n = \Sigma T_n m T_n^{-1}$, where T_n is the diagonal matrix $T_{ii} = \underset{\sim}{g}_i \cdot \underset{\sim}{a}_i$, $\underset{\sim}{g}_i$ is the diffraction vector, and $\underset{\sim}{a}_i$ is the corresponding structure parameter. The matrix m has off diagonal entries deriving from a single atom on the origin; and diagonal entries ζ_i/n. Since it plays a part in dynamical theory somewhat analogous to a scattering factor in kinematical theory this operator which has the same eigen values as the M_n may be described as the single atom matrix.

With the $U_m = \exp\{imz\}|0\rangle$, it is the deviations from $U_m(g)U_m^*(g)$ which contain structural information, so that, for specific structures attention is directed towards particular angular regions in the convergent beam discs.

U_m can of course, be readily evaluated numerically, but it can also be understood qualitatively by utilising Sayre's relations. This is most easily accomplished in direct space.

In estimating $\exp\{i(\sum_n T_n m T_n^{-1})z\}$ an initial reduction to the asymmetric unit can be made, in analogy to kinematical procedures.

The method is illustrated with an example based on the heavy atom technique.