

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

A.W.S. Johnson and F.J. Lincoln,  
Electron Microscopy Centre and Department of Physical  
and Inorganic Chemistry, University of Western Australia,  
Nedlands, Western Australia.

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<sub>2</sub>, 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 isotopic with β-FeSi<sub>2</sub> 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 00*l*,  
*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 periodicity  
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. Neverthe-  
less it seems worthwhile 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  $\Psi = \exp\{iH_z\}\Psi_0$   
in direct space and  $|U\rangle = \exp\{iM_z\}|0\rangle$   
in reciprocal space. For simplicity in notation, suppose  
there is only one atomic species in the structure;  
then  $M = \sum_n M_n = \sum_n T_n m T_n^{-1}$ , where  $T_n$  is the diagonal matrix  
 $T_{ii} = g_i \cdot a_i$ ,  $g_i$  is the diffraction vector, and  $a_i$  is the  
corresponding structure parameter. The matrix *m* has  
off diagonal entries deriving from a single atom on  
the origin; and diagonal entries  $\zeta_i/n$ . 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 kine-  
matical procedures.

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