20. X—1   INTERRELATING   CBED   GROUPS   AND
SPACE GROUPS; A CASE FOR I.T. INCLUSION?
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The symmetries of zero—layer CBED zone—
axis patterns form groups isomorphous
with the Alexander and Hermann space
groups   of   2—dimensional   layers
(Zeits.Krist.(1929) 70,328) . These
groups   in   turn   are   lattice
("klassengleich") subgroups of specific
3—dimensional space groups.

     This suggests a 2—step logic in
space   group identification from CBED
data.

     International Table listings have so
far not included "sub-periodic" groups.
In the case of the layer groups this may
have been advantageous in that, in the
absence of any over—riding necessity,
this has permitted experimentation with
notations suited to different specialist
applications   (e.g.   Wood,E,   Bell
Sys.Tech.Journ.(1964);   Pond R.C.   and
Valchavis,D.S. Proc.Roy.Soc.(1983) A 386
,95).

     Recent experience suggests that, as
with the 3—dimensional space   groups
(Hall,S.R.Acta Cryst. (1981) A37 517), an
explicit,   generator—based listing can
provide a valuable aid to identification
of   space   groups and their   subgroup
relationships.

20. X—2   MODULATED STRUCTURES IN ALLOYS.
By D. Watanabe, Department of Physics, Faculty of
Science, Tohoku University, Sendai, Japan.

A survey is given of the X-ray diffraction and electron
microscopy and diffraction studies on the modulated
structures in ordered alloys. The long-period struc-
tures in alloys often show incommensurate character.
The well-known examples are seen in the one-dimensional
antiphase domain structures (1d-APS) based on the $L1_0$ or
$L1_2$ structure. Antiphase domain sizes M's estimated
from the diffraction patterns are in general non-inte-
gral multiples of the basic cell. The fractional prop-
erty of M value is interpreted in terms of the uniform
mixture of domains with different sizes, and actual mode
of domain mixing revealed by high resolution electron
microscopy study agrees with this prediction. In the
two-dimensional antiphase structures (2d-APS), on the
other hand, it is very difficult to visualize the actual
domain configurations in real space from the diffraction
study alone: the M's in the two directions are generally
not equal and vary with composition. However, high
resolution structure images can reveal the incommensu-
rate structures in an atomic scale, and the technique
has been applied successfully to several alloys, Au-Zn,
Au-Mg, Au-Mn, Cu-Zn-Au, etc. It is particularly inter-
esting that incommensurate structures of the Au-Zn al-
loys containing 16-19 at.% Zn consist of two types of
"domains" with commensurate structures of the same unit
cell size and they are arranged in such a characteristic
way that the incommensurate periods are produced in the
two directions, [100] and [001]. The high resolution
images give information on the density modulations as
well existing in the incommensurate structures. How-
ever, the details of the modulation waves including
displacement modulation are obtained only from the anal-
yses of diffraction data.

20. X—3   POLYTYPISM AND THE OD THEORY
By S. Ďurovič, Centre of Chemical Research,
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ganic Chemistry, 842 36 Bratislava, Czecho-
slovakia.
The phenomenon of polytypism was discovered by
Baumhauer (Z. Krist. (1912) 50, 33; (1915) 55,
249). The chief concern of those investigating
this phenomenon was to find a correct answer
to the generation of almost limitless number
of polytypes of a substance, some of which pos-
sess giant-sized unit cells. A great number of
polytypic substances has since been found, nu-
merous polytypes have been discovered and nota-
tion systems to describe their structures pro-
posed. Recently also physical properties of po-
lytypes attracted attention since these depend
on the actual stacking of layers (e.g. Brafman
and Steinberger, Phys. Rev. (1966) 143, 501),
and thus a "fine tuning" of properties in a pu-
rely structural way, without admixtures, might
well be possible. There is also growing tenden-
cy to use polytypes of some phyllosilicates as
indicators of their genesis (typomorphism). Al-
though polytypists were aware of the peculiar
geometry of their structures, the symmetry of
polytypes was virtually never investigated in
detail.
Independent on polytypism, Dornberger-Schiff
(Acta Cryst. (1956) 9, 593) developed her the-
ory of OD structures to explain the disorder
phenomena exhibited by β-wollastonite and Mad-
rell salt since it became evident that the be-
havior of these structures cannot be adequate-
ly described in terms of space-group crystallo-
graphy. The OD structures consist of 2D-perio-
dic disjunct parts of crystal space a) all geo-
metrically equivalent or relative few in kind,
b) with identical translation groups or with a
common subgroup, c) stacked so that the layer
pairs of the same species remain equivalent in
structures of the same substance (family), and
d) with ambiguity of stacking at every layer
boundary. The letters OD mean that these struc-
tures can be periodic (ordered) as well as ape-
riodic (disordered), but the possibility of be-
ing disordered is inherent to them. In contrast
to fully ordered structures, the set of rele-
vant coincidence operations expressing their
symmetry does not form a group, but only a
groupoid, since some of these operations are
partial. The apparatus of the OD theory con-
tains classification schemes, the list of all
OD groupoid families for structures of equiva-
lent layers, the methods to calculate the num-
ber of equivalent positions of any OD layer re-
lative to its predecessor, the procedures for
systematic derivation of all structures of max-
imum degree of order (MDO structures), for the
choice of OD layers, and procedures to determi-
ne the symmetry principle from diffraction pat-
terns (for references see Dornberger-Schiff,
Cryst. Res. and Technol. (1979) 14, 1027).
An analysis of dozens of structures described
as polytypic revealed that all of them are OD
structures. Hence the OD theory can be consi-
dered as the theory of symmetry of polytypes.
The recognition of these facts can bring advan-
tages for the study of polytypes in an analogy
to those brought by the space-group theory for
the traditional crystallography. Among others,
it makes it possible to correlate the physical
properties of polytypes with their full symmet-
ry, it suggests a new definition of crystalline
substances and thus it opens the way for the
development of a generalized crystallography.