its limiting value. In this case the derivative symmetry group may be of higher order than that given by Hirshfeld, due to extra symmetry of the lattice. Consider, for instance, the space group $P2_1/m$ with its lattice-constant ranges $a \leq c, -a/2c \leq \cos \beta \leq 0$ (Table 3). In the general case $(a < c, -a/2c \leq \cos \beta < 0)$ the derivative group is the Cheshire group $P2/m$ (Hirshfeld, 1968) but it turns to $Pmmm$ if $a < c$ and $\beta = 90°$. Further, for $a = c$ the derivative group is $P2/m$ $4/m$ $2/m$, if $\beta = 90°$, and $P2/m$ $6/m$ $2/m$, if $\beta = 120°$. These groups should be taken instead of $P2/m$ in the corresponding boundary case to derive the molecular parameter ranges.

Thus the boundary case is treated as the general one but requires a 'boundary' derivative group. Since there are too many situations to be considered, we do not systematize them, assuming that obtaining a derivative symmetry group is a trivial procedure for a crystallographer and may be readily undertaken, if necessary, for a particular boundary situation.

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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.

Imaging of polytypes and stacking faults in tetrahedral compounds.

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Abstract

The resolution attained with a JEOL 200CX electron microscope in top-entry configuration has allowed the direct elucidation of the structure of tetrahedrally bonded compounds. Computer simulation methods were used to calculate through-focus series of images at a range of thicknesses and the conditions for which structural features are interpretable on an atomic scale have been ascertained. In particular, various polytypes are differentiated and stacking faults are intuitively interpreted.

A wide variety of compounds crystallize as stacking variants of the diamond lattice. For nearly all of these compounds, ranging from silicon carbide to the quaternary chalcogenides, it is easily seen that, in order to identify specific polytypes directly from electron micrographs, a first requirement is a minimum resolution of about 2.5 Å.

There are, of course, many other requirements, most of which are well known. Using a JEOL 200CX electron microscope in a configuration specifically chosen to maxi-

mize the resolution of lattice images, we have found that all conditions can be satisfied at an accelerating voltage of 200 kV. This is illustrated in Figs. 1(b), (c) with images of 3,3 stacking (*i.e.* pseudo 6H polytype) and 3,4 stacking (*i.e.* pseudo 21R polytype) of the compound CuAsSe (Whitfield, 1981). Our measured value of C_s is somewhat less than 1 mm so that the standard expression for resolution at the Scherzer focus gives a value of 2.3 Å.

As might be anticipated from the micrographs, the technique can be extended much further, for instance to the direct imaging of the intergrowth of polytypes (Fig. 2). Standard multislice calculations (Fig. 1a) have been used in establishing the interpretation. In this example, correspondence between the observed and calculated image is not exact, in that one row of spots in the observed image is somewhat brighter than the rest. This arises from a slight tilt about the c axis, a delicate effect which transforms a glide line into a reflexion line. Effects of this type will be discussed in a forthcoming publication.

The particular material chosen for illustration would appear to be unpromising, since the periodicity in the
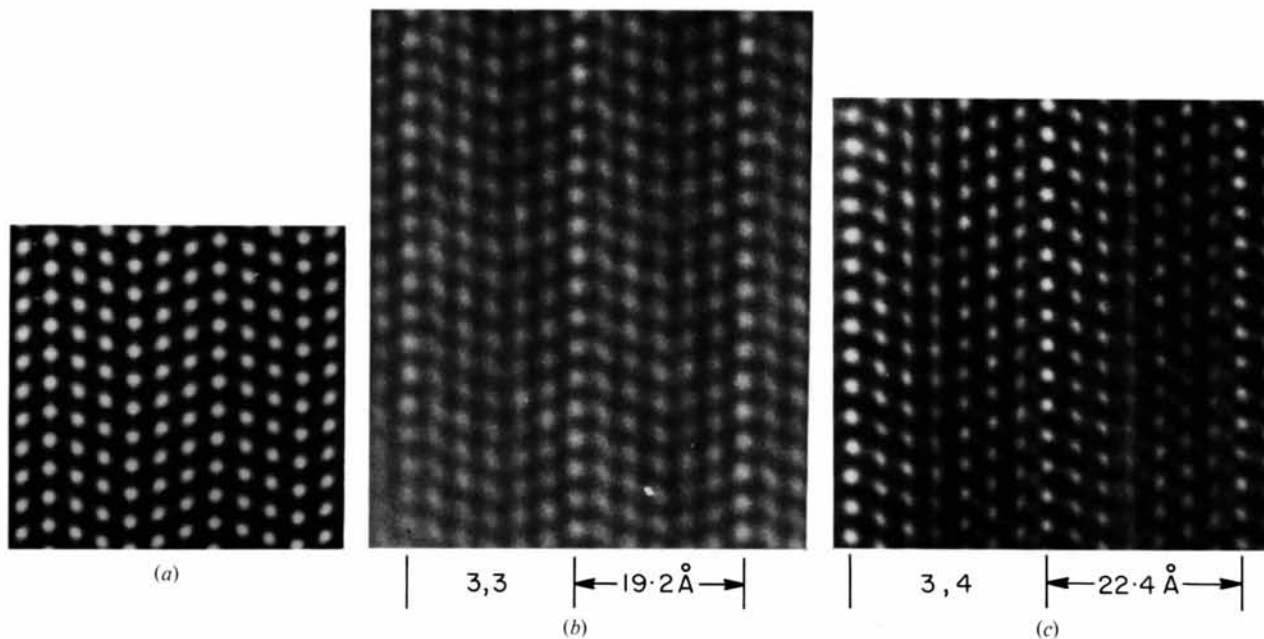
(a)

3,3 ⟵19·2Å⟶

(b)

3,4 ⟵22·4 Å⟶

(c)

Fig. 1. (a) Multislice calculation, using C_s of 0·95 mm and a defect of focus of −950 Å, for a 176 Å thick crystal of the 3,3 (hcc) pseudo 6H polytype of CuAsSe ($a = 11·75$, $b = 6·79$, $c = 19·21$ Å) viewed down the a axis with 200 kV electrons. (b) Experimental observation of 3,3 (hcc) stacking in material of (a). (c) Experimental observation of 3,4 (hcchccc) stacking in the pseudo 21R polytype of CuAsSe.
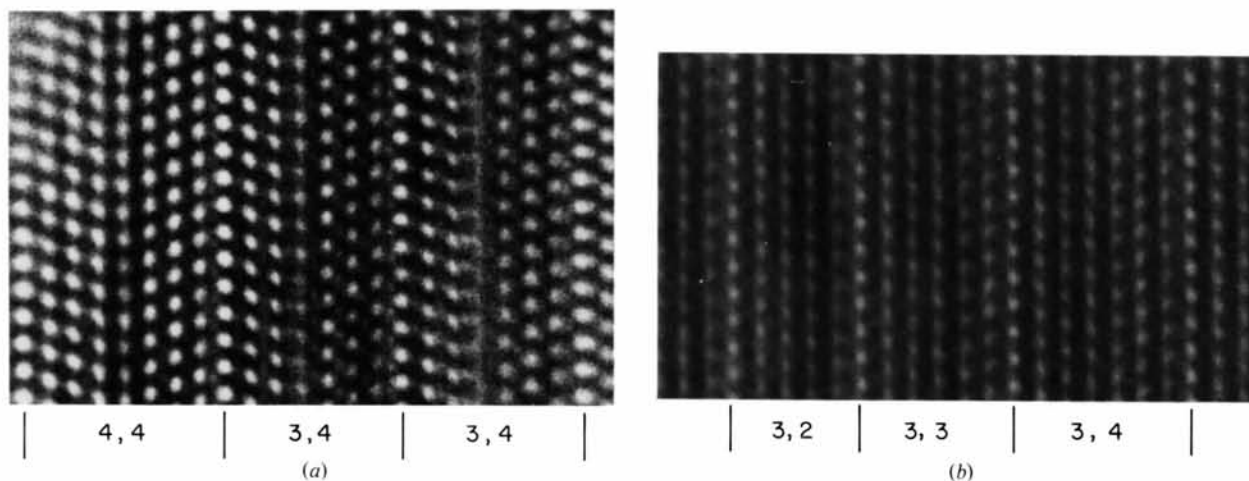

4,4 | 3,4 | 3,4

(a)

3,2 | 3,3 | 3,4

(b)

Fig. 2. Two examples (a) and (b) of experimental observation of stacking faults in the pseudo 21R polytype of CuAsSe with stacking as indicated on the micrograph.

direction of the incident beam is large (11·5 Å). In fact, it is rather easy to choose experimental conditions such that this large periodicity is apparent and this can be of use in more detailed analysis. However, in establishing first-order properties, effects of this type can be suppressed. Crudely, stacking can be 'imaged' almost independently of composition. The situation invites comparison with that involved in the 'direct' imaging of octahedrally coordinated oxides, where a minimum requirement of resolution is 3.4 Å, and in fact the analogy is strong, though not complete. In both octahedral and tetrahedral cases orientations can be found in which there is no overlap of certain defining features in the structure (for instance holes). An application of Sayre's relations to the dynamic equations (Moodie, 1965) then

explains why the disposition of the basic units of the structure can be immediately inferred.

Details of the theory and a description of the particular configuration of the 200CX microscope used to obtain high-resolution lattice images and convergent-beam electron diffraction patterns, together with experimental results on a series of tetrahedrally bonded compounds, will be discussed in a series of forthcoming papers.

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