HREM OF EDGE-ON INTERFACES AND DEFECTS

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INTRODUCTION

The latest generation of intermediate-voltage high-resolution electron microscopes (HREMs) offer the exciting prospect of resolution limits of 2Å or better [1,2]. Moreover, under certain well-defined conditions, it is even possible to deduce useful structural details down to small fractions of this limit [3-5], and some limited chemical information can also be extracted. In this paper, the potentialities and limitations of the high-resolution technique will be considered, with particular reference to edge-on interfaces and defects in various elemental and compound semiconductors. Specific examples described include: i the identification of crystal polarity in <110>-orientated sphalerite materials; ii intensity variations across <100> GaAs/Ga<sub>1-x</sub>Al<sub>x</sub>As interfaces; iii stacking fault symmetry and dislocations; iv refinement of the diamond <100> platelet defect; v distinguishing shuffle and glide models for the Si 30° partial dislocation. Prospects and practical problems associated with the HREM technique, as it applies to imaging semiconductors, are briefly discussed.

CRYSTALLOGRAPHY

The crystal orientations of most interest when imaging elemental or sphalerite compound semiconductors are <100> or <110>. Schematic drawings for the binary sphalerite structure are shown in Fig. 1, together with corresponding diffraction patterns. The sphalerite structure has space group F43m (No. 216). Several relationships between the kinematical structure factors (F<sub>hkl</sub>) have important consequences for imaging these materials. For example, c' or axis related reflections have equal equivalent structure factors due to mirror symmetry, eg. F<sub>T11</sub>=F<sub>T11</sub>. For specific structure factors the following hold:

i h+k+l=4n (n=0,1,2,...) (for example, 220, 400) contain sum terms (f<sub>A</sub>+f<sub>B</sub>) only, and therefore provide no chemical information;

ii h+k+l=4n+2 (for example, 200) contain difference terms (f<sub>A</sub>-f<sub>B</sub>) only. These beams can provide chemical information;

iii h+k+l=4n+1, 4n+3 (for example, 111, 311) contain both sum and difference terms and give information about polarity. The degree of polarity (i.e. non-centrosymmetry) is given by the ratio of (f<sub>A</sub>+f<sub>B</sub>) to (f<sub>A</sub>-f<sub>B</sub>).

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Bijvoet-related reflections, i.e. (hkl), (hKl), are non-equivalent, as a consequence of the crystal's non-centrosymmetry, e.g. \( F_{II} \neq F_{III} \).

The \( \{002\} \) and \( \{020\} \) reflections differ in structure phase by \( 180^\circ \); these relationships are retained under dynamical scattering conditions when the related reflections have equivalent excitation errors; they are utilized later for deriving expressions for image intensity under zone axis imaging conditions. In the \( <110> \) orientation, information from \( \{111\} \) reflections will be used to determine polarity, whereas in the \( <100> \) orientation information from \( \{200\} \) reflections will be used to investigate chemical changes at interfaces.

The \( <110> \) orientation is preferred for the investigation of dislocations in diamond/sphalerite crystals by HREM since the dominant slip system is \( <110> \{111\} \). A \( <110> \) orientation aligns the core of the dislocation parallel to the electron beam and thus provides the most useful projected view of the core. For multilayer structures such as GaAs/GaAl\(_{1-x}\)As, which are grown on \( <100> \), the extent of structural and chemical abruptness at the interface is of critical importance. In order to assess the structural flatness of the interface by HREM, either \( <100> \) or \( <110> \) projections are suitable. However, \( <100> \) is preferred for the determination of chemical information due to the contributions of four chemically-sensitive \( \{002\} \) reflections to the diffraction pattern [6], whereas the two \( \{002\} \) reflections in the \( <110> \) orientation also derive considerable intensity from \( \{111\} \) reflections by double diffraction.

The wurtzite structure, as shown in Fig. 2, has space group \( P6_3\text{mc} \) (No. 186). It consists of two interpenetrating hexagonal-close-packed lattices separated along the c-axis by \( u \), which is a distance ideally equal to \( 3/8 \) in fractional coordinates. Atoms of one atomic species are located on one sublattice at \( (000)(1/3, 2/3, 1/2) \), those of the other species are located on the other sublattice at \( (00u), (1/3, 2/3, 1/2 + u) \). The close-packed \( \{001\} \) planes have a stacking sequence \( \ldots AaBbAaBb \ldots \) compared with the 3-layer sequence \( \ldots AaBbCcAaBbCc \ldots \) of diamond and sphalerite crystals. The structure does not possess a center of symmetry and the \( <0001> \) axis is polar. Important relationships between the structure factors, which again depend upon the choice of origin (see Fig. 2), include the following:

1. Systematic absences of kinematic reflections occur for \( h+k=3n, l=\text{odd} \), e.g. \( \{0001\}, \{3301\} \);
2. The \( \{0004\} \) reflections of wurtzite are chemically sensitive, with structure factors of the form \( F_{0004}=i4\Delta \) and \( F_{0002}=-i4\Delta \), where \( \Delta \) is the difference in electron scattering factors of the two species; and
3. There is a phase difference of \( 180^\circ \) between \( c^*\)-axis mirror-related reflections, due to \( c\)-axis glide plane symmetry, which results in structure