

Polarity reversal and symmetry in semiconducting compounds with the sphalerite and wurtzite structures

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The evidence for the occurrence of polarity reversal domains and inversion twins in compounds with the wurtzite and sphalerite structures is reviewed. Anti-coincidence lattices are defined for orientation relationships such that a fraction of sites of the two lattices coincide, but wrongly, to produce anti-coincidence sites. Proceeding from Friedel's theorem, the range of Friedel indices, l , can be extended to unity and negative odd integers. Polarity reversal domains are characterised by $l = -1$ and n^{th} order inversion twins by $l = -(3)^n$. The partial symmetry operations producing coincidence and anti-coincidence lattices are discussed.

1. Introduction — polarity in the wurtzite and sphalerite structures

Neither the wurtzite nor the sphalerite structures, which are of common occurrence among semiconducting compounds, are centrosymmetric. Hence, as is well-known, these structures exhibit both surface and bulk polarity. For example in the sphalerite structure, in the $[111]a$ direction, the covalent bonds run from an A atom (i.e. one of the lower valence element such as the III atom in a III-V compound) to the B atom. In the $[\bar{1}\bar{1}\bar{1}]b$ direction the bonds run from B to A atoms and the two directions are not equivalent as they are in the simpler diamond cubic structure. This sign convention corresponds to placing the A atoms at the points, at e.g. 000 of the space lattice and the B atoms at the sites displaced from them to e.g. $\frac{1}{4}\frac{1}{4}\frac{1}{4}$. When slices of sphalerite-structure compounds are cut in $\{111\}$ orientation, one side terminates in A atoms triply-bonded to the crystal. Such faces are termed (111) A surfaces and with the present sign convention [1], the $\langle 111 \rangle a$ directions are the outward normals to such faces. The other side of the slice terminates in B atoms triply-bonded to the crystal. The $\langle \bar{1}\bar{1}\bar{1} \rangle b$ directions are outward-drawn normals to such $\{\bar{1}\bar{1}\bar{1}\}$ B faces.

Similarly the wurtzite structure, which has an hexagonal space lattice, is polar in the c -axis direc-

tion $\langle 0001 \rangle$ and on the basal planes $\{0001\}$. The $[0001]a$ direction is the outward normal to the $(0001)A$ face and the $[000\bar{1}]b$ direction is the outward normal to the $(000\bar{1})B$ face.

The surface polar differences are the best known and show up in chemical etching, mechanical damage sensitivity and crystal growth behaviour. A review of the early literature was given by Barber and Heasell [2].

1.1. Polarity reversal

The clearest evidence for polarity reversal is the observation of areas of reversed etching polarity on $\{0001\}$ surfaces of CdS [3], ZnO [4] and on $\{100\}$ surfaces of epitaxial GaAs grown on germanium [5, 6]. This is not solely a surface phenomenon. Piezoelectric polarity reversal was found throughout the domains under the areas of reversed etching behaviour in CdS and ZnO.

The first polarity reversal interpretation of this evidence was in an analysis of the geometry of the interfaces between the domains, which were described as antiphase boundaries (APB) [7], using the ball-and-wire model approach originated by Hornstra [8]. If the occupation of the two sites of the basis unit, at 000 and at $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ in the sphalerite structure, by A and B atoms is interchanged between two volumes, they have reverse polarity.

These volumes are in “antiphase” as the term is used in the field of ordering in metallic alloys. The term can be thought to refer to a periodic occupation function which is positive for A-atom occupied sites and negative for B-occupied sites. These signs are those of the ions, i.e. of the net charges in the Wigner–Seitz cells surrounding the sites, assuming that the bonding is on the ionic side of neutral bonding, as is generally the case. Polarity reversal domains are then separated by APB’s across which the occupation function undergoes “phase” (sign) reversal. It necessarily follows that all bonds crossing APB’s are wrong A–A or B–B bonds, not A–B bonds. The diffraction contrast of APB’s in the sphalerite structure was also treated [7]. The diffraction contrast of APB’s in wurtzite-structure compounds, which were referred to as antistructure boundaries, was analysed by Blank *et al.* [9].

It had earlier been pointed out that to each geometrical type of grain boundary analysed in the diamond structure [10, 11] there corresponded two distinguishable cases in the sphalerite structure [12]. It was recognized that the one could be changed to the other at the join of an APB with the grain boundary as illustrated for the case of the first order twins in sphalerite in Fig. 1. The distinction between an APB across which there is a “phase” reversal of the occupation function only, and inversion twins which involve this and a “twinning” orientation change as well is brought out here. The first order twin can be regarded as produced in various ways. Here it is treated as produced by a tilt about the $\{110\}$ axis normal to the plane of the figure and lying in the $[111]$ interface plane. The two twins in the sphalerite structure corresponding to the single first order twin in the diamond structure are the inversion twin ($\theta = 70^\circ 32'$) and the upright twin ($\Theta = 180^\circ + \theta = 250^\circ 32'$) as shown. For mnemonic convenience A atoms will be represented by alabaster (white) circles or faces and B atoms by black circles or faces in this paper.

1.2. Diffraction contrast studies of APB’s and inversion twins

Inverted twins are those in which the structure is twinned and polarity-reversed relative to the matrix. The twin–matrix interface then has an APB character. As can be seen in Fig. 1, all the cross-interface bonds are wrong (represented by zig-zag lines here). Although inversion twins are to be expected to be of higher energy than upright

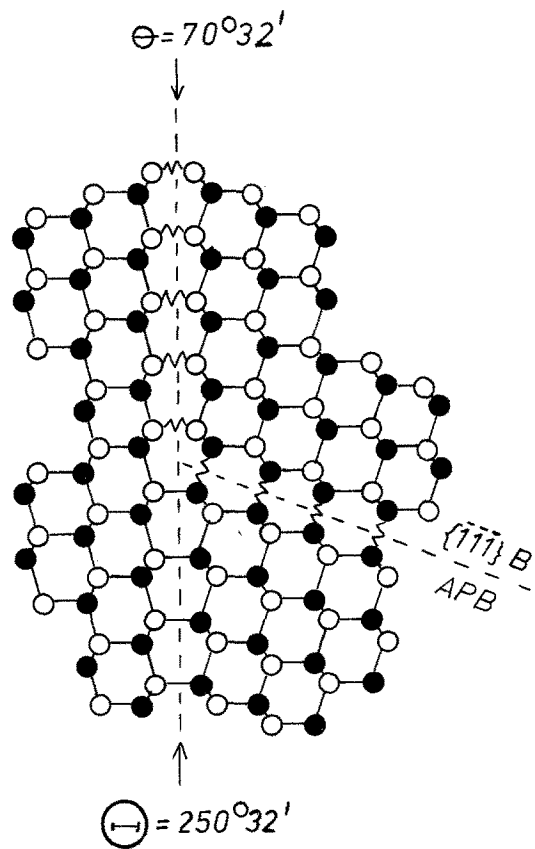


Figure 1 First order $\{111\}$ twin boundaries in the sphalerite structure. Open circles (white sites) represent A atom positions and full circles (black sites) represent B atom positions. Short lines represent bonds and zig-zag lines represent wrong (like atom) bonds. The paratwin or inverted twin ($I = -3$) and the orthotwin or upright twin ($I = 3$) boundary meet at a $\{111\}$ B antiphase boundary ($I = -1$). (After [7]). The Friedel indices, I , are defined later in this paper.

ones, they were found to occur commonly in BeO [13]. Detailed diffraction contrast studies of inversion twin interfaces were carried out in this material using X-ray topography [14].

A prominent “domain-form” structure, found in epitaxial films of sphalerite structure CdS, CdSe and CdTe grown on (110) oriented surfaces of several cubic system substrates was shown, in the case of CdSe, to be due to the growth of polarity reversal domains, apparently arising by the well-known epitaxial growth phenomenon of double position twinning [1]. Beautiful observations of polarity reversal domains in epitaxial GaAs and GaP grown on hemispherical germanium substrates and on silicon in several orientations were made by Morizane [15]. He also carried out transmission electron microscope diffraction contrast analyses

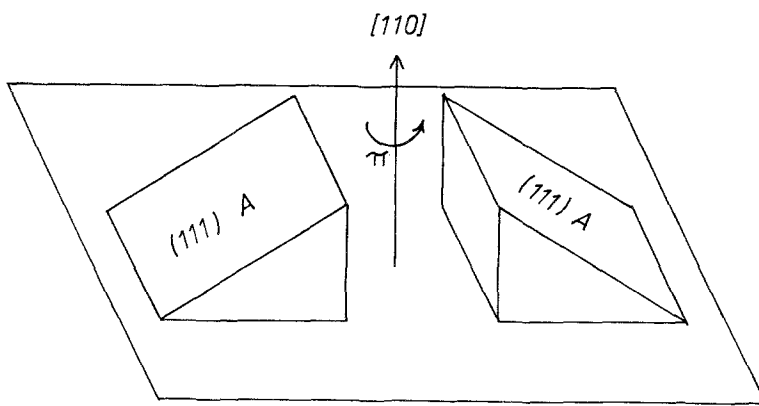


Figure 2 Double positioned "twin" nuclei on a (110) oriented epitaxial growth substrate. Twofold ($2\pi/2$) rotation about the substrate normal puts the nuclei in polarity reversal relation to each other. Each nucleus is equivalently oriented to the substrate. (After [1]).

of the antiphase boundaries in these sphalerite structure materials.

The upright and inverted twins of Fig. 1 differ by a rotation of 180° about a $\langle 110 \rangle$ axis. The double position twins of the domain form structure in epitaxial films of CdSe which turned out to be in antiphase relation also differ by a 180° rotation of the initial nuclei about the $[110]$ substrate surface normal as shown in Fig. 2. Morizane found polarity reversal domains in films grown on (100) and (110) substrates but never in those grown on substrates in (111) orientation.

Neave *et al.* [6] recently observed antiphase domains in epitaxial GaAs films grown on germanium $\{001\}$ substrates, confirming an earlier report [5]. They suggested a nucleation mechanism based on the fact that the first monolayer deposited on germanium during growth is always arsenic. If there occur steps of heights that are half integral multiples of the basis unit height, then on one side the surface germanium atoms occupy fcc lattice (000 type) sites. On the other side of such steps the surface germanium atoms occupy the other sites of the basis unit, i.e. $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ types sites. Arsenic atoms bonding on the first side of the step will occupy $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ sites. On the second side they must, however, occupy 000 sites. The second monolayer of gallium atoms will necessarily occupy 000 sites on the first side of the step, but $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ sites on the other side of the step. That is, nucleation on sites separated by such steps will be in antiphase, with occupation of the basis unit sites interchanged. Neave *et al.* [6] observed the resultant antiphase domains in reversible black-white contrast in TEM micrographs using a new convergent beam diffraction contrast method.

An analysis of polarity-reversal, coloured anti-symmetry operations [16] was suggested by these

observations and serves to account for them. A preliminary account was published previously [17]. A more complete account of the coloured symmetry treatment of these phenomena will be presented later.

2. The polar symmetry of the sphalerite structure

Fig. 3 shows the orientation of the $\{111\}A$ and $\{\bar{1}\bar{1}\bar{1}\}B$ faces in a single crystal of a material with the sphalerite structure. They form a polar octahedron, drawn with its apices at the face centre sites of an fcc unit cell of the structure in Fig. 3a. This illustrates its crystallographic orientation and makes it possible to index the faces and directions involved. The polar octahedron is shown again in Fig. 3b with the three visible $\{\bar{1}\bar{1}\bar{1}\}B$ faces shaded and certain axes and edges indexed. The polar octahedron is drawn in planar form in Fig. 4. The polar octahedron is simpler than two polar tetrahedra [1] and can readily be constructed.

The use of the term double position "twinning" for polarity reversal nucleation is unavoidable in relation to the terminology of epitaxial growth but is open to misinterpretation. It is therefore necessary next to discuss twinning and the Friedel index.

3. Coincidence lattices and the Friedel index

In 1926 Friedel [18] introduced the concept of the twin index and proved a remarkable theorem about coincidence lattices. This work is important for our purposes and is not as well known as it should be. The only account in English is in a simplified form apparently relating to cubic system structures only [19]. Therefore Friedel's argument will be briefly outlined here.

Suppose that two regions of a crystal are

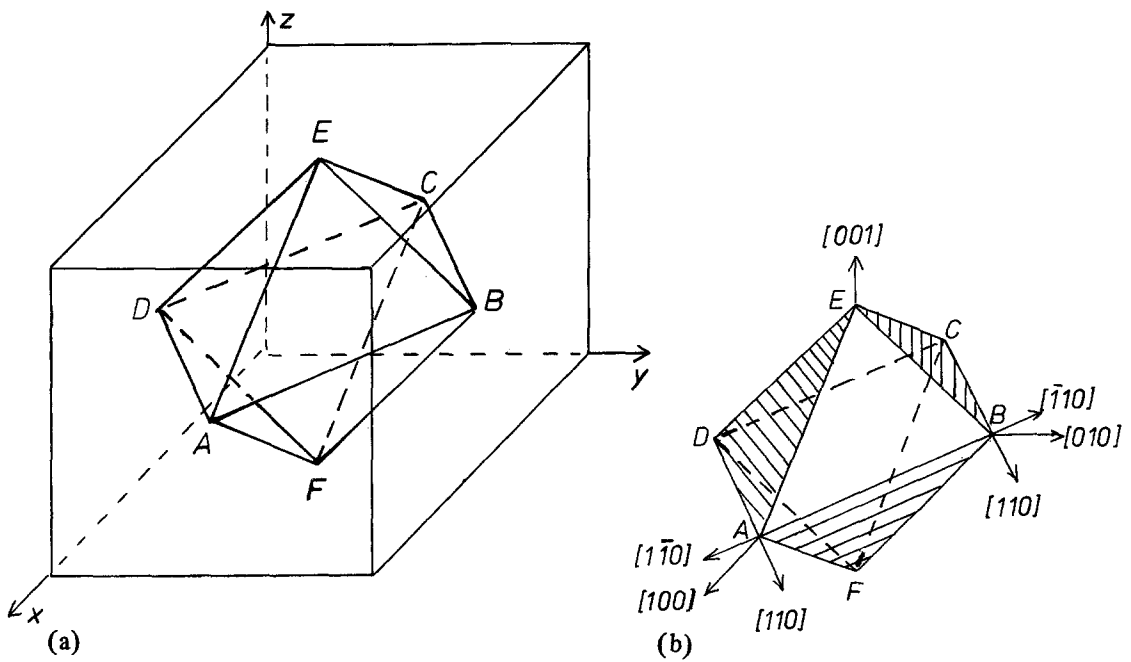


Figure 3 The polar octahedron of $\{111\}$ A and $\{\bar{1}\bar{1}\bar{1}\}$ B faces in the sphalerite structure (a) inscribed in an fcc unit cell for purposes of orientation and indexing and (b) with the three visible $\{\bar{1}\bar{1}\bar{1}\}$ B faces cross hatched and certain directions indexed.

twinned with respect to a mirror plane (pqr) or a twin axis $[ghk]$. Imagine the space lattices of the twin and matrix to be continued through the interface (composition plane). A certain fraction, f , of the lattice sites of the twin and matrix orientations will be found to coincide to constitute a "coincidence lattice" [18, 20]. The super-lattice of coincidence sites has a unit cell of volume V . This is

defined to have as its base the smallest two-dimensional mesh in the mirror plane (pqr) and its height is the coincidence site spacing in the direction $[hkl]$ normal to this plane. Alternatively $[ghk]$ may be the twinning axis and (pqr) the plane normal to it. The volume of the coincidence lattice cell V is an integral multiple of the volume of the unit cell of the original structure, v . Two

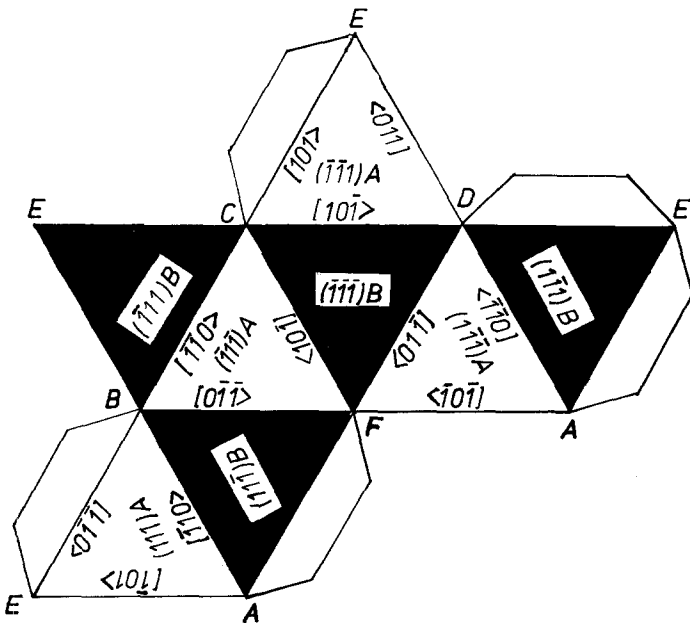


Figure 4 The polar octahedron drawn out flat. The four $\{111\}$ A faces are parallel to the faces of the Thompson's tetrahedron. Accordingly the four $\{111\}$ A faces are indexed as in Hirth and Lothe [36]. However, as the polar octahedron is used to represent macroscopic polar symmetry, the octahedron, unlike Thompson's tetrahedron is not of atomic dimensions, i.e. the edges are not of length $a/2 \langle 110 \rangle$. The symbol $\langle \rangle$ is used, following Hirth and Lothe, to indicate the sense of the direction indexed. The $\langle 111 \rangle a$ directions are the outward drawn normals to the corresponding $\{111\}$ A faces and the $\langle \bar{1}\bar{1}\bar{1} \rangle b$ directions are the outward drawn normals to the $\{\bar{1}\bar{1}\bar{1}\}$ B faces of the same indices.

cases must be distinguished. If V has no site at its centre nor at the centres of its faces other than (pqr) , the twin index is

$$I = V/v. \quad (1)$$

In those cases in which one of the aforementioned conditions do not hold, the twin index is

$$I = V/2v. \quad (2)$$

The twin index is the ratio of the volume per coincidence site to the volume per lattice site. The fraction of coincidence sites is the reciprocal of this, i.e.

$$f = 1/I. \quad (3)$$

Following Friedel, we consider first the case of lattices having primitive cells. Let the origin be at a point O , and g, h, k cleared of common factors. Then, g, h, k are the coordinates of the first coincidence site N on the line $[ghk]$ proceeding from the origin. The plane parallel to (pqr) passing through N has the equation

$$\frac{px}{a} + \frac{qy}{b} + \frac{rz}{c} = pg + qh + rk = \pm \Sigma. \quad (4)$$

The integer Σ is the number of lattice planes included between the plane passing through N and the origin. The volume V of the coincidence lattice cell erected on (pqr) and $[ghk]$ is therefore equal to Σv .

If Σ is odd, the index of the twin having twin plane (pqr) or twin axis $[ghk]$ is therefore

$$I = \Sigma = pg + qh + rk. \quad (5)$$

If Σ is even, there is a plane of the series (pqr) which cuts the line ON at its mid-point. The coincidence lattice cell can still be chosen of such a form that it might have a point at its centre or at the centre of one of its lateral faces. Therefore the conditions require the use of Equation 2 rather than Equation 1 so

$$I = \Sigma/2. \quad (6)$$

Friedel worked through the cases of the coincidence lattice cell being primitive P , (above), or centred on face ab (in the (pqr) plane), C , or body centred, I , or finally face centred, F . The results (recapitulating results 5 and 6 for completeness) were as given in Appendix I.

Thus Friedel proved the powerful theorem that for all Bravais lattices and all orientation relationships between two grains the Friedel index must

always be an odd integer. In other words, for all lattices, the only possible fractions of coincidence lattice sites are $1/3, 1/5, 1/7 \dots$

In the particular case of crystal structures of the cubic system the perpendicular plane and direction have the same Miller indices. Let these be (hkl) and $[hkl]$. Then $[20]$ (substituting into Equation 4)

$$\Sigma = h^2 + k^2 + l^2. \quad (7)$$

In addition, for crystal structures based on the fcc lattice such as the diamond and sphalerite structures the rules of Case D in Appendix I apply.

For the diamond and sphalerite structures the first order twin has, e.g. $(pqr) = (111)$ so that $I = \Sigma = 3$. The second order twin has (pqr) given, for example, by (221) so that $I = \Sigma = 9$. In general the n^{th} order twin has $I = (\Sigma)^n$. Twinning in structures based on the fcc lattice can be regarded as produced by twofold (180°) rotations about $\langle 111 \rangle$ axes. One such rotation produces a first order twin orientation. Two successive such rotations about two different $\langle 111 \rangle$ axes produce a second order twin and so on.

Values of the Friedel index I other than $(3)^n$ such as 5 and 7 correspond to highly symmetrical (high coincidence-site density) orientation relations which are not twinning relations. They are to be expected to have low energy, high coincidence-site area-density, grain boundary interfaces associated with them.

A critical discussion of the coincidence lattice was given by Fletcher [21]. The first systematic treatment of the sub-symmetry operations giving rise to these (partial) coincidence lattices was unpublished work of F. C. Frank in 1958 quoted in [22] and [23]. In this he developed procedures for obtaining coincidence lattices for rotations about $[100]$ and $[111]$ axes in the cubic system. C. G. Dunn and H. Brandhorst in 1959 in further unpublished work [22, 23] developed a procedure for rotations about $[110]$. Raganathan published a generalized treatment for the cubic system and a number of solutions listing the axis and angle of rotation and the relative density of coincidence lattice sites, Σ , have appeared [22, 23]. Later Bollmann and co-workers [24, 25] extended the idea to define other types of derived lattices useful in treating interfaces and orientation relationships. Recent work on the structure of grain boundaries in diamond structure materials employs the coincidence site lattice [26, 27]. In this paper the

idea of the (partial) coincidence lattice and the (partial) symmetry operations corresponding to them will be extended to polarity and its reversal in the cubic sphalerite structure.

4. Anti-coincidence lattices, coloured antisymmetry operations and unity and negative Friedel indices

Coincidence lattices are lattices in which a fraction of the sites of Lattices 1 and 2 coincide and Friedel's index is the reciprocal of this fraction f . The symmetry operations of a crystal structure bring about complete self-coincidence, that is they carry every lattice point to another, and every atom to an equivalent atomic site. The Friedel index can clearly be extended to this case and is then $I = 1$ corresponding to $f = 1$.

An anti-coincidence array or "complex" [28, 29] is one in which a fraction of the atomic sites of the two crystal structures coincide, but in all cases wrongly. In traditional crystal symmetry all lattice sites are equivalent. Coloured symmetry deals with the symmetry of lattices in which points were made distinguishable by colouring say half white and half black. A new class of "antisymmetry" operations are then possible. These carry each lattice site to one of opposite sign or colour [16]. Binary semiconducting compounds have dichromatic (two colour: black and white) symmetry. Antisymmetry operations produce full anti-coincidence, i.e. pure polarity reversal in lattices. Partial antisymmetry operations will produce anti-coincidence of a fraction of sites. Exchange operations produce the corresponding anti-coincidences in crystal structure complexes [17]. A systematic discussion of the dichromatic point group symmetry of the sphalerite and wurtzite structures will be given in relation to the polarity of their physical and chemical properties in a later paper.

Complete polarity-reversal, i.e. antisymmetry exchange operations in crystal structures produce complete anti-coincidences with Friedel index $I = -1$ and represent the "orientation relation" of "antiphase", polarity reversal domains. The colours of all the faces of the polar octahedra of Figs. 3 and 4 are exchanged for $I = -1$.

Polarity reversal twins have Friedel indices $I = -(3)^n$. These orientations are produced from the original, matrix orientation by repeating n times the twinning operation of 2-fold rotation about $\langle 111 \rangle$ axes, no two successive axes being the

same, and an antisymmetry exchange operation. Similarly, high anti-coincidence site density grain orientations have Friedel indices $I = -5, -7 \dots$. They are produced by sub-symmetry operations [22, 23] producing the orientations $I = 5, 7 \dots$ and a polarity reversal, "anti-symmetry" exchange operation.

5. Antiphase domains and polarity reversal twins

The extended range of Friedel indices makes clear the distinction between pure polarity reversal or antiphase domains ($I = -1$) and polarity reversal, inverted or "para" twins ($I = -(3)^n$). This distinction underlines the ambiguity of the term "double position twinning" for the epitaxial nucleation mechanism producing pure polarity reversal.

First order inversion twins in the sphalerite structure were considered by Aminoff and Broome [30] and by Buerger [31]. The latter found that deformation twins were not inverted in minerals. Ball-and-wire model analysis of the core structures of dislocations in the sphalerite structure showed that two forms of dissociated dislocation were possible corresponding to each one in the diamond structure [32]. These differed in that one had an upright stacking fault whereas the other had an inverted stacking fault. The widening of such a dissociated dislocation produces a single double atom layer of inverted material. Passage of a similar partial dislocation over every successive slip plane parallel to the $\{111\}$ twin composition plane would produce a deformation inverted twin. That this was found not to happen [30, 31] shows that, at least under normal circumstances, twinning dislocations in the sphalerite structure are of the type corresponding to upright fault dissociation.

6. Discussion

The notation introduced above makes explicit the distinction between polarity reversal domains for which $I = -1$ and (polarity) inversion twins for which $I = -(3)^n$ where n is the order of the twin. The negative sign indicates antisymmetry exchange, i.e. "antiphase" reversal of the sign of the site occupation function and in general a consequent reversal of the actual sign of the ions at all sites.

Polarity reversal domains (and APB's) are high energy defects and are apparently produced only as growth defects. Growth mechanisms include double position twinning and nucleation on either

side of polarity reversal steps in the substrate in epitaxial deposition. Polarity reversal twin and polarity reversal grain boundaries are also of high energy and form only during growth.

In the case of metal alloys, the antiphase operation can be produced by a shear and dislocation mechanisms are involved in order disorder transformations which proceed by increasing or decreasing the area of APB per unit volume. In the sphalerite structure no antiphase shear exists and although stacking faults of inverted polarity in extended dislocations are geometrically conceivable [32] no macroscopic thermal disorder has ever been observed in binary compounds with these structures. Sphalerite–chalcopyrite structure disorder–order transformations do occur in ternary II IV V₂ and I III VI₂ compounds [33, 34] and there is now some transmission electron microscope evidence for the occurrence of super dislocations containing APB's in ZnSiP₂ [35]. A new “bicrystallographic” coloured symmetry theory [28, 29] can predict the dislocation content of such interfaces. It will be applied to the case of sphalerite on diamond heterojunction interfaces in various orientations in a future paper.

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Appendix 1: Values of the Friedel twin index I

Case A

If the coincidence lattice has a primitive unit cell and Σ is odd then $I = \Sigma$ ([5] above)
but if Σ is even then $I = \Sigma/2$ ([6] above).

Case B

If the coincidence lattice is base (ab) centred and if $p + q$ is odd and ghk unrestricted then
 $I = \Sigma$

and if $p + q$ is even, $g + h$ and k not both even
 $I = \Sigma$ if Σ odd but $I = \Sigma/2$ if Σ even

and if $p + q$ is even, $g + h$ and k both even,
 $I = \Sigma/2$ if $\Sigma/2$ odd and $I = \Sigma/4$ if $\Sigma/2$ even.

Case C

If the coincidence lattice cell is body centred and $p + q + r$ is odd and ghk unrestricted $I = \Sigma$
and if $p + q + r$ is even and ghk are not all odd
 $I = \Sigma$ if Σ odd but $I = \Sigma/2$ if Σ even.

Case D

If the coincidence lattice cell is face centred

and pqr are not all odd and $g + h + k$ is odd $I = \Sigma$
and if pqr are all odd and $g + h + k$ is odd $I = \Sigma$
(necessarily odd)

and if pqr are not all odd and $g + h + k$ is even
 $I = \Sigma$ if Σ is odd $I = \Sigma/2$ if Σ is even

and if pqr are all odd and $g + h + k$ is even $I = \Sigma/2$ if $\Sigma/2$ is odd $I = \Sigma/4$ if $\Sigma/2$ is even.

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