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THE STRUCTURE AND CRYSTALLOGRAPHY OF LATERAL TWIN BOUNDARIES IN SILICON

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Résumé. - La structure de la macle (211) du silicium est discutée. Une structure constituée de cycles à 5 et 7 atomes est proposée ; elle ne comporte pas de liaisons pendantes et ne nécessite qu'une faible distorsion de l'environnement tétraédrique. On montre que le modèle est en excellent accord avec des mesures expérimentales récentes de la position relative des deux cristaux adjacents. L'interface est également étudiée du point de vue cristallographique et toutes les variantes de ce type d'interface sont énumérées.

Abstract. - The structure of lateral twin boundaries in silicon is discussed. A structure comprising five and seven membered rings is proposed which contains no dangling bonds and little distortion of the tetrahedral bonding. The model is shown to be in excellent agreement with recent experimental measurements of the relative position of the adjacent crystals. The crystallography of the interface is also considered, and all the equivalent variants of this type of interface are enumerated.

1. Introduction. - The purpose of this paper is to discuss the structure and crystallography of lateral twin boundaries in silicon. Using the terminology of the coincidence-site-lattice theory, such boundaries are referred to as \( \Sigma = 3 \), \{211\} boundaries. We shall show that recent experimental measurement of the relative position of the adjacent crystals supports a model of the boundary structure which has no dangling bonds and very little distortion of bond lengths and inter-bond angles. The symmetry of lateral twin boundaries is also discussed using a crystallographic methodology developed recently. One advantage of this method is that all the variant forms of a given interfacial structure and their inter-relationships are clearly shown.

The structure of lateral twin boundaries. - The structure of lateral twin boundaries has received considerable attention over the last two decades. Hornstra (1) suggested that the boundary structure is best regarded as a symmetrical tilt boundary comprising partial edge dislocations with Burgers vectors of the type \( 1<211> \). Kohn (2) proposed that the boundary structure is faceted with atomic-scale steps parallel to \{114\} planes(\{110\} planes using the coordinate system of the other crystal). Both these models involve two dangling bonds per period of the boundary. Möller(3) has also considered this boundary recently and, on the basis of an approximate estimation of interfacial energy, concluded that Hornstra's model is less likely since it contains more distorted bonds. Fig. 1 is a schematic representation of a lateral twin boundary viewed along a common \(<011>\) direction. This configuration displays mirror symmetry across the interface and has atoms occupying coincidence positions; this structure resembles closely that suggested by Möller(3). Inspection of the drawing shows that although bond angles and lengths do not appear much distorted, one of the coincidence atoms (per period) has only three immediate three neighbours while the other has five, thereby leading to two dangling bonds per period.
Fig. 1: Schematic drawing of a lateral twin boundary in silicon exhibiting anti-mirror symmetry across the interface. The projection direction is [011], and large and small circles represent the ...ABABA... stacking along this direction.

In a recent study (4), the relative position of the adjacent crystals at lateral twins was measured accurately using transmission electron microscopy. It was found that the relative position of the crystals does not correspond to mirror or mirror-glide symmetry across the interface. Instead, on a (211) boundary, it was found that one crystal was translated away from the coincidence position by \( \mathbf{t} = (0.145, 0.115, 0.115) \). This displacement can conveniently be regarded as comprising two components, one \( 0.125(111) \) parallel to the interface, designated \( t' \), and the second \( 0.01[211] \) which is perpendicular to the interface, designated \( t_\perp \), and which corresponds to the introduction of excess volume at the interface.

Now the experimental method used by Vlachavas and Pond (1981) does not reveal directly the atomic structure at the interface. In particular, the method is insensitive to changes of structure brought about by re-location of the interfacial plane and/or local atomic relaxations. For the measured relative position the three possible structures (excluding symmetry degeneracies) of the (211) boundary obtained by re-locating the interfacial plane but excluding local atomic relaxation were depicted by Vlachavas and Pond (4). They concluded that in none of these structures could all the interfacial atoms be tetrahedrally coordinated without substantial distortion to bond lengths and angles. In the present paper we report the conclusion of a further investigation of these possible structures in which local relaxation has been studied by modelling using balls and springs.

In view of the distortion described above, it was decided to try removing particular atoms from the interfacial region. Fig. 1 shows that the basis of the
structure can be regarded as a pair of atoms separated by $\frac{1}{4}[\overline{111}]$ which is parallel to the interface. The least distorted structure was obtained from the structure depicted in the upper right of fig. 5 of Vlachavas and Pond (1981) by removing the left hand atom from basis pairs in the lowermost layer of the upper crystal and similarly from basis pairs in the uppermost layer of the bottom crystal. On reconstructing the bonds, the resulting ball and spring model was found to be mechanically stable at the experimentally measured relative position, to contain no dangling bonds and to exhibit little distortion. A spoke model of this structure is shown in fig. 2, and the traces of (111) planes have been indicated to show the excellent agreement between the model and the measured value of $t$. Expressed as a proportion of the (111) inter-planar spacing, $d_{\overline{111}}$, the magnitude $|t|_{\overline{111}}$ is $0.38 d_{\overline{111}}$.

Fig. 2 shows that the boundary structure can be regarded as comprising non-equivalent five-member and seven-member rings arranged alternately two per period. The seven-member rings provide rather open channels parallel to $[\overline{111}]$, and the model is consistent with the small magnitude of the measured component $t_{11}$. We note that Fontaine and Smith (5) have also proposed a structure for this boundary comprising five and seven-member rings, although no supporting experimental observations were obtained, and the relative translation, $t_{x}$, and high symmetry they suggest are not consistent with the present model.

Fig. 2: Spoke model of relaxed lateral twin boundary exhibiting no dangling bonds and little distortion.
Crystallography of lateral twin boundaries.- The symmetry of interfacial structures has been treated recently (6,7) using the theory of composite entities. In the case of grain boundaries the two entities, which can be the two crystal lattices or the two crystals themselves, are crystallographically equivalent. If, as in the present case, these equivalent entities are related by a symmetry operation (symmetrising operation), the symmetry group of the composite is given by the intersection of the symmetry groups of the components extended by the symmetrising group (which must be of order 2 in the case where there are 2 components). In addition, if we regard one entity as being black and the other as white, symmetrising operations are readily distinguished from ordinary operations since they involve colour-reversal (antisymmetry operations). The crystallographic methodology employed is to find the highest possible symmetry group for the composite, called the embracing group, and to investigate subsequent reduction of symmetry (dissymmetrisation) in the stages leading to the relaxed minimum energy interfacial structure. Each stage of dissymmetrisation leads to the existence of crystallographic variants, and by using the law of symmetry compensation we can identify the number and inter-relation of the variant forms. It is convenient to consider four stages of dissymmetrisation leading to four types of variants, viz. orientational, complex, morphological and relaxational, and these are discussed below.

I) Orientational variants. - Consider a white and a black fcc lattice (space group Fd3m) having a coincident origin and which are relatively rotated by 180° about <211>, i.e. to be in a Ë=3 twin orientation. Let this orientation relationship be represented by the matrix operator, R', where the prime indicates colour reversal. Let the 48 point symmetry operations of the space group of the black and white lattices be designated D*(u) and D*(λ), respectively. The pattern of black and white sites is called a dichromatic pattern, and the ordinary symmetry operations of this pattern are given by the solutions of D*(λ) = R'D*(u)R' -1. In the present case there are twelve solutions, designated D*(p), which correspond to the point group 3m. Since R' corresponds to an antisymmetry operation, 2', the antisymmetry group of the dichromatic pattern can be regarded as 3m extended by 2', i.e. to correspond to 6mm'; the space group of the dichromatic pattern is P6'mm'(6). Thus, the dichromatic pattern has point symmetry comprising twelve ordinary operations, D*(p), and twelve antisymmetry operations, designated D*(p)', given by D*(p)' = D*(p), R'; one of this latter set is, for example, a rotation of 60° about [111] corresponding to the operation 6'.

It is seen that by bringing together the black and white lattices all the elements D*(λ) and D*(u) which do not correspond to ordinary elements D*(p) have been destroyed. Now according to the law of symmetry compensation such reduction of symmetry leads to the possibility of crystallographic variants, and the operations relating the variants can be obtained by decomposing the original group, Fd3m, which has order 48, with respect to the group 3m, which has order 12. The result of this decomposition is the group 4 = (1,2,41,42), where 42 denotes a rotation of 90° about [001]; in other words four orientation variants exist where the orientation relationships are given by (1,2,41,42)6'. Fig. 3(a) shows schematically black and white cubes which are twin related by rotation of 60° about a common body diagonal. The above analysis corresponds to the well known result that the four orientation variants would be obtained by rotations of 60° about the four body diagonals.

II) Complex variants. - A silicon crystal has a structure which is described most concisely by considering it to comprise one basis, which consists of a pair of atoms separated by 1<111>, located at each fcc lattice point. The symmetry group of the black or white lattice-complex (as opposed to the lattice) is Fd3m, which is holosymmetric but non-symmorphic. When a dichromatic complex is formed, i.e. the pattern of interpenetrant lattice-complexes, it may be dissymmetrised (with respect to the dichromatic pattern) by the presence of non-symmorphic operations in its components, as, for example, occurs in the case of rotations about [001] (7). However, in the Ë=3 case the dichromatic complex and pattern have identical symmetry and thus no complex variants exist.
Fig. 3: a) Interpenetrant black and white twinned cubes; the arrow indicates the common <111> axis. b) As (a) but viewed along the common <111> axis to show that the point symmetry of the aggregate is $6' \text{mm}'$.

iii) Morphological variants. - An ideal bicrystal can be created from a dichromatic complex by selecting the interfacial plane and discarding white bases on one side of the interface and black ones on the other. A possible form of a holosymmetric bicrystal obtained on (211) in this way is shown in fig. 1. This composite object has the layer spatial group p2'\text{mm}' (i.e. a spatial group with only two dimensional translation symmetry). Since this process of creating a bicrystal in this way has caused dissymmetrisation, variant bicrystal forms with crystallographically equivalent interfacial orientations, designated morphological variants, exist, and the inter-relation of these can be obtained by decomposing p2'\text{mm}' with respect to p2'\text{mm}' (see 7 for details). Six morphological variants exist corresponding to bicrystals with interfaces parallel to the three (211) planes containing the ordinary three fold axis of the dichromatic complex and their colour reversed counterparts.

These six morphological variants are depicted schematically in fig. 3(b) which shows a projection along the ordinary three-fold axis of the twinned cubes in fig.3(a). The (211) interfaces correspond to the vertical antimirror planes; three variants are seen in the upper part of the diagram, and the three colour reversed forms are below the (111) antimirror plane which is parallel to the page. We note that the complete composite shown in fig.3. displays the point symmetry $6' \text{mm}'$, and corresponds to six black and six twin-related white crystallites each exhibiting mirror symmetry in their external morphology and arranged in an aggregate with (211) and (111) antimirror variant interfaces. It is interesting to speculate that twinned crystals which display the morphology of fig. 3(a), such as fluorite (8), actually have an internal structure as discussed here.

iv) Relaxational variants. - Realistic boundary structures can be obtained from ideal holosymmetric bicrystals by allowing relaxations such as changes of the relative position of the adjacent crystals and local atomic relaxation. The relaxations involved in the creation of the favourable structure, shown in fig. 2, from the idealised structure of fig. 1 have been described. The spatial group for the
favourable structure is pml, and thus dissymmetrisation has occurred. The variants are designated relaxation variants, and two such variants exist related by the operation m' (or 2'). These two variants are depicted schematically in fig. 4.,

![Schematic illustration of relaxational variants](image)

where the black and white motifs represent one period of the interfacial structure. Such variants can exist on the same interfacial plane, and since t_\# has opposite sign for each structure, they would be separated by a dislocation with Burgers vector equal to 2t_\# + b_{dsc}, where b_{dsc} is either zero or some vector of the dsc lattice. For example, a dislocation with Burgers vector = \frac{1}{3}[111] could dissociate as follows (putting t_\# = \frac{1}{8}[111])

$$\frac{1}{3}[111] + \frac{1}{4}[111] + \frac{1}{12}[111]$$

The two partial grain boundary dislocations would separate domains of variant structures, and a step one (422) plane high would be associated with the \frac{1}{3}[111] dislocation. Dissociations of this type were not observed experimentally (4), unlike the case of crystallographically equivalent boundaries in aluminium (9), and an investigation of the core structure of such grain boundary dislocations is in progress.

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