TWINNING IN DERIVATIVE STRUCTURES OF BCC AND FCC

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Introduction

The literature on the deformation twinning of superlattice structures is rather sparse and usually concerns specific examples rather than the general theory. Early demonstrations (1-3) that the simple shears of the normal bcc and fcc deformation twinning modes produce orthorhombic structures when applied to the ordered cubic B2 and $L1_2$ structures respectively have led some authors to conclude (incorrectly) that these modes cannot give true twins in any superlattice. Moreover, although geometrically possible twinning modes of higher shear have been identified in the two structures just mentioned (3), it is sometimes incorrectly implied that such modes do not exist for other superlattices, e.g. DO_3. In this paper, we briefly note some general rules governing the possible twinning modes of both cubic and non-cubic superlattice structures derived from disordered bcc or fcc solid solutions.

Our treatment is based on the Bilby-Crocker (4) and Bevis-Crocker (5,6) formulation of the theory of deformation twinning, and we make the simplifying assumption that the twinning shear must reproduce the superlattice structure in a new orientation without any atomic "shuffles". (In a full treatment, which will be published elsewhere, shuffle modes have to be considered as possibilities, and there is recent experimental evidence (7) for the operation of such a mode in the B2 structure.) We are concerned only with modes which produce twins in both the superlattice structure and the ideally disordered structure, so that we exclude "order twins" as defined by Hanssom and Barnes (8); these are essentially anti-phase domain boundaries, and the hypothetical shear which could produce them in the superlattice corresponds to homogeneous slip in the disordered structure.

Laves (9) distinguished between true twinning and pseudo twinning (or between twinning and "twinning"); a pseudo twin will have its atomic sites in twin relation to those of its parent crystal but the occupancy of these sites will be incorrect. Cahn (10) points out that in a strict sense there are not true twins, but we think, nevertheless, that the distinction between true twinning and pseudo twinning in ideal, perfectly ordered superlattices may be important in real materials. Pseudo twinning will be discussed only in relation to the normal deformation twinning modes of the bcc and fcc structures; if all variants of this mode are pseudo modes in the superlattice structure, we consider what other modes (necessarily of higher shear) will give true twins. Consider first superlattice structures of stoichiometric composition A_nB with only one formula unit per primitive unit cell so that the lattice points of the fully ordered structure may be defined by the complete set of B atoms. The condition for a given mode to represent a true twin is then simply that all B atoms are carried into correct twin positions by the shear. Hence, it is sufficient to ensure that there are no "lattice shuffles"; "structure shuffles" (11) need not be considered. For any mode variant, the parameters q and $\overline{q}$ defined in (4) may be derived analytically or by examination of the positions of the B atoms in a unit cell defined by η_1, η_2 and the normal to the plane of shear. The mode is then a pseudo twin if both q and $\overline{q}$ are greater than 2. If there is more than one B atom in the smallest unit cell, as in the B32 superlattice structure, for example, it is necessary to examine whether both B atoms are sheared into correct twin positions, i.e. to consider whether structure shuffles are required. The condition for the absence of such shuffles is that the motif unit lies within the K_1 or K_2 planes, and this is specified for the B32 modes considered here.

Cubic Superlattice Structures

In the ground state diagrams of Richards and Cahn (12) which are based on first and second nearest neighbour pairwise interactions, there are three cubic superlattices of the bcc structure and one of the fcc structure. The bcc superlattices may be readily related to each other by using the enlarged 16 atom unit cell shown in Fig. 1. The atom sites are regarded as situated on four interpenetrating fcc lattices, different occupancy of which gives the B2 and B32 structures of composition AB and the DO_3 structure of composition A_3B. The usual twinning mode of the bcc structure has K_1 and K_2 planes of type {112} and the two corresponding shear directions η_1 and η_2 are of the type ⟨111⟩. In a pure

metal or a completely disordered solid solution, the smallest lattice vectors parallel to these directions are nearest neighbour vectors and cross two lattice planes of type {112} so that q and $\bar{q}$ are both equal to 2. However, this vector is doubled in the B2 structure and quadrupled in the other two ordered structures, so that $q,\bar{q}$ are respectively 4 and 8 for this mode which can not give rise to a true twin without shuffles in any of the superlattices. Two other hypothetical twinning modes which have the same K_1 plane but different η_2 are now of interest. If η_2 is parallel to <001> and the direction of η_1 is reversed, the so-called "anti-twinning" mode of the bcc structure is obtained; it has a shear twice as large as the normal mode, and as has previously been demonstrated, could give rise to a true twin in B2 but not in B32 or DO_3. However, examination of Fig. 1 shows that a shear on {112} in the normal sense but of four times the normal magnitude has η_2 in a <110> direction and $q,\bar{q}=2$ for all the superlattice structures. Thus this improbably large shear could geometrically produce a true twin in all three superlattice structures.

Arunchalaman and Sargent (3) pointed out that some of these results may be deduced directly from the list of twinning modes in cubic lattices given in Table 1 of the second Bevis and Crocker paper (6). Each entry in this table actually represents four possible modes made up of two mode pairs. The modes of a pair are conjugate or reciprocal to each other and are related by interchanging the two undistorted planes K_1 and K_2 and their associated shear directions. The second mode pair is obtained from the first by interchanging the indices of K_1 and η_1 and K_2 and η_2 and changing the sign of η_1 and K_2. This transposed mode pair is equivalent to a change from direct to reciprocal lattice, i.e. from bcc to fcc or vice versa. For greater clarity, we distinguish between a mode pair and its transpose by adding the superscript T, so that the normal fcc mode is any variant of Bevis and Crocker's mode 2.2, and the normal bcc mode is any variant of 2.2^T. The values of m, m_I and m_F given in Table 1 of (6) are the reciprocal fractions of lattice points sheared directly into twin positions for simple cubic, bcc and fcc lattices respectively, and have values, 2, 4 and 1 for mode 2.2 and 2, 1 and 4 for mode 2.2^T. It follows that for mode 2.2^T, only one-half of the B atoms are sheared to correct twin positions in a B2 structure, since this is simple cubic, and only one-quarter in the B32 or DO_3 structures which are both face-centred. The lowest shear mode which could give a true twin in a B2 structure is 1.3^T of the Bevis and Crocker table, but one-half of the lattice points of the superlattices with fcc symmetry are still incorrectly placed. The mode of even larger shear which could, in principle, twin B32 and DO_3 is not listed in Table 1 of (6) since this table is cut off at a smaller shear magnitude, but examination of the correspondence matrices shows that it is mode 1.9, listed in Table 2 of (5). This mode and its transpose 1.9^T both represent no-shuffle modes in simple cubic, bcc and fcc lattices.

In a similar way, the $L1_2$ superlattice structure forms only a pseudo twin in the usual fcc mode 2.2 but forms true twins in modes 1.3, 1.9^T and 1.9. Specific variants of the modes we have derived are listed in full in Table 1, where S represents the plane of shear and g the magnitude of the shear. The Bilby-Crocker sign convention (4) is used.

TABLE 1

True Twinning Modes (Without Shuffles) in Cubic Superlattice Structures

B-C mode (6)	S	K_1	K_2	η_1	η_2	g^2	True twin in
1.3	(110)	$(1\bar{1}1)$	(001)	$[\bar{1}12]$	$[1\bar{1}0]$	2	$L1_2$
1.3^T	(110)	$(\bar{1}12)$	$(\bar{1}10)$	$[\bar{1}1\bar{1}]$	[001]	2	B2
1.9	$(\bar{1}\bar{1}0)$	$(\bar{1}12)$	(001)	$[1\bar{1}1]$	$[\bar{1}10]$	8	$B2,B32,DO_3,L1_2$
1.9^T	$(\bar{1}\bar{1}0)$	$(1\bar{1}1)$	$(1\bar{1}0)$	$[1\bar{1}\bar{2}]$	[001]	8	$L1_2,B2,B32,DO_3$

Finally, we note that since mode 2.2 is a no-shuffle mode only for a fcc lattice, and 2.2^T only for a bcc lattice, the normal mode of a disordered solid solution of either type can not act as a true twinning mode for a cubic superlattice unless the lattice retains the same Bravais symmetry. This is only possible if the lattice parameter of the cubic unit cell is an integral multiple t of that of the disordered cell, so that the superlattice can form only at stoichiometric compositions A_7B, $A_{26}B$, $A_{63}B...A_nB...$ where $n=t^3-1$. Clearly, such superlattices are improbable, although a structure Ca_7Ge has been reported (13) and Khachaturyan (14) discusses a possible Pt_7Cu superlattice.

Non-Cubic Superlattice Structures

When the formation of the superlattice results in a non-cubic symmetry, it is immediately obvious that some variants of the normal mode will still give true twins in the superlattice. Consider, for example, the CuPt superlattice structure in which alternate parallel planes of a single close-packed set are entirely occupied by Cu and Pt atoms respectively. Choice of these particular planes as the K_1 planes of mode 2.2 will then obviously lead to a true twin. In general, the six equivalent pairs of variants of the normal twinning modes break up into non-equivalent smaller groups, some of which give rise to true twinning modes of the superlattice structure whilst others correspond to pseudo modes. Several non-cubic superlattices are derived from fcc disordered solutions (12) and have various symmetries down to monoclinic. Detailed consideration of the various superlattices will be given elsewhere; here, we briefly summarise the results and give one example.

All modes derived from 2.2 are necessarily compound in the usual definition of this term for deformation twinning, i.e. the indices of the crystallographic planes and directions defining the mode are all rational. The structures are also all centrosymmetric, so that only two orientation relations need be considered. In some cases, however, these orientations are distinct, a possibility not envisaged for compound twins in many elementary discussions, so that there are two types of compound (true) twins derived from mode 2.2. We distinguish these as "combined" and "I/II" (or "II/I"). Combined means that the superlattice plane derived from the plane of shear, S , remains a mirror plane of the superlattice, and there is then only one possible orientation relation. I/II means that a type I orientation is produced in the direction mode without shuffles, whereas a type II relation could only be obtained by some additional shuffling, and the reverse is true of the conjugate or reciprocal mode.

As an example, consider the orthorhombic Pt_2Mo type superlattice which has space group Immm with six atoms in the body-centered orthorhombic unit cell. The base vectors of this cell may be defined by the fcc cubic vectors $1/2[\bar{1}10]$, [001] and 1/2[330]; these correspond to those given in (12) except that the sign of the first vector has been reversed to keep the set right-handed. Table 2 shows the three different types of modes which result from variants of the 2.2 mode and give rise respectively to combined, I/II and pseudo twins of the superlattice structure.

TABLE 2
True Twins and Pseudo Twins in Pt_2Mo Superlattice Structure

S (cubic)	S (superlattice)	K_1	K_2	η_1	η_2	g	$\bar{g}$	Type
(110)	(001)	(110)	$(1\bar{1}0)$	$[1\bar{1}0]$	[110]	2	2	Combined
$(01\bar{1})$	$(1\bar{2}3)$	(013)	(110)	$[93\bar{1}]$	$[\bar{1}11]$	2	6	I/II
$(\bar{1}10)$	(100)	$(0\bar{1}3)$	(013)	[031]	$[0\bar{3}1]$	6	6	Pseudo

In the superlattice structure, two of the cubic {111} planes become {110} planes of the orthorhombic lattice, and the other two become {013} planes. Fig. 2(a) shows that all 1/2<112> repeat vectors of the disordered fcc structure in the first type of close-packed plane remain repeat vectors of the superlattice, but Fig. 2(b) shows that in the second type, such vectors are only one-third of superlattice repeat vectors. Fig. 3 shows perspective views of the unit cells of the original structure which are sheared into equivalent cells of the twinned structure for variants which lead to genuine twins. The twin with a "combined" orientation relation (Fig. 3(a)) has both K_1 and K_2 planes of the first type, and the orthorhombic (001) planes of shear each consist entirely of either A atoms or B atoms in a six-plane repeating sequence ...BAABAA... . A type I orientation relation results if the K_2 plane is of the type shown in Fig. 2(a) and the K_1 plane is of the type shown in Fig. 2(b) (see Fig. 3(b)); if these planes are interchanged, the orientation relation is of type II. Note that four of the six variant pairs give type I/II twins. The corresponding representation of the pseudo mode is shown in Fig. 4.

If the atom positions remain unchanged on the formation of the superlattice, $g^2=1/2$ for all true and pseudo modes derived from 2.2 or $2.2^{\dagger}$. However, relaxation of the atomic positions on ordering will lead to new lattice parameters consistent with the symmetry of the structure, and if this symmetry is non-cubic, the magnitude of g may be slightly changed. Thus in the Pt_2Mo structure, the shears for the three modes of Table 2 may be written respectively as $g = r-r^{-1}$, $g = 1/2(9p^{-2}+r^{-2}+p^2r^{-2}+9p^{-2}r^{-2}-6)^{1/2}$ and $g = (p^2r^{-2}+81p^{-2}r^2-18)^{1/2}/3$ where p=c/a and r=b/a. Without relaxation, the ideal values are p=3 and $r=2^{1/2}$ and all three expressions for g then reduce to $2^{-1/2}$.

It may seem illogical to exclude shuffles since many crystals of symmetry lower than cubic are known to twin by shuffle modes. Clearly, however, interatomic interchange must be excluded in the present context; if it were permitted, the problem addressed here would disappear since the pseudo twin could always re-order to form a true twin. Thus a distinction has to be made for superlattice structures between "interchange" and other shuffles, and we deal with this in another paper.

Acknowledgements

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References

1. F. Laves, *Naturwissenschaften* **39**, 546 (1952).
2. R. W. Cahn and J. A. Coll, *Acta Met.* **9**, 138 (1961).
3. V. S. Arunchalaman and G. M. Sargent, *Scripta Met.* **5**, 949 (1971).
4. B. A. Bilby and A. G. Crocker, *Proc. Roy. Soc.* [A] **288**, 240 (1965).
5. M. Bevis and A. G. Crocker, *Proc. Roy. Soc.* [A] **304**, 123 (1968).
6. M. Bevis and A. G. Crocker, *Proc. Roy. Soc.* [A] **312**, 509 (1969).
7. E. Goo, T. Duerig, K. Melton and R. Sinclair, *Acta Met.* **33**, 1725 (1985).
8. B. Hanssom and R. S. Barnes, *Acta Met.* **12**, 315 (1965).
9. F. Laves, *Acta Met.* **14**, 58 (1966).
10. J. W. Cahn, *Acta Met.* **25**, 1021 (1977).
11. J. W. Christian, *The Theory of Transformations in Metals and Alloys,* Ch. 20, Pergamon Press, Oxford (1965).
12. M. J. Richards and J. W. Cahn, *Acta Met.* **19**, 1263 (1971).
13. O. Helleis, H. Kandler, E. Leicht, W. Quiring and E. Wolfel, *Z. Anorg. Chemie* **320**, 87 (1963).
14. A. G. Khachaturyan, *Progr. in Mater. Sci.* **22**, 1 (1978).

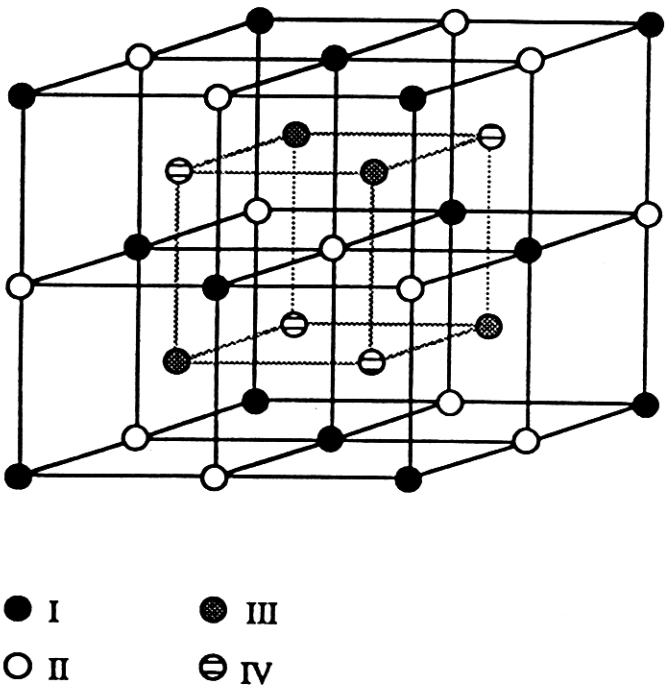

Figure 1. Atomic Site Occupancy for B2, B32 and DO_3 Cubic Superlattices. The sites occupied by B atoms are I and II in the B2 structure, I and III in the B32 structure, and I in the DO_3 structure.

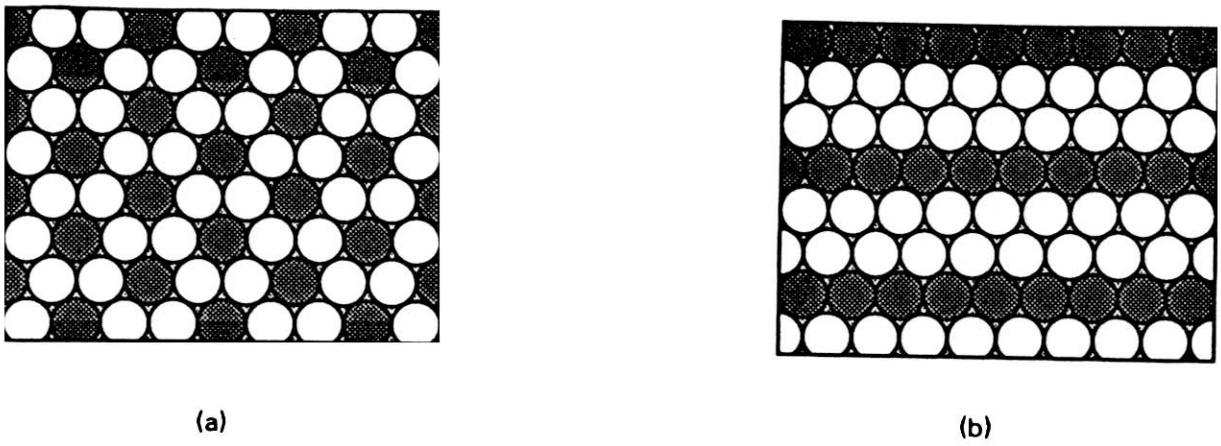

Figure 2. Site Occupancy in Close-Packed Planes of Pt_2Mo Structure. (a) Superlattice {110} planes. (b) Superlattice {031} planes. Shaded circles are Mo atoms, open circles Pt atoms.

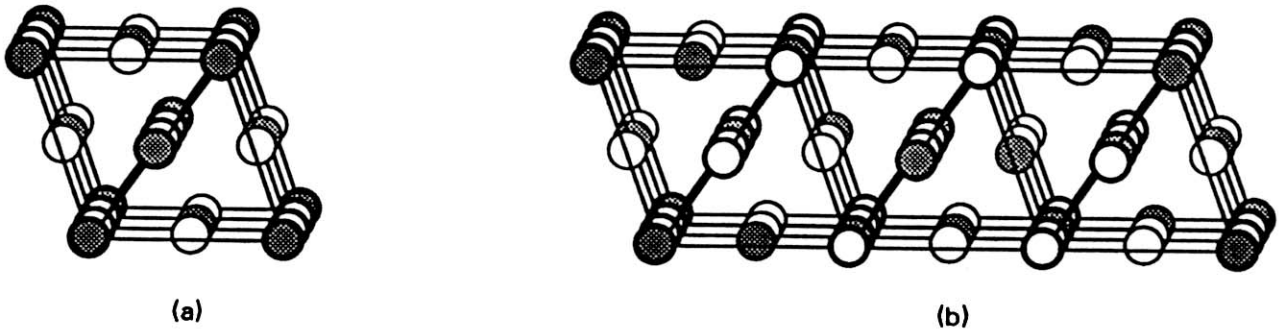

Figure 3. Perspective View of Pt_2Mo Structure for Mode 2.2 Variants Which Lead to Genuine Twins. (a) Combined Mode. (b) I/II Mode. Symbols as in Fig. 2.

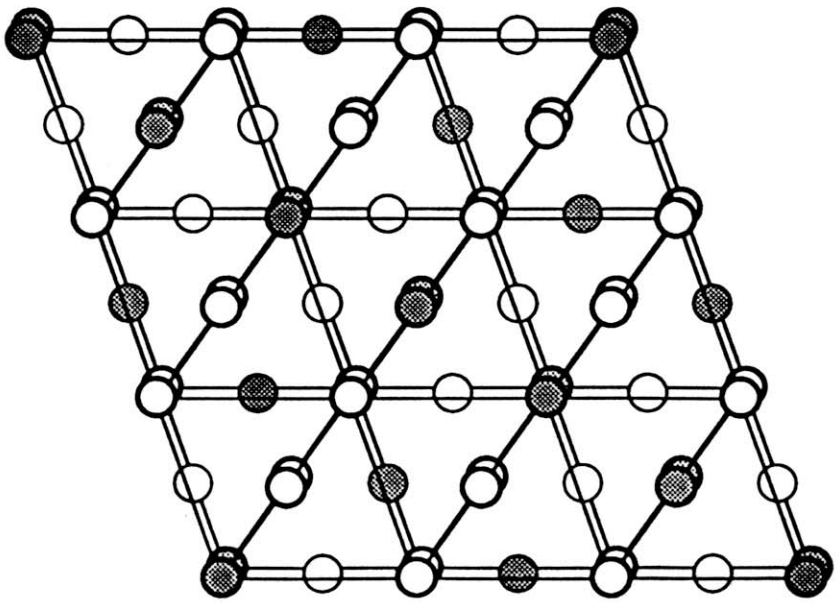

Figure 4. Perspective View of Pseudo-Mode in Pt_2Mo. Symbols as in Fig. 2.