Acta metall. Vol. 36, No. 7, pp. 1617–1642, 1988
Printed in Great Britain.

0001-6160/88 $3.00 + 0.00

OVERVIEW NO. 67

THE DEFORMATION TWINNING OF SUPERLATTICE STRUCTURES DERIVED FROM DISORDERED B.C.C. OR F.C.C. SOLID SOLUTIONS

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(*Received* 23 *November* 1987)

Abstract—The theory of deformation twinning is developed and applied to superlattice structures. With the exception of some hypothetical structures at rather improbable stoichiometric compositions, the normal b.c.c. or f.c.c. twinning shears always lead to "pseudo modes" when applied without "shuffles" to a cubic superlattice. In non-cubic superlattices, however, some variants of the usual disordered mode correspond to true twins whereas others give pseudo twins. True twins in non-cubic superlattices may have type I, type II or "combined" orientation relations, even though all twinning elements are rational, so that all twins are "compound" in the conventional definition. True twins in cubic superlattices may form (geometrically) by non-shuffle modes of higher shear or by modes requiring some "non-interchange" shuffling; there is recent experimental evidence for the operation of such a shuffle mode in a B2 superlattice structure. The paper includes a full discussion of the various true and pseudo twinning modes in all the cubic and non-cubic superlattices which appear in the Richards and Cahn ground state diagrams. Recent experimental work has shown that twinning is often an important deformation mode in superlattices; these experimental results are discussed and shown to be in general agreement with the theory.

Résumé—Nous développons la théorie du maclage de déformation et nous l'appliquons aux surstructures. A l'exception de quelques structures hypothétiques de composition stoechiométrique plutôt improbable, les cisaillements de maclage dans les structures cfc ou cc normales conduisent à des "pseudomodes" quand on les applique à une surstructure cubique sans introduire de déplacements latéraux. Dans les surstructures non cubiques, cependant, quelques variantes du mode désordonné usuel correspondent à des macles véritables, alors que d'autres donnent des pseudomacles. Pour les macles véritables dans les surstructures non cubiques, les relations d'orientation peuvent être de type I, de type II, ou une combinaison des deux, même si tous les éléments de macle sont rationnels; toutes ces macles sont alors "composées" suivant la définition classique. Des macles véritables peuvent être formées (géométriquement) dans les surstructures cubiques par des modes sans déplacement à cisaillement plus important, ou par des modes nécessitant un déplacement sans échange. Des expériences récentes ont montré que ce mode avec déplacement était actif dans une surstructure B2. Nous présentons dans cet article une discussion complète des différents modes de maclage véritable et de pseudomaclage dans toutes les surstructures cubiques et non cubiques présentes dans les diagrammes d'états fondamentaux de Richards et Cahn. L'expérience a montré récemment que le maclage est souvent un mode de déformation important dans les surstructures; nous discutons ces résultats expérimentaux et nous montrons qu'ils sont en bon accord avec la théorie.

Zusammenfassung—Es wird die Theorie der Bildung von Verformungszwillingen entwickelt und auf Übergitterstrukturen angewendet. Die normale Zwillingsscherung im krz und kfz Gitter führt immer zu "Pseudomoden", wenn sie auf kubische Übergitter ohne "Stufung" angewendet werden; ausgenommen sind einige hypothetische Strukturen mit ziemlich unwahrscheinlicher stöchiometrischer Zusammensetzung. Einige Varianten der gewöhnlichen entordneten Mode entsprechen in nichtkubischen Übergittern jedoch wahren Zwillingen, wohingegen andere Varianten Pseudozwillinge ergeben. Wahre Zwillinge können in nichtkubischen Übergittern Orientierungbeziehungen vom Typ I, vom Typ II oder "kombinierte" aufweisen, auch wenn alle Zwillingselemente rational sind, so daß alle Zwillinge im herkömmlichen Sinne "zusammengesetzt" sind. Wahre Zwillinge können sich in kubischen Übergittern (geometrisch) bilden über nicht-gestufte Moden mit höherer Scherung oder über Moden, die eine gewisse "nicht-wechselwirkende" Stufung erfordern. Es gibt neuere experimentelle Hinweise darauf, daß eine solche Stufungsmode in einer B2-Übergitterstruktur auftritt. Die vorliegende Arbeit enthält eine vollständige Diskussion der verschiedenen wahren und Pseudo-Zwillingsmoden in allen kubischen und nichtkubischen Übergittern, die im den Grundzustandsdiagrammen von Richards und Cahn auftreten. Neuere Experimente haben gezeigt, daß die Zillingsbildung häufig eine wichtige Verformungsart in Übergittern ist; die Diskussion zeigt, daß diese experimentellen Ergebnisse mit der Theorie im allgemeinen übereinstimmen.

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1. INTRODUCTION

Our aim in this paper is to develop and apply the general theory of the crystallography of deformation twinning to superlattice structures of both cubic and non-cubic symmetry, and thereby to remove some confusion in the existing literature. Most papers have dealt only with cubic superlattices, and although it has often been stated or implied that such a superlattice cannot be mechanically twinned by utilising the twinning mode of the disordered b.c.c. or f.c.c. structure on which the superlattice is based, a formal proof does not appear to have been given. The original and much cited discussion of Laves [1] is brief and incomplete, and (R.W.) Cahn and Coll [2] and Bolling and Richman [3] considered only particular examples. The result is implicit in the discussions of Arunchalam and Sargent [4] and (J.W.) Cahn [5] but is not explicitly stated. We show in Section 3 that the statement is valid for all cubic superlattices except for a very limited class in which the new structure has the same Bravais lattice and point group symmetry as the disordered structure.

Most recent papers on deformation twinning in superlattices distinguish between "true" twinning and "pseudo" twinning (or between twinning and "twinning"), both terminologies having been suggested by Laves [6]. Cahn [5] argues that true twinning is impossible; he concludes that since there are no truly pure metals, random solid solutions or stoichiometric compounds with perfect long range order, "what we call deformation twinning always entails some structural and symmetry changes". Whilst recognising the purist validity of this statement, we think it self evident that it is useful to distinguish the minor changes due to incomplete order in a superlattice from the major change caused by a shear which does not reproduce the structure even in the ideal, perfectly ordered superlattice of exact stoichiometric composition. Thus we distinguish between true twinning and pseudo twinning for ideal superlattice structures in the belief that this distinction may also be important in real materials. Pseudo twinning, as has often been emphasised, is essentially a stress-induced martensitic transformation; however, it produces (at least before atomic relaxation is allowed) a structure which is fully coherent with the parent phase and which has the same specific volume. We think this merits a special designation and so we shall continue to use the term pseudo twin. Although, in principle, pseudo twinning might arise from various shear systems, we shall generally be concerned only with that particular shear mode which corresponds to the normally observed true mode of the ideal disordered lattice. Thus we shall be interested in four main questions, namely (a) does a particular variant of the disordered mode give a true twin or a pseudo twin in the superlattice structure; (b) what are the structures of any pseudo twins which may be formed; (c) in the event that no true twins may be formed by utilising the normal mode of the disordered structure, what other geometrically possible shears (without shuffles) are available to give true twins in the superlattice, and (d) are there any alternative possible true modes involving some shuffling? We shall consider all those superlattices which appear in the ground state diagrams derived by Richards and (J.W.) Cahn [7] for the binary b.c.c. and f.c.c. solid solutions. Their ground states are based on pairwise first and second near neighbour interactions; de Fontaine [8] has shown how other assumptions such as those made by Khachaturyan [9] can lead to exclusion of some superlattice structures and inclusion of others, but those in the Richards and Cahn paper include all the important structures observed in practice.

One further point should be clarified. In a non-cubic superlattice, it is, in principle, possible to generate a special type of twinned structure from an originally disordered single crystal simply by varying the occupancy of the atom sites. For example, an originally disordered f.c.c. structure of equiatomic composition may form a $L1_0$ (CuAu I type) superlattice by a rearrangement in which alternate atomic planes of any one of the three sets of {100} f.c.c. planes are occupied entirely by atoms of one species. If the ordering produces no relaxation in the interatomic distances, different choices of the {100} planes will produce differently orientated superlattices with the c axes of the tetragonal $L1_0$ structure at 90° to each other in any two regions. These two superlattices are then related by any of the four reflection or rotation relations of the classical theory of twinning. Clearly, as with all forms of twinning, such a configuration could arise from the growing together of independently nucleated regions, but Hannson and Barnes [10] pointed out that deformation twins of this type are also possible. In the $L1_0$ structure, a deformation twin could be produced by glide of a dislocation with a f.c.c. Burgers vector of $\frac{1}{2}\langle 10\bar{1}\rangle$ through each plane of the original f.c.c. {101} set. These displacements correspond to homogeneous slip in the disordered structure and produce a macroscopic simple shear of magnitude $g = 2$. The same displacements in the (unrelaxed) ordered structure give the same simple shear, but now produce a twin of the superlattice. In practice, the lattice parameters change slightly on ordering so that the c axis is no longer equal in length to the original a axes (i.e. the simple tetragonal $L1_0$ cell no longer has its ideal axial ratio of $2^{1/2}$); this slightly changes the magnitude of the twinning shear and the c axes of two twinned regions are no longer exactly perpendicular to each other.

Hannson and Barnes introduced the term "order twins" for twins of this special type, and they have also been called "transformation twins" [11], although many authors reserve this latter term for twins formed during martensitic transformation. From our example of the CuAu I structure, it is clear that the displacement $\frac{1}{2}\langle 10\bar{1}\rangle$ applied across a single

{101} plane will produce an antiphase domain, so that an order twin may be regarded as an array of antiphase domain boundaries, whereas an ordinary twin is similarly modelled as an array of stacking faults. Order twinning by deformation may not appear physically very probable since the slip plane is not a usual slip plane of the disordered structure, and the shear is large. However, if interfaces between order twins exist in any structure, their migration requires either toleration of this large shear or reordering by interatomic interchange ("interchange shuffling"; see below). In this paper, we shall not discuss order twinning further. Deformation twinning, as defined here, thus means modes which give true twins in the disordered structure. In other words, there is a change in the spatial arrangement of the atoms and not just, as in ideal order twins, in the occupancy of a common set of atom sites.

Many published papers on deformation twinning in superlattice structures contain statements which we believe to be erroneous or contradictory. Some examples are (i) cubic superlattices are unable to form true twins by deformation, (ii) true twinning is geometrically possible in some cubic superlattices, but not in others, (iii) twinning (or martensitic transformation) always leads to a lowering of symmetry, and (iv) atomic shuffles are not permissible in the deformation twinning of superlattices. In Section 2, we develop the general theory of deformation twinning in a form suitable for application to superlattices, and in Section 3 we apply this theory to cubic superlattices, deriving the possible true modes of minimum shear without shuffles and also considering modes which require some shuffles. For non-cubic superlattices, the situation is more complex; some variants of the usual disordered mode will give true twins when applied to the superlattice, whilst others will not. We discuss in Section 4 the various true and pseudo modes for all the non-cubic superlattices in the Richards and Cahn ground state diagram. The available experimental evidence is discussed in Section 5.

2. GENERAL THEORY

We specify a deformation twinning mode by the usual crystallographic elements K_1, K_2, η_1, η_2, together with the plane of shear, S, the shear magnitude, g, and the shuffle parameters q and $\bar{q}$. As defined by Bilby and Crocker [12], q is the number of K_1 lattice planes crossed by a primitive lattice vector parallel to η_2, and $\bar{q}$ is the number of K_2 lattice planes crossed by a primitive lattice vector parallel to η_1. When discussing a particular variant of any mode, we shall use the Bilby–Crocker sign convention (shown in Fig. 1 of their paper) in which the angle between the positive directions of η_1 and η_2 is obtuse in the parent crystal, the angles between η_1 and the positive normal to K_2 and between η_2 and the positive normal to K_1 are both acute, and the directions of η_1, η_2 and the positive normal to S form a right handed set. A mode is usually considered to be of type I, type II or compound according to whether (a) K_1 and η_2, (b) K_2 and η_1 or (c) all four elements are rational, and the value of q or $\bar{q}$ is then relevant to any further shuffling of lattice points which may be necessary to complete the twinning operation. (We do not need, within the ranges of shear and shuffle magnitude discussed here, to consider the possibility of "non-classical" modes [13–15] which may have either three or four irrational elements.) If $q = 1$ or 2, all lattice points are sheared into their correct positions for type I or type IV orientation relations which may be described respectively as a reflection in K_1 and a rotation of π about the normal to K_1, these two operations being equivalent, for all centrosymmetric structures, and in particular for lattices. Similarly, all lattice points are sheared into correct positions for a type II or type III orientation relation (a rotation of π about η_1 and a reflection in the plane normal to η_1 respectively) if $\bar{q} = 1$ or 2. More generally, a fraction q^{-1} (q odd) or $2q^{-1}$ (q even) of the lattice points are sheared into the correct positions for a type I orientation, and similarly for general values of $\bar{q}$ and a type II orientation. The normal twinning modes of the disordered b.c.c. and f.c.c. structures are both compound with $q = \bar{q} = 2$, and the relative orientations of parent and twin may be described by any of the four classical relations which are all equivalent since S is a mirror plane.

If the direction indices of any vector and the Miller indices of any plane with respect to the original cubic axes are written as column and row matrices $[u]^c$ and $(h)^c$ respectively, the corresponding indices referred to axes defined by a unit cell of the superlattice are given by

$$[u]^s = \mathbf{J}[u]^c \quad \text{and} \quad (h)^s = (h)^c\mathbf{J}^{-1}$$

where $\mathbf{J}$, $\mathbf{J}^{-1}$ are 3×3 matrices expressing the relation between the two bases, so that the columns of $\mathbf{J}^{-1}$ are the cubic components of the base vectors of the chosen superlattice cell. The effect of applying to the superlattice structure the shear corresponding to any particular variant pair (i.e. a particular variant and its conjugate) of any deformation twinning mode of the disordered structure may be examined by referring the planes and direction of the variant pair to the superlattice basis and then calculating the values of q and $\bar{q}$ from the equations

$$q = (I'/I)(K_1)[\eta_2] \quad \text{and} \quad \bar{q} = (I'/I)(K_2)[\eta_1]$$

where the column matrices $[\eta_1]$, $[\eta_2]$ and the row matrices (K_1), (K_2) are formed from relatively prime indices in the superlattice basis, and I' and I are the so-called "cell factors" [15]. The value of I' is $\frac{1}{2}$ for body-centred lattices if the direction indices are all odd, for face-centred lattices if the sum of the direction indices is even, and for base-centred (or side-centred) lattices if both direction indices for the axes defining the centred face are odd and the third index

is even; in all other cases $I' = 1$. Similarly, $I = \frac{1}{2}$ for body-centred lattices if the Miller indices have an odd sum, for face-centred lattices if the indices are mixed odd and even, and for base-centred lattices if the two appropriate indices have an odd sum; otherwise $I = 1$.

For most superlattice structures, the condition that the lattice points are sheared directly to twin positions is sufficient to ensure that a true twin is formed. In such cases, we thus have a pseudo twin if both q and $\bar{q}$ exceed 2, and a true twin otherwise. (We use the definition suggested by Laves [6] and Goo *et al.* [16] that a pseudo twin has the atomic sites in twin positions, but that these sites are incorrectly occupied.) The true twins may be further classified as types I/II (or II/I) or "combined". Here I/II means the direct variant gives a twin with a type I (or equivalently IV) orientation relation, and the conjugate gives a type II (or equivalently III) relation, whilst the combined twin is one for which all four classical orientations are equivalent. The classification is similar to the conventional division into type I, type II and compound twins, but we have introduced the new term "combined" for the orientation relations since all the twinning modes have rational crystallographic elements and so are "compound" in the strict sense of the usual definition. This distinction between the orientations and the conventional rules for classification of deformation twins has been made previously by Rowlands *et al.* [17] who refer to a "type II, compound mode".

The Bilby–Crocker rules give the condition for the absence of atomic shuffling in the twinning of "single lattice" structures, but when the primitive unit cell contains more than one atom, consideration has to be given to "multiple lattice" [12] or "structure" [15] shuffles. Previous treatments of both lattice and structure shuffles have analysed the additional displacements needed to carry some of the atoms from (putatively) wrongly occupied sites in the sheared crystal to correct sites which in the sheared crystal are (putatively) unoccupied. Such displacements are generally through distances appreciably smaller than an interatomic distance, and shuffling of this kind is known to take place during the deformation twinning of many real materials. It is presumed that the atomic displacements occur spontaneously at the moving interface, so that the separation into shear and shuffle components is only a mathematical convenience and does not imply kinetically separate processes.

Suppose that each atom is first given the displacement appropriate to the homogeneous simple shear, i.e. treat the atoms as embedded in a sheared continuum. The structure may be defined by a motif unit repeated at each lattice point, and, in general, further relative displacements of the various atoms within a motif unit will be required to complete the twinning operation and restore the original structure. These structure shuffles may be avoided, however, if the motif unit satisfies a restrictive condition which, for a non-centrosymmetric structure in which S is not a mirror plane, is different for each of the four possible orientations of the twin. Thus a type I or a type III orientation may be produced by shear without accompanying shuffling if the motif unit may be chosen as a planar set of atoms within K_1 or K_2 respectively,† whereas for a type II or IV orientation, it is required that a possible choice of motif is a linear unit parallel to η_1 and η_2 respectively. For centrosymmetric structures, as already noted, IV = I and III = II, and either choice of motif will eliminate the need for shuffles in both cases. If S is a mirror plane, II = I and IV = III, and shuffles will then be absent for motif units in K_1 or K_2 respectively. The overall condition for absence of atomic shuffling may be obtained by combining the rules for absence of lattice and structure shuffles, or equivalently by considering the unit cell defined by η_1, η_2 and the normal to S (which is sheared into an equivalent cell) as either primitive or base-centred (for q odd and even), and treating all the atoms within this cell as part of a motif unit which must conform to the above (structure shuffle) rules.

Use of the above rules enables a decision to be made about any particular shear which is under investigation as a potential true twinning mode of a superlattice. As noted above, however, most of the shears which we shall consider will produce, without shuffling, a set of atomic sites corresponding to a true twin in the disordered structure (or in a pure component), and it is only the occupancy of these sites which determines whether or not a true twin has been produced in the superlattice. If the occupancy is incorrect, the necessary shuffles take the form of atomic interchanges and thus might be compared with the unit processes in ordering or in atomic diffusion. It is improbable that such shuffles could occur sufficiently rapidly to accompany the shear during deformation twinning, and it is usually tacitly assumed that they must be excluded; this is indeed the basis for the proposal that pseudo twins may form in superlattices subjected to the twinning shear of the disordered structure. In order to make this distinction clearer, we suggest that the term "interchange shuffling" or "order shuffling" might be used for this particular type of shuffling. Figures 1–3 show how for the hypothetical case of cubic twinning on a {120}

†In [15], the condition for no structure shuffles in type II twinning is stated to be a motif unit in the plane perpendicular to η_1 rather than in K_2. This is because in the conventional analysis of such shears given by Bilby and Crocker, the lattice points are displaced by the shear, but the motif units are carried rigidly with the lattice points. This analysis simplifies the discussion if the shuffles involve displacements of less than half of an interatomic distance, but the alternative assumption that each atom undergoes an individual shear displacement is more appropriate in the superlattice case. It is this alternative assumption which leads to the condition that the motif unit must lie in K_2. The example illustrates that the factorisation into shear plus shuffle is to some extent arbitrary.

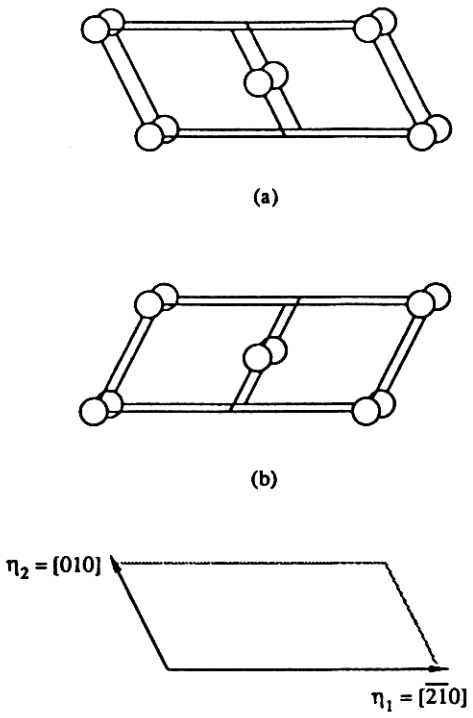


Fig. 1. Formation of twin by hypothetical shear on $(1\bar{2}0)$ plane of simple cubic structure. (a) Parent. (b) Twin. (c) Orientation of parent cell. The perspective view along the negative normal to S shows the parent unit cell defined by primitive lattice vectors parallel to η_1, η_2 and the positive normal to S. This cell is sheared into an equivalent cell, and no shuffles are required to produce a twin.

plane no shuffles are required for a simple cubic structure, lattice shuffles are required for a disordered b.c.c. structure or (equivalent) structure shuffles for a B2 superlattice, and a combination of lattice, structure and interchange shuffles are needed to produce a true twin in the DO_3 and B32 superlattices. We shall assume that interchange shuffling is always forbidden, but in view of recent experimental results [16] we shall consider the possibility of twinning modes which require some non-interchange shuffling in cubic superlattices.

All of the superlattices which appear in the Richards and Cahn diagrams are centrosymmetric and have stoichiometric compositions of type A_nB. Moreover, with two exceptions, which will be discussed individually when they arise, there is 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. Thus in almost all cases any shear which gives a true twin in the disordered structure will also give a true twin in the superlattice with a type I ($\equiv$ IV) orientation provided the minimum separation of the B atoms along the η_2 direction does not cross more than two lattice planes of type K_1 (i.e. atomic K_1 planes containing B atoms). A similar statement applies to twins with a type II ($\equiv$ III) orientation if η_1 and K_2 are substituted for η_2 and K_1, and if both conditions are satisfied all orientation relations are equivalent. The plane of shear is then a mirror plane of both the disordered and superlattice structures. In terms of the general theory, these results arise because the A atoms are at special points rather than general points of the ideal superlattice cell, and any relaxation in the atomic positions on formation of the superlattice is assumed not to move the atoms off these special positions. In some cases, this condition is imposed by symmetry; in others, it may be only approximately true, so that, in principle, very small shuffle displacements could also be required.

In summary, the following rules may be applied to any potential twinning mode, as given, for example, by the various correspondence matrices listed by Bevis and Crocker [13, 14]. Provided there is only one B atom per primitive unit cell, the condition that both disordered and ordered *lattices* can twin in a given mode without shuffles automatically incorporates the absence of structure and interchange shuffles in the superlattice structure. A possible mode without lat-

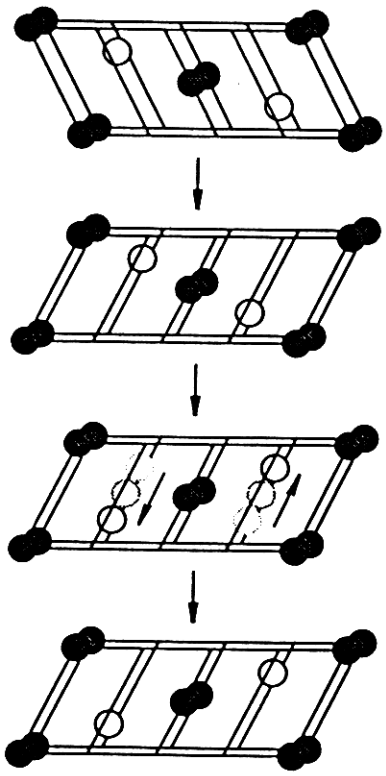


Fig. 2. Formation of $(1\bar{2}0)$ twin in b.c.c. or B2 structure. The successive figures show an analysis of the overall change from parent to twin into a shear followed by shuffles. The open and shaded symbols indicate atoms on two successive planes of shear, and also, in the case of the B2 structure, A and B atoms respectively. For both structures, the formation of a twin requires additional relative translations of the open and shaded atoms. The shuffles shown represent only one of several possibilities, but in each case there are no "interchange" shuffles.

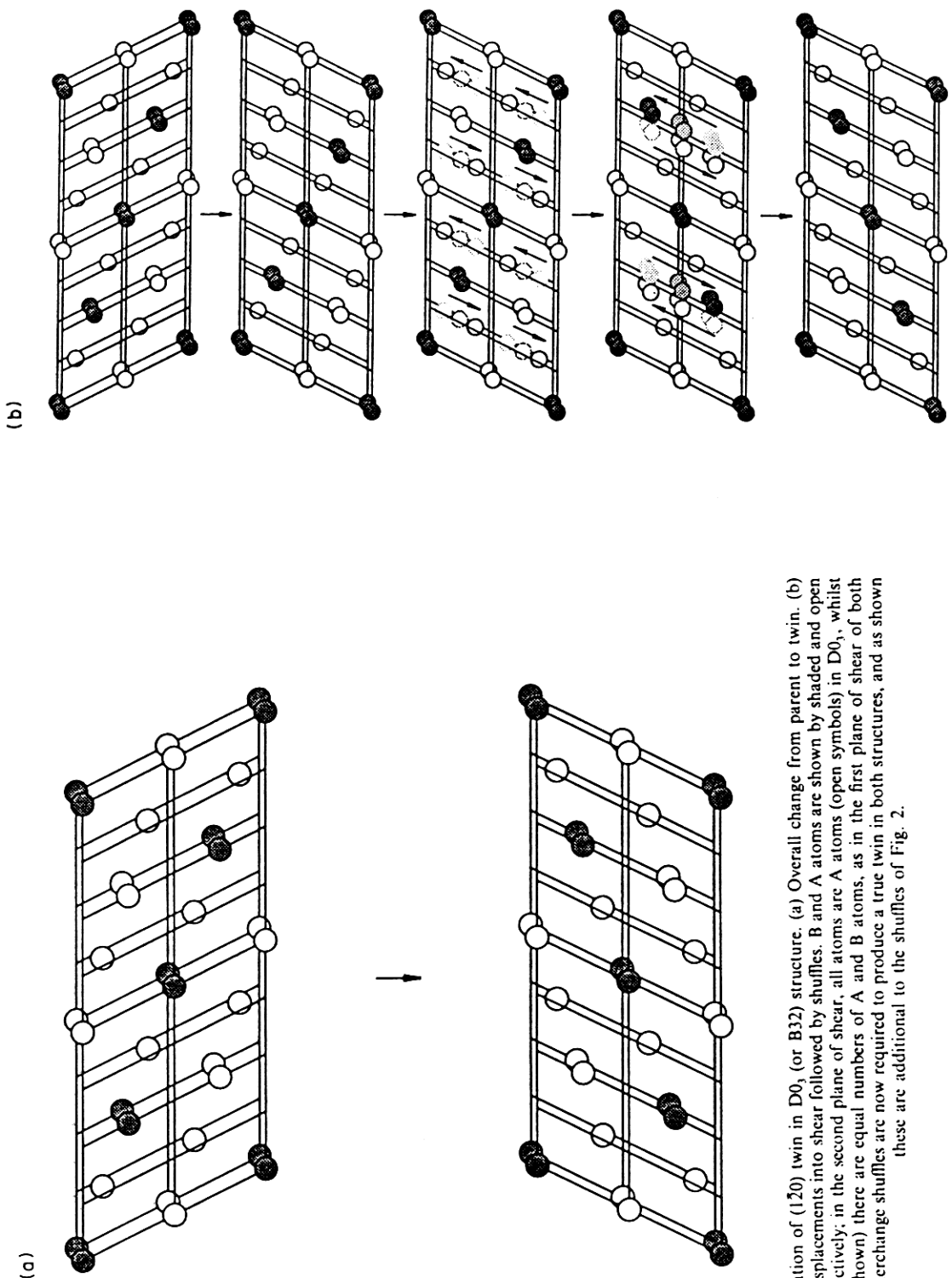


Fig. 3. Formation of $(1\bar{2}0)$ twin in DO_3 (or B32) structure. (a) Overall change from parent to twin. (b) Analysis of displacements into shear followed by shuffles. B and A atoms are shown by shaded and open symbols respectively; in the second plane of shear, all atoms are A atoms (open symbols) in DO_3, whilst in B32 (not shown) there are equal numbers of A and B atoms, as in the first plane of shear of both structures. Interchange shuffles are now required to produce a true twin in both structures, and as shown these are additional to the shuffles of Fig. 2.

Table 1. Pseudo twins in cubic superlattices

Disordered structure	Twin mode (Table 2)	Composition	Superlattice structure	Space group	t	$q, \bar{q}$
b.c.c.	2.2^T	AB	B2 (CsCl type)	$Pm\bar{3}m$	1	4, 4
b.c.c.	2.2^T	AB	B32 (NaTl type)	$Fd\bar{3}m$	2	8, 8
b.c.c.	2.2^T	A_3B	$D0_3$ (BiF_3 type)	$Fm\bar{3}m$	2	8, 8
f.c.c.	2.2	A_3B	$L1_2$ (Cu_3Au type)	$Pm\bar{3}m$	1	4, 4

tice shuffles in the superlattice will require structure shuffles (but not interchange shuffles) in order to produce a true twin if the underlying disordered lattice requires lattice shuffles in that mode. Conversely, a true twin cannot be obtained without interchange shuffles if the superlattice requires a higher fraction of lattice shuffles than does the disordered structure. Finally, if both structures require the same fraction of lattice shuffles, further investigation is required to discover whether any of the superlattice shuffles are interchange shuffles. The motif unit must also be examined in cases where there is more than one B atom per primitive unit cell.

3. FORMATION OF TRUE AND PSEUDO TWINS IN CUBIC SUPERLATTICES

Superlattices with cubic symmetry must have the cube axes parallel to the axes of the disordered cubic structure from which they are formed, so that the matrices J and $\mathbf{J}^{-1}$ are necessarily of the form $\mathbf{I}/t$ and $t\mathbf{I}$ respectively where t is an integer and I is the unit matrix. There are three cubic superlattices of the b.c.c. structure predicted by Richards and Cahn, and one of the f.c.c. structure; these are listed in Table 1 together with the values of q and $\bar{q}$ for a shear system derived from the ordinary twinning mode of the disordered structure. It will be seen that in each case, the values of q and $\bar{q}$ exceed 2 in the superlattice because of the change in symmetry to simple cubic or f.c.c. for the b.c.c. superlattices and to simple cubic for the f.c.c. superlattice. Thus it follows that if interchange shuffles are forbidden, this mode cannot give a true twin in any cubic superlattice unless it has the same Bravais lattice and point group symmetry as the disordered structure. For both b.c.c. and f.c.c. structures, a superlattice of similar symmetry could form only at stoichiometric compositions A_7B, $A_{26}B$, $A_{63}B$, ... A_nB ... where $n = p^3 - 1$. Although theoretically possible, only very long range and unusual forms of atomic interaction could stabilise such superlattices and none of them are predicted by the Richards and Cahn model which considers only first and second neighbour interactions. A face-centred superlattice of this type (Pt_7Cu) is discussed by Khachaturyan [9].

The result just derived is also implicit in the Bevis and Crocker treatment of twinning [13, 14] which is a development of the Bilby Crocker approach. In particular, Table 1 of their second paper shows that mode 2.2 which represents in their notation the observed twinning mode for both the f.c.c. and b.c.c. disordered structures would correctly shear only one-half of the lattice points in a simple cubic superlattice of either structure and only one-quarter of the lattice points in a f.c.c. superlattice of the b.c.c. structure, or vice versa. Thus only by preservation of the disordered lattice symmetry can the ordinary twinning mode of the disordered structure remain a true mode of the superlattice.

The results of Bevis and Crocker may also readily be used to deduce the possible true twinning modes for the various cubic superlattices. Since the observed mode for both b.c.c. and f.c.c. structures is that of minimum shear without shuffles, it follows that a true mode of the superlattice structure must involve either a higher shear or some shuffling. We shall consider the possibility that one-half of the atoms shuffle, but exclude higher fractions as improbable. The modes of interest are listed in Table 2 and have either been taken directly from Table 1 of [14] and Tables 1 and 2 of [18] or have been calculated from Table 2 of [13]. In Table 2, the mode number, denoted $m.n$, is the Bevis–Crocker designation, except that, for ease of description, we have introduced the additional notation $m.n^T$ to mean the "transposed" mode obtained by interchanging K_1 and η_1 and K_2 and η_2 and changing the signs of the new K_2 and η_1. Thus $m.n$ now designates a mode pair (i.e. a mode and its conjugate, or reciprocal, mode in which K_1 is interchanged with K_2 and η_1 with η_2 and the sign of S is changed) and $m.n^T$ represents the related mode pair specified as above. The shuffle parameters m, m_I and m_F specify the minimum reciprocal fractions of lattice sites which are carried directly to twin positions without shuffles in simple cubic, b.c.c. and f.c.c. lattices respectively.

The modes listed in [13] extended up to shear magnitudes of 3, $(3.5)^{1/2}$ and 1.5 in cases where none, one-half or three-quarters respectively of the lattice points in a simple cubic lattice must shuffle to give a twin; within these limits, we have included in Table 2 all the modes which could occur without shuffles in either b.c.c. or f.c.c. lattices up to shear magnitude $g = 8^{1/2}$ and the modes in which one-half of the atoms must shuffle up to shear magnitude $g = 1$. Our limits are chosen to allow us to list at least one non-shuffle and one 50% shuffle mode for each superlattice structure. Bevis *et al.* [18] have previously listed modes for b.c.c. lattices with shear limits of 2 and 1 for non-shuffle and 50% shuffle conditions respectively, and since they use a different $m.n$ designation

Table 2. Twinning modes in cubic lattices

Mode no. [13, 14]	b.c.c. mode no. [18]	g^2	Shuffle parameters m	m_I	m_F	Orientation relation
4.2	—	$\frac{1}{6}$	4	8	2	comb.
4.2^T	2.1	$\frac{1}{6}$	4	2	8	comb.
4.5	2.2	$\frac{3}{6}$	4	2	8	II
4.5^T	—	$\frac{3}{6}$	4	8	2	I
2.2	—	$\frac{1}{2}$	2	4	1	comb.
2.2^T	1.1	$\frac{1}{2}$	2	1	4	comb.
2.3	—	$\frac{1}{2}$	2	4	2	comb.
2.3^T	2.3	$\frac{1}{2}$	2	2	4	comb.
4.10	—	$\frac{7}{6}$	4	8	2	I
4.10^T	2.4	$\frac{7}{6}$	4	2	8	II
1.2	—	1	1	2	2	comb.
2.5	2.5	1	2	2	2	comb.
2.8	1.2	$\frac{3}{2}$	2	1	4	I
2.8^T	—	$\frac{3}{2}$	2	4	1	II
1.3	—	2	1	2	1	comb.
1.3^T	1.3	2	1	1	2	comb.
2.18	—	$\frac{7}{2}$	2	4	1	I–II
2.18^T	1.4	$\frac{7}{2}$	2	1	4	II–I
1.9	—	8	1	1	1	comb.
1.9^T	—	8	1	1	1	comb.

(with $m = m_I$ of the Bevis and Crocker list), their notation where relevant is given in the second column of Table 2. Table 1 of [14] has previously been used [4] to predict true twinning modes in cubic superlattices but it covers only a selection of modes and excludes 1.9, 4.2, 4.5 and 4.10 and their conjugates which appear in our table. Mode 1.5, although included in [14] as a zero shuffle mode for all three cubic lattices, is omitted from our Table 2 since it represents a shear to the identity in all cubic lattices and hence need not be considered further as a twin. Such a homogeneous shear could, of course, conceivably occur as a physical deformation and in a non-cubic superlattice could give an order twin. In fact, 1.5 is the mode already discussed as an example of order twinning for the $L1_0$ superlattice.

For most of the modes listed in Table 2, the values of q and $\bar{q}$ are equal, and the values of m, m_I and m_F are then simply q or $\frac{1}{2}q$ for odd and even values of q respectively. For those modes in which q and $\bar{q}$ are not equal, the smaller value is used to obtain m, m_I and m_F and if shuffles are involved, as in modes 4.5, 4.10, 2.8, 2.18 and their transposes, these minimum shuffles are obtained with either a type I or a type II orientation relation. In principle, the conjugate mode then has the other type of orientation relation with the minimum shuffling indicated in the table, but in the first three of the cases just cited the conjugate modes do not actually represent twins since either K_1 is then a mirror plane or η_1 is a two-fold axis of the parent structure. Thus such modes are marked either as I or II in the orientation column, whereas modes such as 2.18 where both the direct mode and its conjugate represent twins are noted as I–II or II–I. Although there is only one I–II mode in Table 2, we shall find many examples of such modes in the non-cubic superlattices.

As is clear from the table, if a mode $m.n$ gives only a type I orientation with minimum shuffles, it follows that $m.n^T$ gives a type II relation with the same fraction of shuffles. For example, mode 4.5 gives a type II orientation if only half of the atoms shuffle, and five-sixths of the atoms would have to shuffle to give a type I relation; the opposite is true of 4.5^T. Obviously also it is arbitrary which set of elements define $m.n$ and $m.n^T$ respectively; the labelling in our Table 2 is based on the correspondence matrices of Table 2 of [13].

For the B2, $D0_3$ and $L1_2$ superlattices, a true twinning mode without shuffles is now predicted if a 1 appears in the shuffle columns for both the disordered and the superlattice symmetries; this is also a necessary condition for a no-shuffle mode for B32 but further examination is then required since the primitive unit cell of this structure contains two B atoms. This gives for the superlattices of the b.c.c. structure the possible modes 1.3^T, 1.9 and 1.9^T for B2, and 1.9 and 1.9^T for both $D0_3$ and B32. In the case of B32, the two B atoms which share a lattice point are displaced from each other in a $\langle 111 \rangle$ direction, and, since this is in K_1 for 1.9 and K_2 for 1.9^T, no additional shuffling is required. The 1.9 modes were not considered by Arunchalam and Sargent [4] because they used Table 1 of [4] which cuts off at $g = 5^{1/2}$; presumably this is why they concluded that true twinning in $D0_3$ is impossible. Similarly, for the $L1_2$ superlattice of the f.c.c. structure, possible true twinning modes are 1.3, 1.9 and 1.9^T; 1.3 is the mode predicted by Arunchalam and Sargent. Note that 1.3, 1.3^T, 1.9 and 1.9^T each represent only one possible mode since the conjugate mode in each case has a mirror plane as K_1 and a two-fold axis as η_1.

In view of the large shear magnitudes of these predicted modes, we now consider the possibility of

Table 3. Possible true twinning modes in cubic superlattices

Mode no.	S	K_1	K_2	η_1	η_2	g^2	True twin in
(a) *Modes without shuffles*							
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, $D0_3$, $L1_2$
1.9^T	($\bar{1}\bar{1}$0)	(1$\bar{1}$1)	(1$\bar{1}$0)	[1$\bar{1}\bar{2}$]	[001]	8	B2, B32, $D0_3$, $L1_2$
(b) *Modes with 50% (non-interchange) shuffles*							
2.3^T	(110)	(1$\bar{1}\bar{4}$)	(1$\bar{1}$0)	[22$\bar{1}$]	[00$\bar{1}$]	$\frac{1}{2}$	B2
1.2	(001)	(1$\bar{2}$0)	(100)	[210]	[0$\bar{1}$0]	1	B2, $L1_2$
2.5	(001)	($\bar{1}$30)	(110)	[310]	[$\bar{1}$10]	1	B2, B32, $D0_3$
1.3	(110)	(1$\bar{1}$1)	(001)	[$\bar{1}$12]	[1$\bar{1}$0]	2	B2, B32, $D0_3$
1.3^T	(110)	($\bar{1}$12)	($\bar{1}$10)	[$\bar{1}$1$\bar{1}$]	[001]	2	$L1_2$

true twinning modes in which one-half of the atoms must undergo (non-interchange) shuffles. Such a shuffle mode exists if a "2" appears in the "shuffle" column of Table 2 appropriate to the disordered structure and a "1" in that for the superlattice structure. This indicates that no lattice points (i.e. B atoms, except for the B32 superlattice) need shuffle, and hence that the only shuffles are the non-interchange shuffles of the A atoms. This rule gives the additional modes 1.2 and 1.3 for the B2 structure, 1.3 for the $D0_3$ and B32 structures and 1.2 and 1.3^T for the $L1_2$ structure; examination of the motif unit of B32 confirms that no interchange shuffles are involved in mode 1.3. Figures 2 and 3 illustrate how mode 1.2 can lead to twinning without interchange shuffles for B2 but not for $D0_3$ and B32. Further possible modes can occur if there is a 2 in the shuffle columns of Table 2 for both disordered and ordered symmetries. This means, however, that some B atoms must shuffle and it is necessary to examine each case to determine whether or not interchange shuffling is implied. This can be done by determining the plane of the motif unit, or (equivalently) whether or not the minimum lattice vectors in the η_1 and η_2 directions are increased in magnitude when the superlattice is formed. The modes of this type which produce true twins without interchange shuffles are 2.3^T and 2.5 for B2 and 2.5 for $D0_3$ and B32, but modes 1.2 for $D0_3$ and B32 and 2.3 and 2.5 for $L1_2$ all involve interchange shuffles.

The predicted true twinning modes are gathered together in Table 3. Modes without shuffles have minimum shears of $2^{1/2}$ for B2 and $L1_2$ and $8^{1/2}$ for $D0_3$ and B32; modes with 50% shuffles have minimum shears of $2^{-1/2}$ for B2, and unity for the other three superlattices.

We shall illustrate the true and pseudo twinning modes mainly by perspective drawings of the occupancy of the sites in a unit cell defined by lattice vectors parallel to η_1 and η_2 and normal to S. As already illustrated in Figs 1–3, such a cell is sheared into a new cell of equivalent size and shape, and it is obvious from the figure whether or not shuffles will be required to produce a true twin. Figures 4–7 show the unit cell for each of the four cubic superlattices in the pseudo-modes derived from the basic modes of the b.c.c. and f.c.c. structures (2.2^T and 2.2 respectively) and in each mode of Table 4 which gives a true twin without shuffles. Consideration of the shuffle modes is deferred to the discussion. It is also useful when considering the non-cubic superlattices derived from f.c.c. to consider the occupancy of the various $\{111\}^c$ planes which could serve as K_1 or K_2 of the 2.2 mode; the {111} planes of the $L1_2$ structure have the configuration shown in Fig. 8(f).

4. FORMATION OF TRUE AND PSEUDO TWINS IN NON-CUBIC SUPERLATTICES

There are six equivalent conjugate pairs of variants of the usual b.c.c. and f.c.c. modes, each pair having a different {110} plane of shear, S. When the symmetry is lowered, these six pairs break up into non-equivalent smaller groups, some of which are transformed into true twinning modes of the superlattice whilst others are not. Any true superlattice twinning modes derived in this way are necessarily no-shuffle modes of minimum shear, and may thus be expected to be preferred over other possible modes of higher shear, or of smaller shear but requiring shuffles. For non-cubic superlattice structures we shall, therefore, discuss only modes derived from the basic disordered mode.

There are, in fact no non-cubic superlattices in the ground state diagram for binary b.c.c. alloys derived by Richards and Cahn, but there are several non-cubic superlattices in that for f.c.c. alloys. Examination of these structures shows that in those of lowest symmetry (monoclinic) there are four different types of true or pseudo mode derived from the cubic modes, so that in order to discuss every case we need to list at least four variant pairs of the original cubic mode. We have chosen the following:

Variant	S	K_1	K_2	η_1	η_2
A	(110)	($\bar{1}$11)	($\bar{1}$1$\bar{1}$)	[$\bar{1}\bar{1}\bar{2}$]	[$\bar{1}$12]
B	($\bar{1}$10)	(11$\bar{1}$)	(111)	[112]	[11$\bar{2}$]
C	(01$\bar{1}$)	(111)	($\bar{1}$11)	[$\bar{2}$11]	[211]
D	($\bar{1}$01)	(111)	(1$\bar{1}$1)	[1$\bar{2}$1]	[121]

The remaining two variant pairs, E and F with planes of shear (S) of (011) and (101) respectively will be equivalent in all cases to one of the modes derived from A–D.

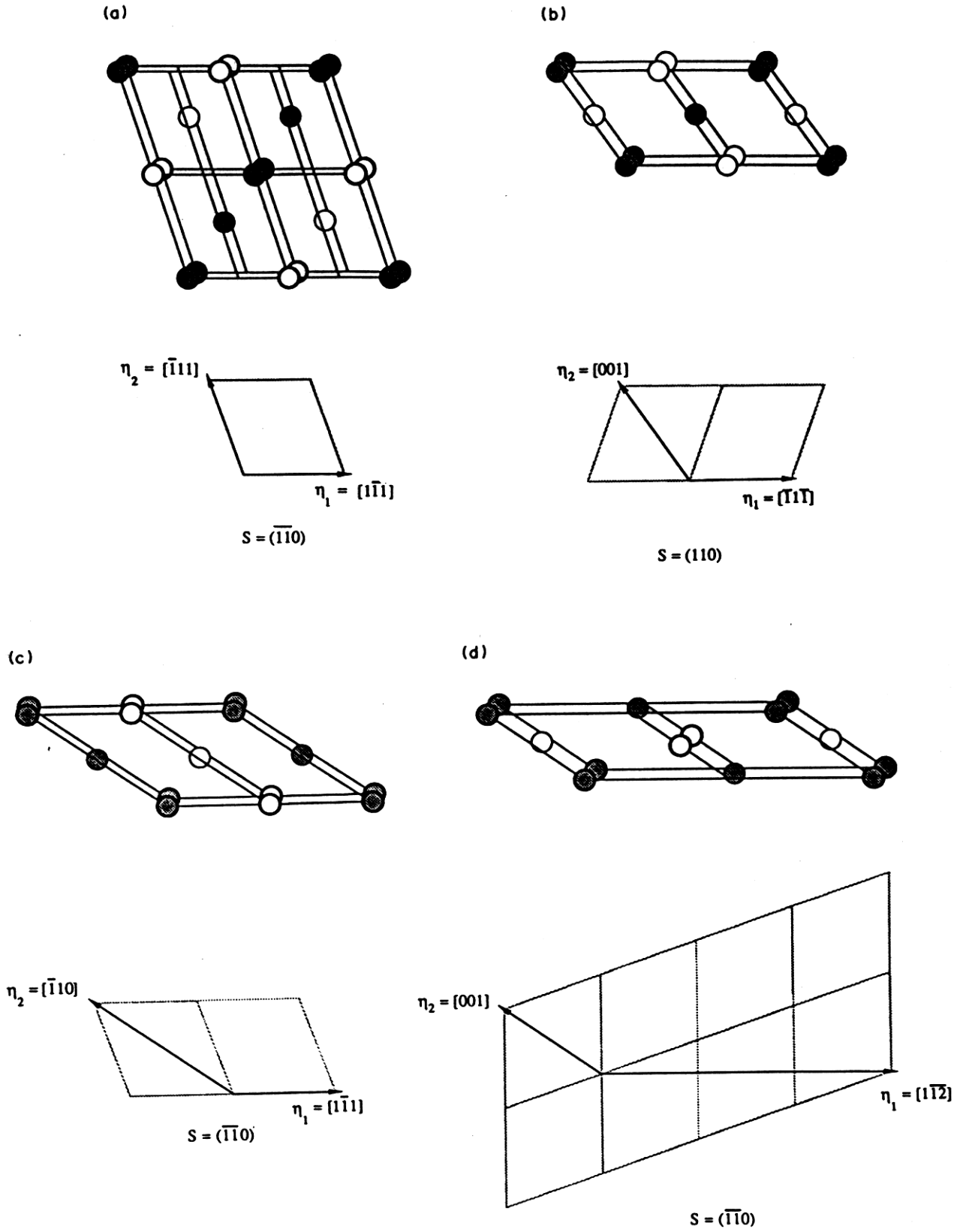


Fig. 4. Perspective views of appropriate unit cells defined as above for various shear modes of the B2 structure. (a) Pseudo twins (mode 2.2^T). (b) True twins (1.3^T). (c) True twins (1.9). (d) True twins (1.9^T). Symbols as in Fig. 3.

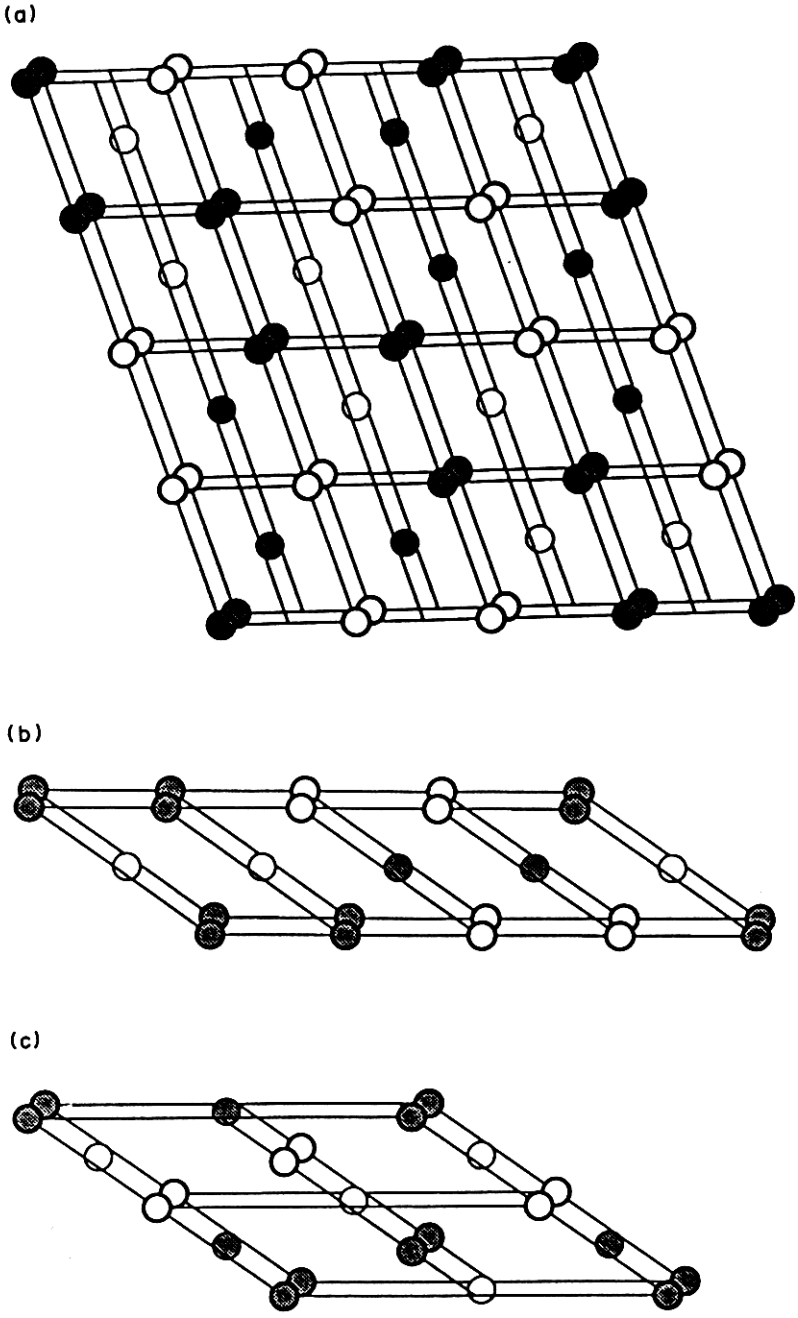


Fig. 5. Perspective views of appropriate unit cells for shear modes of the B32 structure. (a) Pseudo twins (2.2^{T}). (b) True twins (1.9). (c) True twins (1.9^{T}). Symbols as in Fig. 3.

In the disordered structure, primitive vectors parallel to η_1 and η_2 are of type $\frac{1}{2}\langle 112\rangle^{c}$ with $q, \bar{q} = 2$ and in most cases, the restriction on q and $\bar{q}$ in the superlattice amounts to considering whether or not these vectors remain as lattice repeat vectors. However, if some planes of a particular $\{111\}^{c}$ set are entirely composed of A atoms in the superlattice structure, it is possible for the primitive lattice vector in a $\langle 112\rangle^{c}$ direction which crosses this set to be increased in magnitude without increasing q. Thus, for example, in the monoclinic structure with composition A_3B and space-group $B2/m$ discussed below, alternate $(\bar{1}11)$ planes are entirely A-atomic planes, and are crossed by primitve vectors of the superlattice which are derived from $\frac{1}{2}[\bar{2}11]^{c}$, $\frac{1}{2}[\bar{1}21]^{c}$ and $[\bar{1}12]^{c}$ respectively. The first two lead to $q = 1$ modes of the superlattice whilst the third leads to a $q = 2$ mode, but since the corresponding values of $\bar{q}$ are 4, 4 and 2 only the third mode is "combined".

An alternative procedure is to examine the

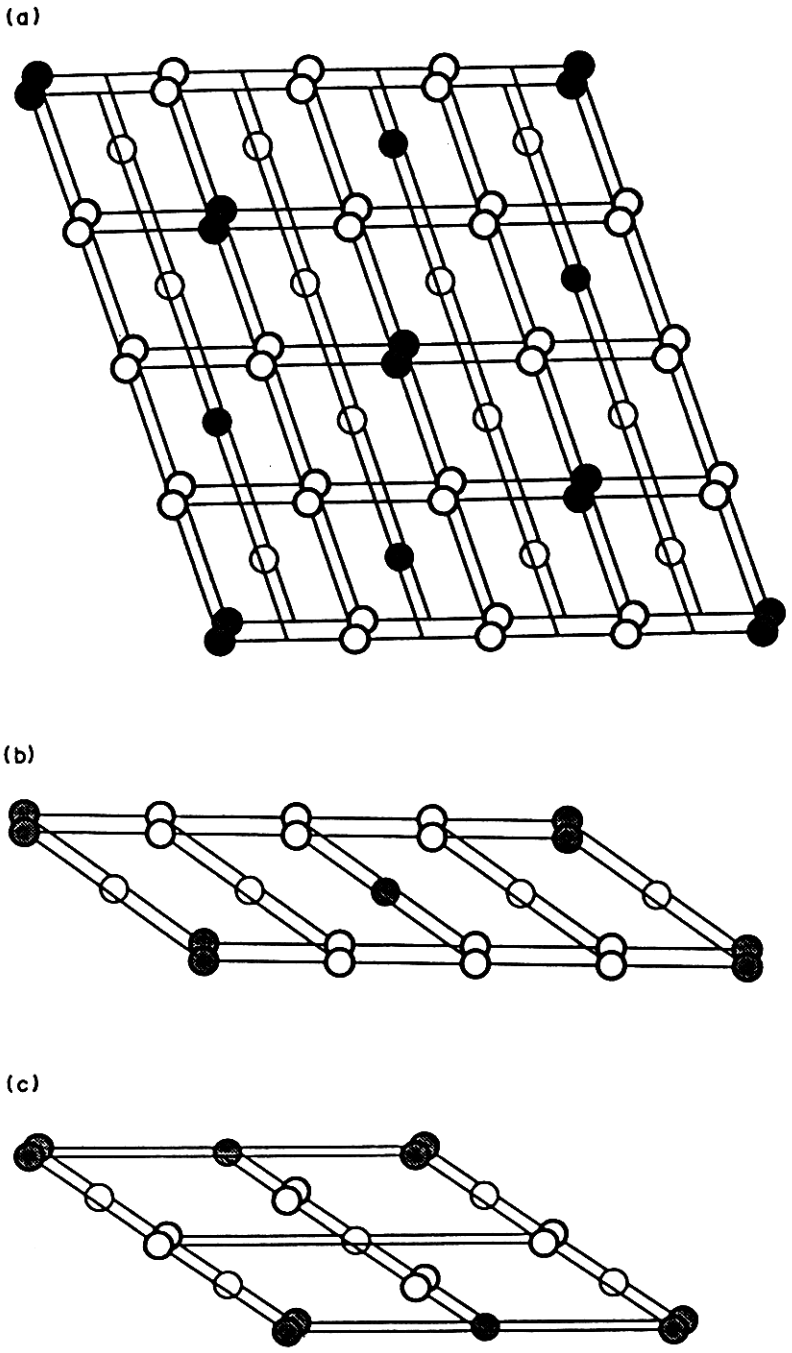


Fig. 6. Perspective views of appropriate unit cells for shear modes of the DO_3 structure. (a) Pseudo twins (2.2^T). (b) True twins (1.9). (c) True twins (1.9^T). Symbols as in Fig. 3.

occupancy of the atomic sites in the various possible $\{110\}^c$ planes of shear or in the various $\{111\}^c$ planes which correspond to K_1 and K_2. In the following discussion, the systematic approach is used for classification but the occupancy of the relevant planes is also shown. The base vectors specified by Richards and Cahn [7] in their Table 2 are generally used to define the ideal cells of a particular variant of the superlattice, but in some cases we have had to make changes in these vectors in order to correct errors or to conform with crystallographic conventions. For each superlattice structure, the crystallographic parameters are listed in terms of the superlattice cell for those of the cubic mode variant-pairs A–D which need to be distinguished, and it is indicated whether the corresponding shear-pair in the superlattice produces true twins which are combined (cb) or of type I-type II (I–II or II–I) or produces pseudo twins (ps).

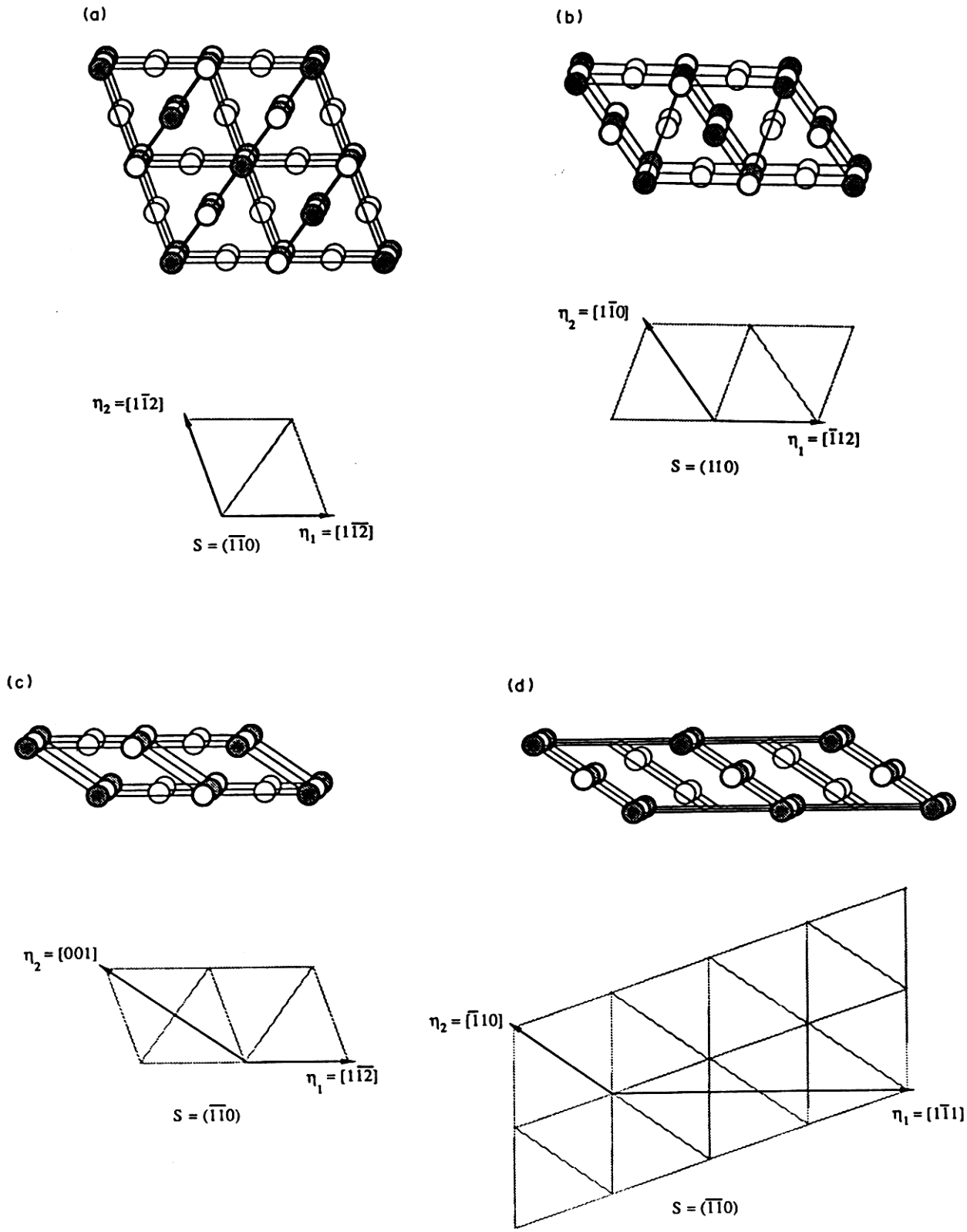


Fig. 7. Perspective views of appropriate unit cells for shear modes of the $L1_2$ structure. (a) Pseudo twins (2.2). (b) True twins (1.3). (c) True twins (1.9^T). (d) True twins (1.9). Symbols as in Fig. 3.

The parameters listed include the values of q and $\bar{q}$ which establish these distinctions and the shear magnitude, g, in terms of the superlattice cell parameters.

The shear magnitude calls for some comment. If on the formation of the superlattice, the atom positions remain unchanged then g always equals $2^{-1/2}$ as in the disordered structure and in the pseudo modes of the cubic superlattice structures. In practice, however, the ideal base vectors of a unit cell, defined by Cahn and Richards in terms of the disordered cell parameter a_0, are likely to relax to slightly different, new values consistent with the symmetry of the new structure.

Thus for completeness, we list the new value of g which will depend upon the axial ratio $p = c/a$ for tetragonal and hexagonal cells, upon $c = \cos\alpha$ for rhombohedral cells, upon p and $r = b/a$ for orthorhombic cells, and upon p, r and $c = \cos\gamma$ for monoclinic unit cells; in the latter case, we also use $s = \sin\gamma$ to simplify the algebraic expressions. The "ideal" values of these parameters are given in each case, and the various expressions for g all reduce to $2^{-1/2}$ when these ideal values are used.

The various superlattices are all of the form A_nB at stoichiometric compositions and will be considered in order of increasing n.

(i) *Composition AB $L1_0$ (CuAu I type) P4/mmm*

The superlattice is simple tetragonal with two atoms in the primitive cell which has ideal axial ratio $p = 2^{1/2}$. However, the base vectors given by Richards and Cahn form a left-handed set if the cubic axes are right-handed, and to avoid any possible misunderstanding, the sign of their second vector has been reversed so that $\mathbf{a}_2$ is derived from $[\bar{1}10]^c$. The relevant matrices are then

$$\mathbf{J} = \begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{J}^{-1} = \frac{1}{2}\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

All of the $\{111\}^c$ planes become $\{101\}^s$ planes. Two $\{110\}^c$ planes of shear become $\{100\}^c$ planes and the associated modes are true, combined modes of the superlattice; the remaining four $\{110\}^c$ planes become $\{112\}^s$ planes and the associated modes are not true twinning modes of the superlattice. Details are as follows:

Cubic var.	*Superlattice mode pair*							
	S	K_1	K_2	η_1	η_2	$q, \bar{q}$	g	*Type*
A ($\equiv$B)	(100)	(011)	(01$\bar{1}$)	[01$\bar{1}$]	[011]	2, 2	$p - p^{-1}$	cb.
C ($\equiv$D, E, F)	(11$\bar{2}$)	(101)	(011)	[$\bar{1}$31]	[3$\bar{1}$1]	4, 4	$\frac{1}{2}(p^2 + 10p^{-2} - 5)^{1/2}$	ps.

In the combined mode, the atomic planes of shear are alternately composed entirely of A atoms and entirely of B atoms. Each $\{111\}^c$ plane has the configuration shown in Fig. 8(b); the combined modes are those in which the close-packed rows consisting entirely of B or A atoms respectively are normal to the plane of shear and the pseudo modes are those in which the other $\langle 110\rangle^c$ directions are normal to the plane of shear. Plane of shear projections are shown in Figs 9(a) and 11(a) respectively.

(ii) *Composition AB $L1_1$ (CuPt type) $R\bar{3}m$*

The structure is rhombohedral but the hexagonal axes given by Richards and Cahn are incorrect since their **c** and **a** axes are not perpendicular. We retain $[111]^c$ as the direction of the **c** axis, but choose the **a** axes of the ideal hexagonal cell as $\frac{1}{2}[10\bar{1}]$ and $\frac{1}{2}[\bar{1}10]$. The positive directions of the two **a** axes are thus at 120°, in accordance with usual crystallographic convention, rather than at 60° as in the axes given by Richards and Cahn. [Equivalent $\{h, k, l\}$ planes in the hexagonal system are, of course, obtained by permutation of the first three axes of the Miller–Bravais indices $\{h, k, \overline{h+k}, l\}$.] The hexagonal cell contains six atoms and has ideal axial ratio $p = (24)^{1/2}$. It gives the transformation matrices

$$\mathbf{J} = \frac{1}{6}\begin{pmatrix} 4 & 4 & \bar{8} \\ \bar{4} & 8 & \bar{4} \\ 1 & 1 & 1 \end{pmatrix} \quad \mathbf{J}^{-1} = \frac{1}{2}\begin{pmatrix} 1 & \bar{1} & 4 \\ 0 & 1 & 4 \\ \bar{1} & 0 & 4 \end{pmatrix}.$$

The $(111)^c$ planes which are entirely occupied by either A atoms or B atoms become $(001)^S$ planes and the remaining $\{111\}^c$ planes become $\{102\}^s$ planes. Three of the $\{110\}^c$ planes become $\{110\}^S$ planes and give rise to true (combined) twin modes: the other three are transformed into $\{108\}^S$ planes and do not generate true modes.

The symmetry of this structure is alternatively displayed by choosing a rhombohedral unit cell defined by three equal axes $\frac{1}{2}[211]^c$, $\frac{1}{2}[121]^c$ and $\frac{1}{2}[112]^c$. This is a primitive cell containing two atoms which is characterised by the rhombohedral angle α where $c = \cos\alpha$ has the ideal value of $\frac{5}{6}$. With this choice of cell)

$$\mathbf{J} = \frac{1}{2}\begin{pmatrix} 3 & \bar{1} & \bar{1} \\ \bar{1} & 3 & \bar{1} \\ \bar{1} & \bar{1} & 3 \end{pmatrix} \quad \mathbf{J}^{-1} = \frac{1}{2}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}.$$

The $(111)^c$ plane now becomes $(111)^R$ and the other planes of this type become $\{110\}^R$. The true twinning modes have planes of shear of type $\{\bar{1}10\}^R$, and the pseudo modes of type $\{332\}^R$. The following table

gives full details of the derived modes in both axis systems:

Cubic var.	*Axes*	*Superlattice mode pair*							
		S	K_1	K_2	η_1	η_2	$q, \bar{q}$	g	*Type*
A (≡E, F)	H	(108)	$(\bar{1}12)$	$(01\bar{2})$	$[8, 10, \bar{1}]$	$[\bar{8}21]$	4, 4	$3^{-1/2}(3^{-1/2}p^2 + 84p^{-2} - 7)^{1/2}$	
	R	(332)	(011)	$(\bar{1}0\bar{1})$	$[\bar{1}3\bar{3}]$	$(\bar{3}13]$	4, 4	$\left[\frac{(19-18c)(1-c)}{2(1-3c^2+2c^3)} - 4\right]^{1/2}$	ps.
B (≡C, D)	H	$(\bar{1}20)$	(102)	(001)	$[\bar{2}\bar{1}1]$	[210]	2, 1	$(12)^{1/2}p^{-1}$	
	R	$(\bar{1}10)$	(110)	(111)	[001]	$[11\bar{2}]$	2, 1	$2\left[\frac{3(1-c^2)}{1-3c^2+2c^3} - 1\right]^{1/2}$	cb.

The $(111)^c$ planes are alternately pure A and pure B [Fig. 8(a)] whilst the remaining $\{111\}^c$ planes are of the type shown in Fig. 8(b). The combined modes are again those in which the close-packed rows are normal to the plane of shear, which then has the equiatomic configuration of Fig. 9(b) whilst the pseudo-modes have the remaining three $\langle 110\rangle^c$ directions normal to the plane of shear which appears as in Fig. 11(b).

(iii) Composition AB (NbP type) $I4_1/amd$

The structure has eight atoms in the body-centred tetragonal unit cell which has an ideal axial ratio $p = 2$. This cell is identical with that of the $D0_{22}$–I4/mmm structure considered below in (v), but the motif unit at each lattice point is here A_2B_2 instead of A_3B. Thus this is one of the two superlattice structures on our list with more than one B atom in the primitive unit cell (the other is the cubic B32 structure). In the Richards and Cahn ground state, both this structure and the $D0_{22}$ structure are stable for positive ratios in the range 0–0.5 of the second:first neighbour interaction potentials. There is then a continuous change with composition, the structure varying from A_3B (I4/mmm) via A_2B_2 ($I4_1$/amd) to AB_3 (I4/mmm) as B atoms are substituted for A atoms; at intermediate (non-stoichiometric) compositions, the symmetry is side-centred monoclinic (B2). The cell change is specified by the matrices given below for $D0_{22}$, and the same four pseudo mode pairs and two true mode pairs are obtained.

Each $\{111\}^c$ plane has the configuration shown in Fig. 8(c), and as in Fig. 8(b) there is a single $\frac{1}{2}\langle 112\rangle^c$ vector in the plane which remains a lattice vector on formation of the superlattice structure. The true (combined orientation) modes are those in which two such directions form η_1 and η_2. The planes of shear in these modes then all contain equal numbers of A and B atoms, as in Fig. 9(b), but are now stacked in a four plane sequence [Fig. 9(c)]. The absence of shuffles is confirmed by the choice of a linear motif unit along a $\langle 021\rangle$ direction which is contained within either K_1 or K_2. The planes of shear in the pseudo modes have an eight plane repeat and are shown in Fig. 11(c).

(iv) Composition A_2B. (Pt_2Mo type) Immm

The structure is body-centred orthorhombic with six atoms in the body-centred cell which has ideal axial ratios of $p = 3$ and $r = 2^{1/2}$. The base vectors given by Richards and Cahn form a left-handed set if the cubic axes are right-handed, and the sign of their first vector has thus been reversed so that $\mathbf{a}^s$ is derived from $\frac{1}{2}[\bar{1}10]^c$.

This gives

$$\mathbf{J} = \frac{1}{3}\begin{pmatrix} \bar{3} & 3 & 0 \\ 0 & 0 & 3 \\ 1 & 1 & 0 \end{pmatrix} \quad \mathbf{J}^{-1} = \frac{1}{2}\begin{pmatrix} \bar{1} & 0 & 3 \\ 1 & 0 & 3 \\ 0 & 2 & 0 \end{pmatrix}.$$

Two of the $\{111\}^c$ planes become $\{110\}^s$ planes and the other two become $\{013\}^s$ planes. One of the $\{110\}^c$ planes becomes $(001)^s$ and this leads to a true (combined) twinning mode, another plane becomes $(100)^s$ and the derived mode does not give a true twin. The remaining four $\{110\}^c$ planes all become planes of type $\{123\}^s$ and lead to type I–type II true twinning mode pairs in the superlattice. The characteristics of these three types are:

Cubic var.	*Superlattice mode pair*							
	S	K_1	K_2	η_1	η_2	$q, \bar{q}$	g	*Type*
A	(001)	(110)	$(1\bar{1}0)$	$[1\bar{1}0]$	[110]	2, 2	$r - r^{-1}$	cb.
B	(100)	$(0\bar{1}3)$	(013)	[031]	$[0\bar{3}1]$	6, 6	$(\frac{1}{3})(p^2r^{-2} + 81p^{-2}r^2 - 18)^{1/2}$	ps.
C (≡D, E, F)	$(1\bar{2}3)$	(013)	(110)	$[93\bar{1}]$	$[\bar{1}11]$	2, 6	$\frac{1}{2}(9p^{-2} + r^{-2} + p^2r^{-2} + 9p^{-2}r^2 - 6)^{1/2}$	I–II

Figures 8(d) and (e) show the two types of $\{111\}^c$ plane in the ordered structure, in which the $\frac{1}{2}a\langle 112\rangle^c$ vectors become respectively repeat vectors and

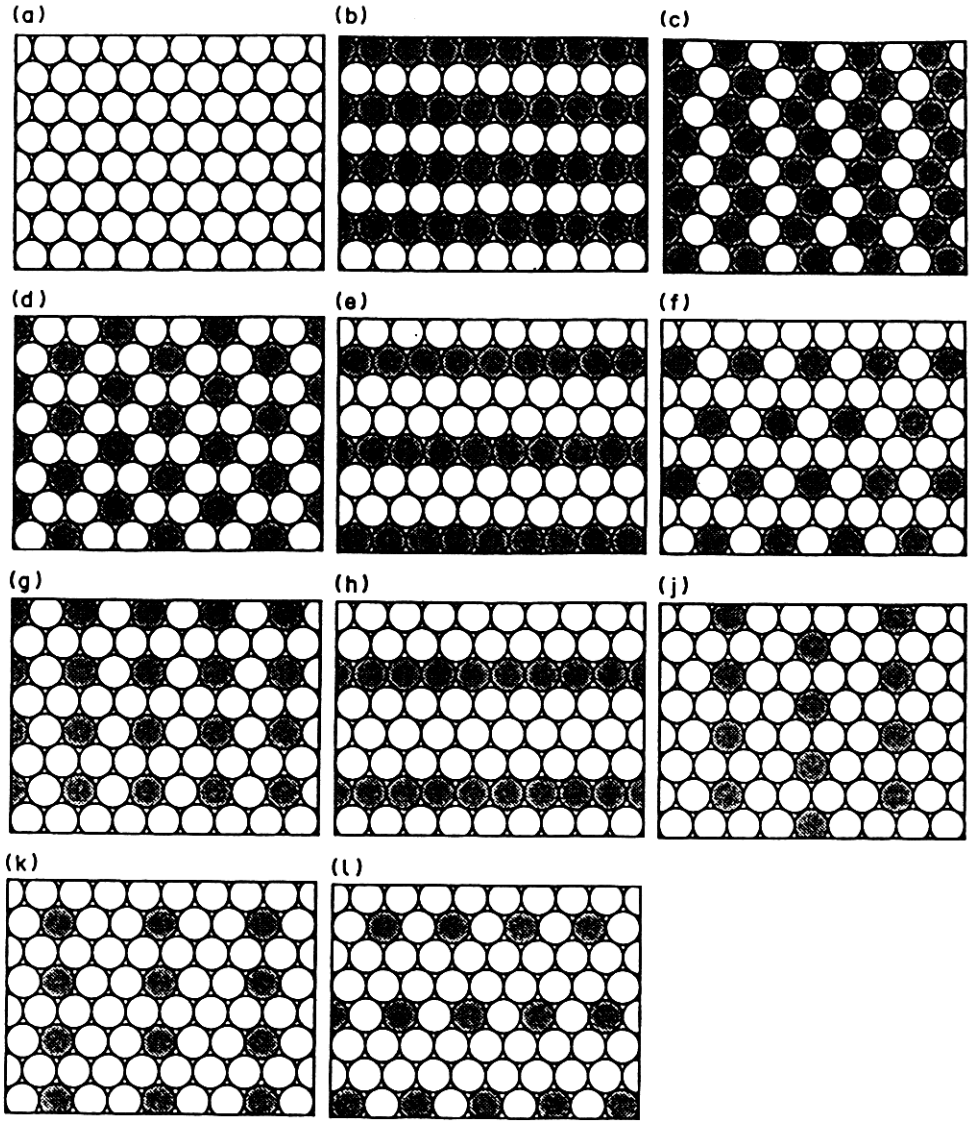


Fig. 8. Atomic configuration of close-packed $\{111\}^c$ planes for superlattice structures formed from f.c.c. B and A atoms are shown by shaded and open symbols respectively. (a) Pure A planes. Such planes are alternate $(111)^c$ of $L1_1$, $(\bar{1}11)^c$ of monoclinic A_3B and $(\bar{1}11)^c$ of A_5B. Pure B planes (not shown) are alternate $(111)^c$ of $L1_1$. (b) Equiatomic planes. All $\{111\}^c$ planes of $L1_0$ are of this form, as are also all planes except $(111)^c$ of $L1_1$ and alternate $(\bar{1}11)^c$ planes of monoclinic A_3B. (c) Equiatomic planes. All planes of the NbP ($I4_1/amd$) superlattice structure have this form. (d) Planes of composition A_2B in which $\frac{1}{2}\langle 112\rangle^c$ vectors are also lattice vectors of the superlattice. The $(\bar{1}11)^c$ and $(\bar{1}1\bar{1})^c$ planes of Pt_2Mo are of this form, as are also alternate $(\bar{1}11)^c$ planes of A_5B. (e) Planes of composition A_2B in which there are no $\frac{1}{2}\langle 112\rangle^c$ vectors which remain lattice vectors of the superlattice. The $(111)^c$ and $(11\bar{1})^c$ planes of Pt_2Mo are of this form. (f) Planes of composition A_3B. All $\{111\}^c$ planes of the cubic superlattice $L1_2$ are of this form. (g) Planes of composition A_3B. All $\{111\}^c$ planes of $D0_{22}$ are of this form, as are also $(111)^c$ and $(11\bar{1})^c$ of monoclinic A_3B. (h) Planes of composition A_3B. The $(\bar{1}1\bar{1})^c$ planes of monoclinic A_3B have this form. (j) Planes of composition A_4B. All planes of Dla are like this. (k) Planes of composition A_5B corresponding to the $(\bar{1}1\bar{1})^c$ planes of the monoclinic A_5B superlattice. (l) Planes of composition A_5B. The $(111)^c$ and $(11\bar{1})^c$ planes of the A_5B superlattice have this form.

$\frac{1}{3}\times$ repeat vectors of the superlattice. In the combined twinning mode of the superlattice, both the K_1 and K_2 planes are of the first type, and the $(001)^S$ atomic planes consist entirely of A atoms or B atoms in a repeating sequence of six planes ... BAABAA ... [Fig. 9(d)]. If both K_1 and K_2 planes are of the second type, the derived mode is not a superlattice twinning mode, and the plane of shear projection is shown in Fig. 11(d). The remaining four mode pairs each have the first type of $\{111\}^c$ plane as the K_2 plane which gives a true twin in a type I orientation relation [see Fig. 10(a)], or (in the conjugate to each mode listed) the first type of $\{111\}^c$ plane is the K_1 plane, leading to a type II orientation relation.

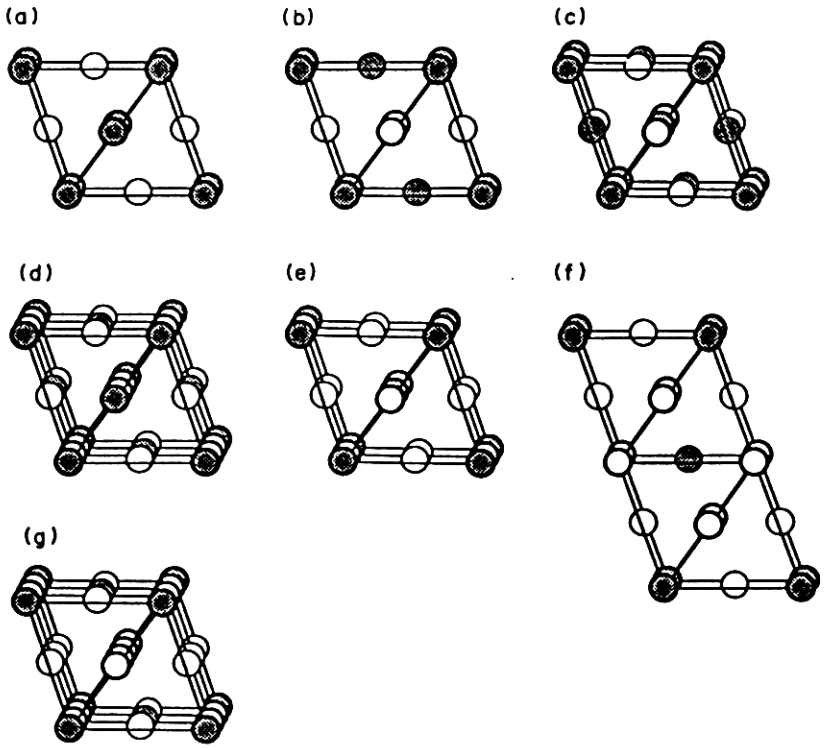


Fig. 9. Perspective views of true (combined) modes. Symbols as in Fig. 3. (a) $L1_0$ structure. (b) $L1_1$ structure. (c) NbP structure. (d) Pt_2Mo structure. (e) $D0_{22}$ structure. (f) Monoclinic A_3B structure. (g) Monoclinic A_5B structure.

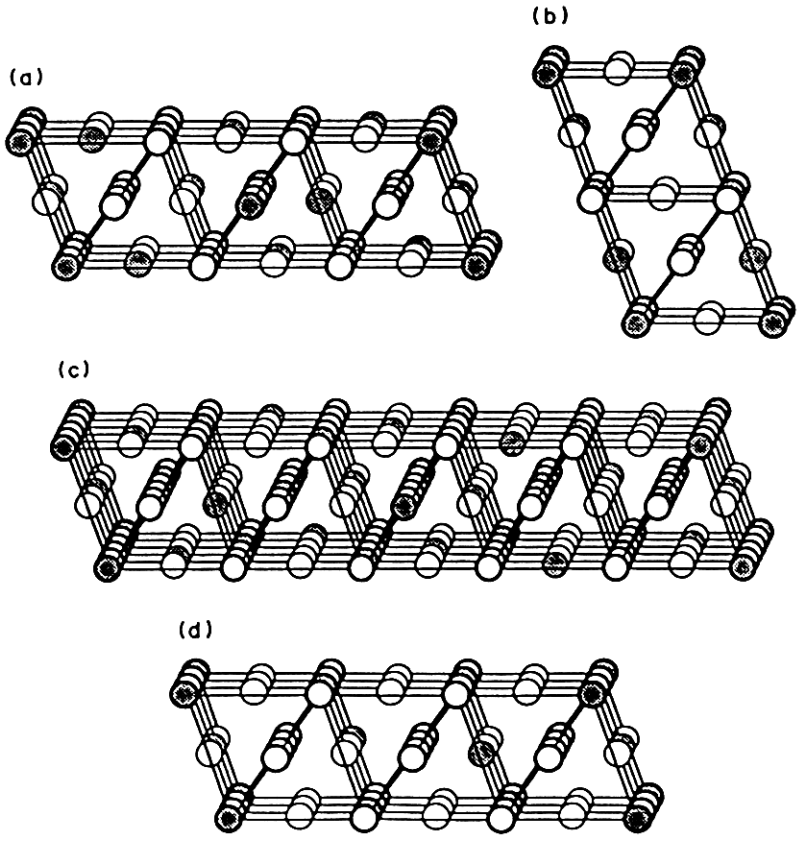


Fig. 10. Perspective views of true (I–II) modes. Symbols as in Fig. 3. (a) Pt_2Mo structure. (b) Monoclinic A_3B structure (shown as type II mode to conform with text). (c) Dla structure. (d) Monoclinic A_5B structure.

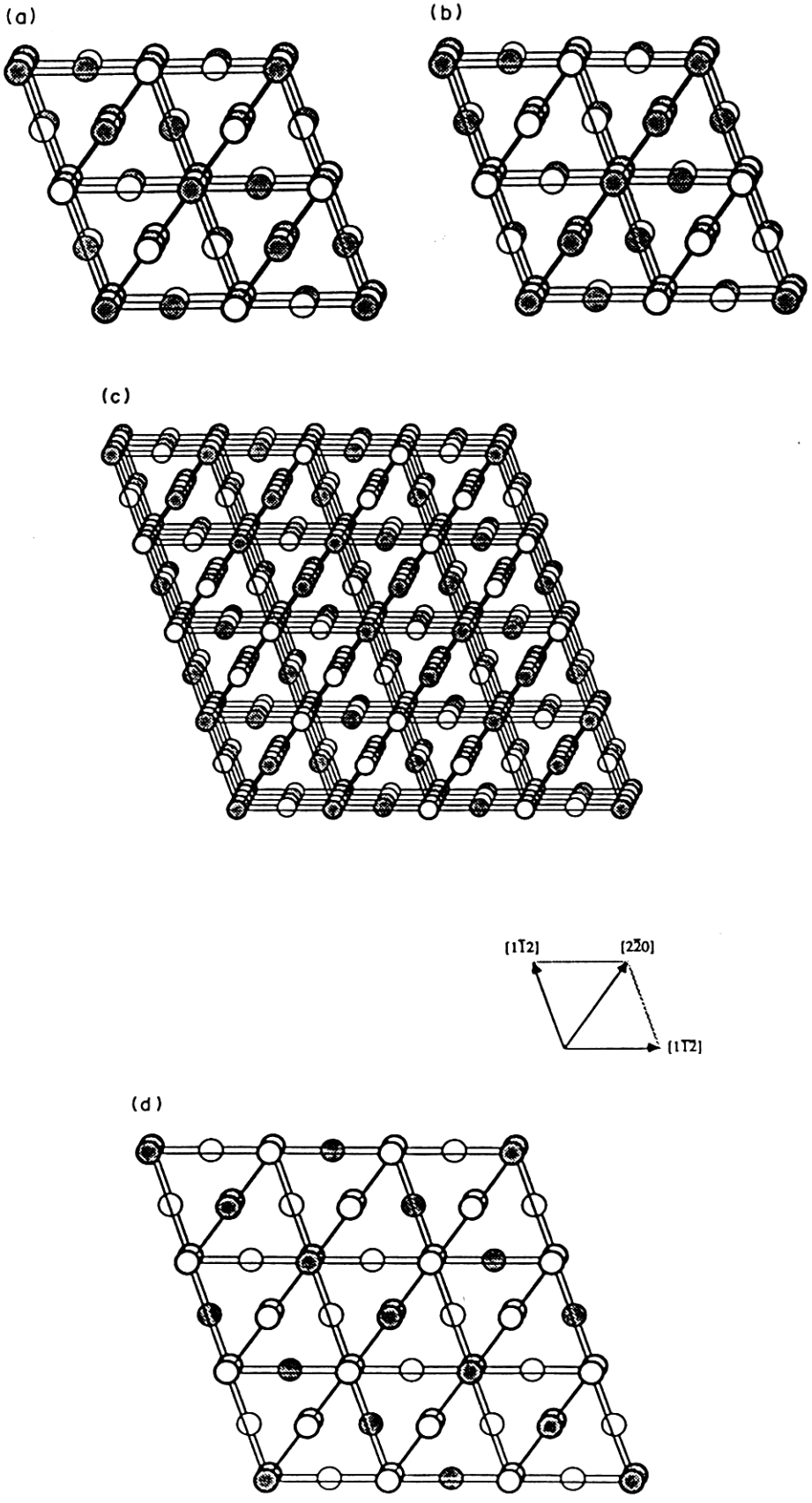


Fig. 11a–d. *Caption on p. 1637.*

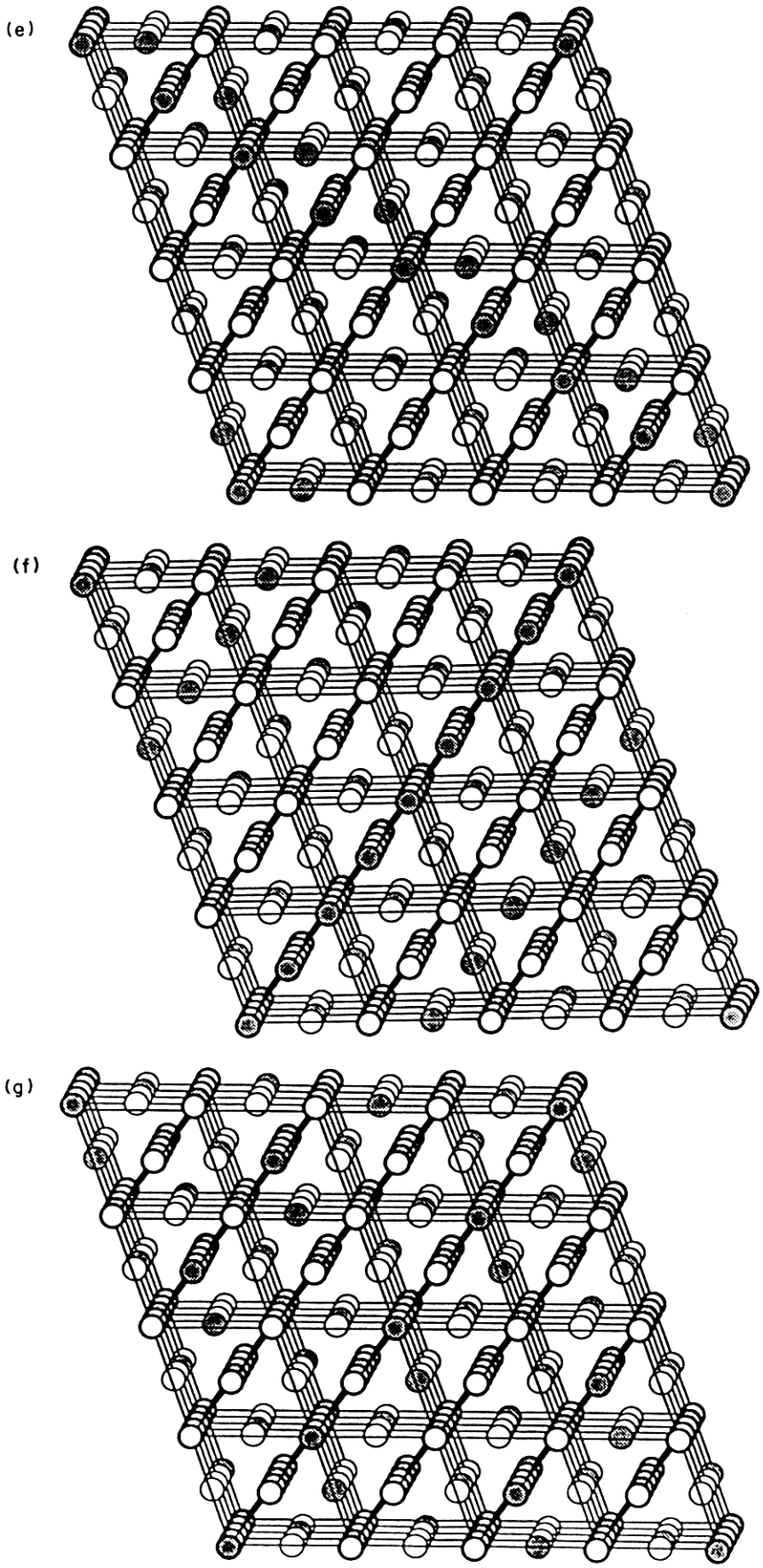
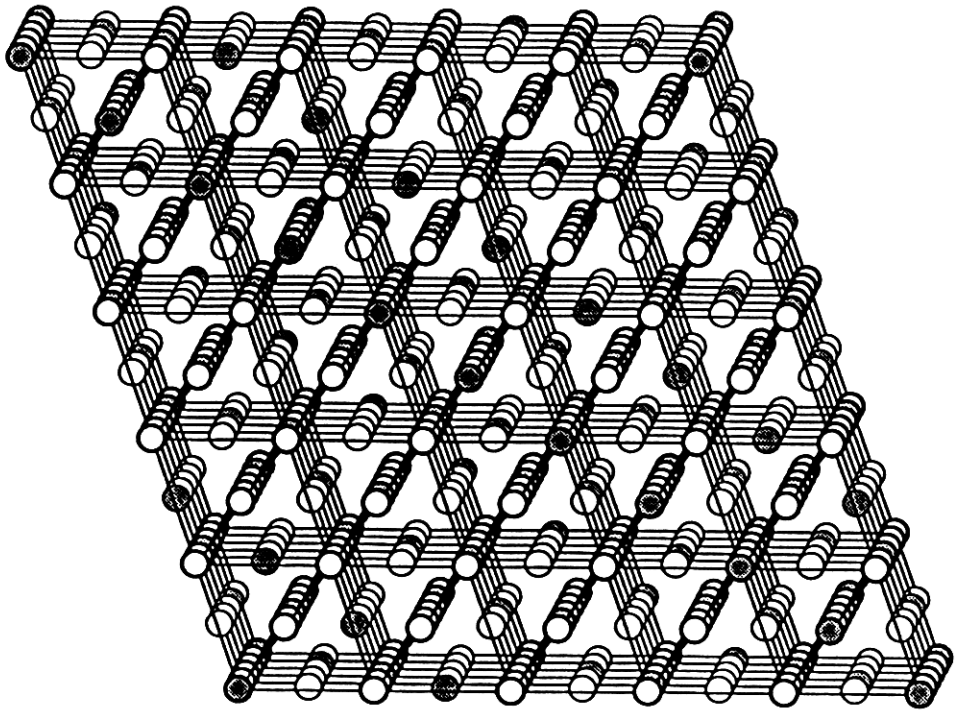


Fig. 11e g.

(h)



(j)

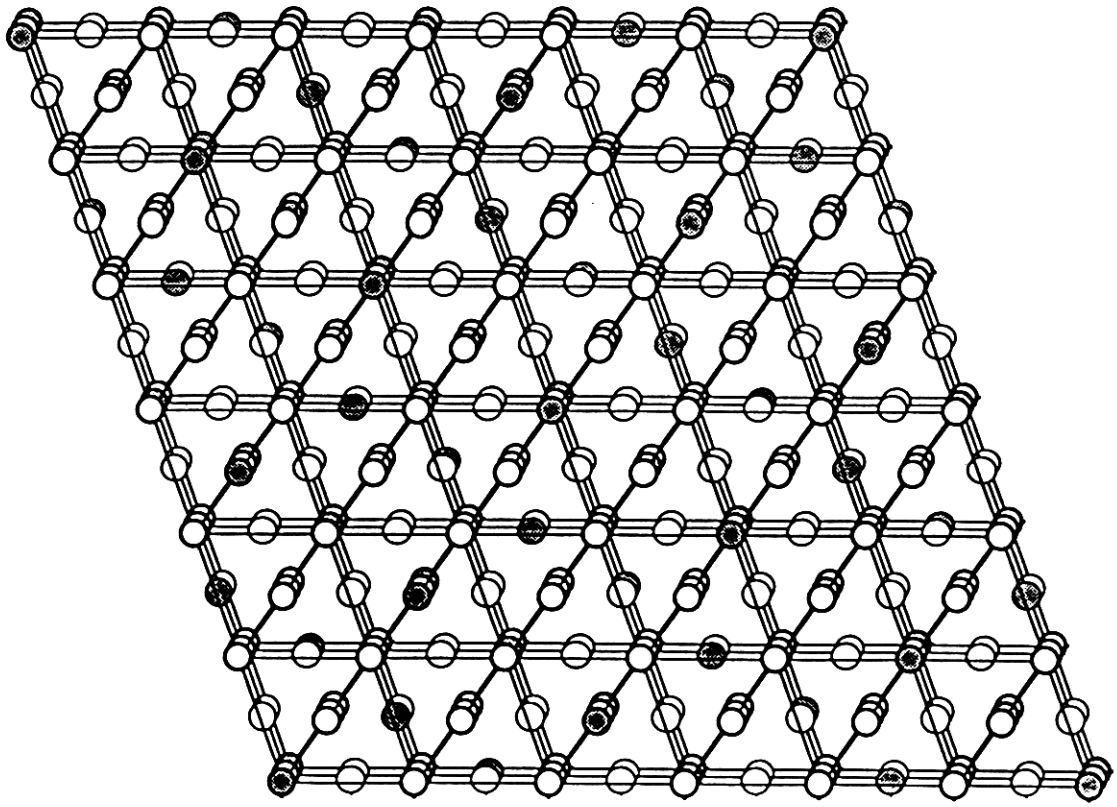


Fig. 11h and j.

(k)

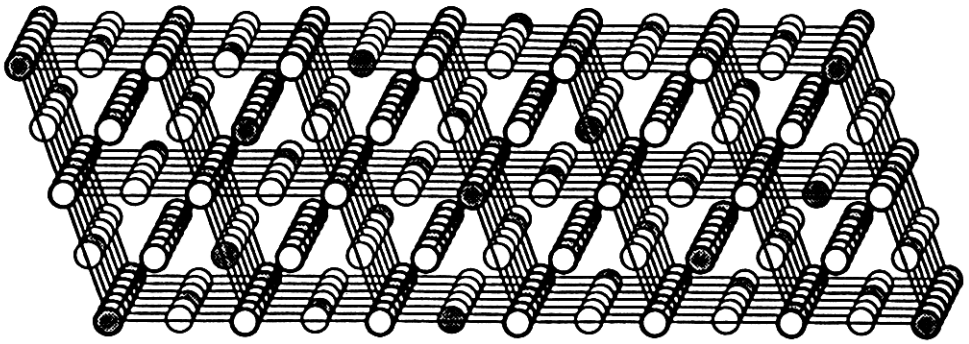


Fig. 11. Perspective views of pseudo modes. Symbols as in Fig. 3. (a) $L1_0$ structure. (b) $L1_1$ structure. (c) NbP structure. (d) Pt_2Mo structure. (e) $D0_{22}$ structure. (f) Monoclinic A_3B structure (variant B). (g) Monoclinic A_3B structure (variant D). (h) Dla structure. (j) Monoclinic A_5B structure (variant B). (k) Monoclinic A_5B structure (variant D).

(v) Composition A_3B. $D0_{22}$ ($TiAl_3$ type) I4/mmm

The structure is body-centred tetragonal with eight atoms in the unit cell which has an ideal axial ratio $p = 2$. The change is specified by

$$\mathbf{J} = \frac{1}{2}\begin{pmatrix} 0 & 2 & 0 \\ 0 & 0 & 2 \\ 1 & 0 & 0 \end{pmatrix} \quad \mathbf{J}^{-1} = \begin{pmatrix} 0 & 0 & 2 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

All of the $\{111\}^c$ planes become $\{112\}^S$ planes. Two $\{110\}^c$ planes of shear become $\{110\}^S$ planes and the associated twinning modes change into true (combined) modes of the superlattice; the remaining four $\{110\}^c$ planes become $\{102\}^S$ planes and the associated superlattice modes are not true twinning modes. Details are as follows:

Cubic var.	*Superlattice mode pair*							
	S	K_1	K_2	η_1	η_2	$q, \bar{q}$	g	*Type*
A (=B, D, F)	(102)	(11$\bar{2}$)	(1$\bar{1}\bar{2}$)	[2$\bar{4}\bar{1}$]	[24$\bar{1}$]	8, 8	$\frac{1}{4}(2p^2 + 80p^{-2} - 20)^{1/2}$	ps.
C (=E)	(1$\bar{1}$0)	(112)	(11$\bar{2}$)	[11$\bar{1}$]	[111]	2, 2	$\frac{1}{2}(2p^2 + 8p^{-2} - 8)^{1/2}$	cb.

In the combined mode, the superlattice planes of shear are alternately of the equiatomic type [Fig. 9(b)] and pure A. Each $\{111\}^c$ plane has the structure shown in Fig 8(g). The combined modes are those in which two of the four $\frac{1}{2}\langle 112\rangle^c$ vectors (one to each $\{111\}^c$ plane) which remain as repeat vectors of the superlattice form the η_1 and η_2 directions, and the planes of shear then have a repeating four-plane sequence $(A_{1/2}B_{1/2})A(B_{1/2}A_{1/2})A$ [Fig. 9(e)]. The planes of shear in the pseudo modes are shown in Fig. 11(e).

(vi) Composition A_3B. B2/m

The structure is side-centred monoclinic with eight atoms in the unit cell which has ideal axial ratios of $p = (27)^{-1/2}$, $r = 4/(27)^{1/2}$ and an ideal value of $c = \cos\gamma = 5/(27)^{1/2}$. The transformation matrices are

$$\mathbf{J} = \frac{1}{4}\begin{pmatrix} 0 & 0 & 4 \\ 1 & \bar{1} & \bar{3} \\ 4 & 4 & 0 \end{pmatrix} \quad \mathbf{J}^{-1} = \frac{1}{2}\begin{pmatrix} 5 & 4 & 1 \\ \bar{3} & \bar{4} & 1 \\ 2 & 0 & 0 \end{pmatrix}.$$

Two of the $\{111\}^c$ planes become equivalent $\{101\}^S$ planes and the other two become $(110)^S$ and $(320)^S$ respectively. One $\{110\}^c$ plane changes into $(001)^S$ and gives rise to a true combined twinning mode, whilst another changes into $(540)^S$ and the derived mode pair does not then produce true twins in the superlattice. The remaining four $(110)^c$ planes consist of two equivalent pairs, leading to $\{341\}^S$ and $(741)^S$ planes of shear. The derived modes with $\{341\}^S$ planes of shear do not correspond to true superlattice twinning modes, whilst those with $\{741\}^S$ planes of shear correspond to type II–type I mode pairs. Details are as follows:

Cubic var.	*Superlattice mode pair*							
	S	K_1	K_2	η_1	η_2	$q, \bar{q}$	g	*Type*
A	(001)	($\bar{1}\bar{1}$0)	($\bar{3}\bar{2}$0)	[$\bar{1}$10]	[2$\bar{3}$0]	2, 2	$2[(4 + 9r^2 - 12rc)(1 + r^{-2} - 2r^{-1}c)s^{-2} - 1]^{1/2}$	cb.
B	($\bar{5}\bar{3}$0)	($\bar{1}$01)	(101)	[4$\bar{5}$4]	[$\bar{4}$54]	8, 8	$\frac{1}{4}[(16 + 16p^2 + 25r^2 - 40rc)(p^{-2} + s^{-2}) - 64]^{1/2}$	ps.
C (≡F)	($\bar{7}\bar{4}$1)	(101)	($\bar{1}\bar{1}$0)	[1$\bar{2}\bar{1}$]	[1$\bar{1}$3]	4, 1	$2[(1 + p^2 + 4r^2 - 4rc)(1 + r^{-2} - 2r^{-1}c)s^{-2} - 1]^{1/2}$	II–I
D (≡E)	($\bar{3}\bar{4}$1)	(101)	(320)	[2$\bar{1}\bar{2}$]	[2$\bar{3}$6]	8, 8	$\frac{1}{4}[(4 + 36p^2 + 9r^2 - 12rc)(p^{-2} + s^{-2}) - 64]^{1/2}$	ps.

The $(\bar{1}11)^c$ atomic planes consist alternately of the configurations of Fig. 8(b) and (a) (the latter being entirely A planes) and become the K_1 planes of the compound mode. The $(\bar{1}1\bar{1})^c$ planes are shown in Fig. 8(h); although they do not contain any $\frac{1}{2}\langle 112\rangle$ vectors which remain lattice vectors, the $(\bar{1}11)^c$ and $(\bar{1}1\bar{1})^c$ planes are nevertheless able to yield a single combined mode in the superlattice as mentioned earlier. The other $\{111\}^c$ type planes are equivalent to those in the $D0_{22}$ superlattice shown in Fig. 8(g); combinations of these planes with each other or with the $(\bar{1}1\bar{1})$ planes lead to shear modes which are not true twins but combinations with the $(\bar{1}11)^c$ planes give true type II–type I twins. The plane of shear of the combined twins is shown in Fig. 9(f), of the type II–I mode pair in Fig. 10(b) and of the two types of pseudo mode in Fig. 11(f) and (g).

(vii) Composition A_4B Dla (Ni_4Mo type) I4/m

The structure is body-centred tetragonal with ten atoms in the unit cell at ideal axial ratio $p = (2/5)^{1/2}$ and

$$\mathbf{J} = \frac{1}{5}\begin{pmatrix} 3 & \bar{1} & 0 \\ 1 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix} \quad \mathbf{J}^{-1} = \frac{1}{2}\begin{pmatrix} 3 & 1 & 0 \\ \bar{1} & 3 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

All of the $\{111\}^c$ planes become $\{211\}^S$ planes. Two of the $\{110\}^c$ planes become $\{210\}^S$ planes and do not lead to true twins of the superlattice; the remaining four $\{110\}^c$ planes become $\{312\}^S$ planes and each such mode pair becomes a type I–type II mode pair of the superlattice. Details are

Cubic var.							*Superlattice mode pair*	
	S	K_1	K_2	η_1	η_2	$q, \bar{q}$	g	*Type*
A	(001)	$(0\bar{1}0)$	$(\bar{1}\bar{1}0)$	$[\bar{1}00]$	$[1\bar{1}0]$	1, 2	$2[(r^{-2} - 2r^{-1}c + 1)s^{-2} - 1]^{1/2}$	cb.
B	$(\bar{1}\bar{2}0)$	$(\bar{1}03)$	(103)	$[6\bar{3}2]$	$[\bar{6}32]$	12, 12	$[\{9p^{-2} + s^{-2}\}\{1 + (r^2/4) - rc + (p^2/9)\} - 4]^{1/2}$	ps.
C (≡F)	$(\bar{3}\bar{2}3)$	(103)	$(0\bar{1}0)$	$[3\bar{6}\bar{1}]$	[101]	2, 3	$\frac{1}{2}[(1 + p^2)s^{-2} + 9p^{-2} - 7]^{1/2}$	I–II
D (≡E)	$(1\bar{2}\bar{3})$	(103)	(110)	$[33\bar{1}]$	$[1\bar{1}1]$	4, 12	$\frac{1}{2}[(1 + p^2 + r^2 - 2rc)(9p^{-2} + s^{-2}) - 16]^{1/2}$	ps.

(viii) Composition A_5B B2/m

This structure is side-centred monoclinic with 12 atoms in the unit cell which has ideal axial ratios $p = 3^{1/2}$, $r = 2/3^{1/2}$, and an ideal value of $c = \cos\gamma = 1/3^{1/2}$. The transformation matrices are

$$\mathbf{J} = \frac{1}{6}\begin{pmatrix} 0 & 0 & 6 \\ 3 & \bar{3} & \bar{3} \\ 2 & 2 & 0 \end{pmatrix} \quad \mathbf{J}^{-1} = \frac{1}{2}\begin{pmatrix} 1 & 2 & 3 \\ \bar{1} & \bar{2} & 3 \\ 2 & 0 & 0 \end{pmatrix}.$$

Two of the $\{111\}^c$ planes become equivalent $\{103\}^S$ planes and the other two become $(110)^S$ and $(010)^S$ respectively. One of the $\{110\}^c$ planes changes into $(001)^S$, giving a true twinning mode of the superlattice, and another becomes $(120)^S$, which does not give a true twinning mode. The remaining four $\{110\}^c$ planes consist of two equivalent pairs leading to $\{323\}^S$ and $\{123\}^S$ planes of shear; the former corresponds to a type I–type II mode pair and the latter gives a pseudo mode. Details are as follows:

Cubic var.							*Superlattice mode pair*	
	S	K_1	K_2	η_1	η_2	$q, \bar{q}$	g	*Type*
A	(001)	$(0\bar{1}0)$	$(\bar{1}\bar{1}0)$	$[\bar{1}00]$	$[1\bar{1}0]$	1, 2	$2[(r^{-2} - 2r^{-1}c + 1)s^{-2} - 1]^{1/2}$	cb.
B	$(\bar{1}\bar{2}0)$	$(\bar{1}03)$	(103)	$[6\bar{3}2]$	$[\bar{6}32]$	12, 12	$[\{9p^{-2} + s^{-2}\}\{1 + (r^2/4) - rc + (p^2/9)\} - 4]^{1/2}$	ps.
C (≡F)	$(\bar{3}\bar{2}3)$	(103)	$(0\bar{1}0)$	$[3\bar{6}\bar{1}]$	[101]	2, 3	$\frac{1}{2}[(1 + p^2)s^{-2} + 9p^{-2} - 7]^{1/2}$	I–II
D (≡E)	$(1\bar{2}\bar{3})$	(103)	(110)	$[33\bar{1}]$	$[1\bar{1}1]$	4, 12	$\frac{1}{2}[(1 + p^2 + r^2 - 2rc)(9p^{-2} + s^{-2}) - 16]^{1/2}$	ps.

In the superlattice structure, the $(\bar{1}11)$ planes are alternately pure A and the type shown in Fig. 8(d) whilst the $(\bar{1}1\bar{1})$ planes have the configuration shown in Fig. 8(k). All of the $\frac{1}{2}\langle 112\rangle^c$ lattice vectors in the $(\bar{1}11)$ plane are lattice vectors of the superlattice, and since one lattice vector of this type in the $(\bar{1}1\bar{1})^c$ plane is also a superlattice vector, the variant pair utilising these two planes remains as a combined superlattice mode; the projection of the structure on the $(110)^c$ plane of shear is shown in Fig. 9(g) and consists of a 6-plane repeat of type $(A_{1/2}B_{1/2})AA(B_{1/2}A_{1/2})AA\ldots$. The remaining two $\{111\}^c$ planes both have the configuration shown in Fig. 8(l) in which there are no lattice vectors derived from $\frac{1}{2}\langle 112\rangle^c$ vectors. Combinations of these planes with each other thus give only pseudo modes of the superlattice; the plane of shear projection is given in Fig. 11(j). Combination of either of these planes with the $(\bar{1}1\bar{1})$ plane also gives a pseudo mode, as shown in Fig. 11(k), but combination with $(\bar{1}11)^c$ gives a true type I type II twin, see Fig. 10(d).

Cubic var.							*Superlattice mode pair*	
	S	K_1	K_2	η_1	η_2	$q, \bar{q}$	g	*Type*
A (≡B)	(120)	$(\bar{2}11)$	$(\bar{2}1\bar{1})$	$[\bar{2}\bar{1}5]$	$[\bar{2}15]$	10, 10	$[(25p^2 + p^{-2} - 10)/5]^{1/2}$	ps.
C (≡D, E, F)	$(\bar{1}3\bar{2})$	(121)	$(\bar{2}11)$	$[\bar{7}15]$	[111]	2, 10	$\frac{1}{2}(5p^2 + 2p^{-2} - 5)^{1/2}$	I–II

All of the $\{111\}^c$ planes are of the type shown in Fig. 8(j) and contain a single lattice vector derived from $\frac{1}{2}\langle 112\rangle^c$, whilst the other two vectors of this type are $\frac{1}{5}\times$ lattice vectors of the superlattice. The true type I–type II twins have η_2 and η_1 respectively parallel to the direction in which B atoms are nearest to each other, whilst in the pseudo modes both η_1 and η_2 have lattice repeat distances which are appreciably larger than in the disordered structure. Projections of the superlattice structure in the plane of shear are shown in Figs 10(c) and 11(h).

5. DISCUSSION

Slip in a superlattice is usually more difficult than in the random solid solution since the motion of lattice dislocations of the disordered structure generally creates antiphase boundaries in the superlattice, and perfect dislocations of the superlattice must have increased Burgers vectors. Twinning is similarly inhibited since the normal mode of the disordered structure frequently leads to the production of a region of incorrect order when applied to the superlattice, and a true twinning mode requires a higher shear. As we have seen, this applies to all variants of the normal twinning mode in almost all cubic superlattices, but only to some of the variants in a non-cubic superlattice. In the same way, some variants of the normal slip system may operate without producing antiphase boundaries in non-cubic superlattices.

For the B2 and $L1_2$ cubic superlattices, the true twinning modes without shuffles predicted in Table 3 require shears in the opposite sense to the normal shear of the disordered structure and of twice the normal magnitude. True twinning of the $D0_3$ and B32 structure requires shears in the same sense as the normal mode but of four times the normal magnitude. The available experimental evidence on deformation twinning in general indicates a strong preference for modes of low shear combined with simple (where possible, zero) shuffles, and it might be expected that the atomic displacements required to produce the twins of Table 3 will not readily take place. In fact, the only mode in part (a) of Table 3 for which there is any experimental evidence is the 1.3 mode for the $L1_2$ structure.

Deformation twinning has been observed in both copper–gold alloys and nickel-based superalloys containing phases with the $L1_2$ structure. Mikkola and (J.B.) Cohen [19] found twins in shock-loaded specimens of both disordered and ordered Cu_3Au, and neither electron diffraction photographs nor measurements of diffuse X-ray scattering revealed the additional peaks expected if the twins in the ordered structure were in fact pseudo twins. Rather similar indirect evidence of the operation of a true twinning mode (presumably 1.3) has been reported for nickel superalloys by Guimier and Strudel [20] and by Kear *et al.* [21, 22]. The superalloys contain coherent precipitates of the γ' $Ni_3(Al, Ti)$ phase in a solid solution (γ) matrix and the microtwins appear to be continuous across the γ–γ' boundaries. Chakraborty and Starke [23] found that for imperfectly ordered Cu_3Au crystals deformed in compression the twinning stress first falls slightly with increasing order and then rises steeply as the order approaches 100%. These twins were believed to form in the normal f.c.c. mode, the initial decrease in stress being ascribed to a decrease in stacking fault energy with order, and the sharp increase to the higher energy of the product of the pseudo mode in specimens with relatively high degrees of order. In these compression specimens, twinning was only observed after some plastic deformation by slip, so that even initially fully ordered crystals were somewhat disordered when twinning began. However, some tensile specimens twinned in the early stages of deformation at relatively low stresses, and the authors interpret this as evidence that the 1.3 mode was operating in the fully ordered crystals, the decrease in stress again being attributed to the effect of the order on stacking fault energy.

All of these results thus indicate some probability that fully ordered $L1_2$ structures may form true deformation twins, but the evidence is not complete and in particular there is no experimental confirmation of the shear magnitude. Measurements of the tilt produced on pre-polished surfaces or of the deviation of marker lines are required but are obviously very difficult since the twins observed are usually very narrow. The twin habit plane does appear always to be {111} in cases where it has been determined, and this would be expected since the only alternative in Table 3 is a shuffle mode with quite a high shear.

Many authors have discussed the possibility of twinning of the B2 structure by the mode 1.3^T but, to our knowledge, no experimental evidence for this mode has been obtained. Pseudo twinning, however, is well established in iron–beryllium alloys [3, 24]. The alloys with up to 25 at.% beryllium were originally thought to have ordered structures based on $D0_3$ but were later shown to have modulated structures consisting of the primary solid solution and an ordered B2 phase. The pseudo twinning produces a well-studied superelastic effect, and the structure of a pseudo twin was confirmed as side-centred orthorhombic [24]. As may be seen from Fig. 4(a), this structure is obtained if alternate planes of a single {110} set are occupied solely by A atoms and B atoms respectively. (It is occasionally wrongly reported [2, 16] that this structure is tetragonal because the a and b axes are of equal length in the ideal (unrelaxed) unit cell.) Rather similar but less complete results have been obtained with iron–aluminium alloys variously reported to have either the B2 or $D0_3$ structure. Cahn and Coll [2] found that alloys with imperfect long range order (less than 50%) form pseudo twins, but that twinning is suppressed at higher degrees of order. Guedo and Rieu [25] obtained visual evidence of twinning and, on unloading, of subsequent detwinning for some alloys with B2 structures, but superelasticity was only observed in alloys with $D0_3$ structures and there was then no visible twinning. The superelasticity was provisionally ascribed to the formation and removal of very small pseudo twins, but in a later paper [26] from the same laboratory, superelastic effects in iron–aluminium alloys were attributed largely to dislocation interactions.

Very recently, some experimental evidence for deformation twinning of the B2 structure using the shuffle mode 2.3^T of Table 3 has been obtained for titanium–nickel and titanium–iron–nickel alloys [16].

A possible complication is that the specimens twinned most readily when cycled through the martensitic transformation under stress, so that some form of transformation twinning may have been involved. Nevertheless, both pseudo twins and true twins with the {114} habit of mode 2.3^T were also observed in stressed single phase specimens. Figure 12 shows possible shuffle mechanisms in which one-half of the atoms move relatively to the others through a distance $a/2$ in a $\langle 100 \rangle^c$ direction; compare with the hypothetical mode 1.2 twinning of Fig. 2. The atoms which must shuffle are alternately A and B on successive planes of shear and are contained in alternate K_2 ($\{110\}$ type) planes normal to the plane of shear. Goo *et al.* [16] suggest that these atoms are all displaced in the same direction [Fig. 12(c) i]; alternative possibilities in which the atoms move in opposite directions in successive K_2 shuffle planes or in successive rows of one shuffle plane are shown in (ii) and (iii). Goo *et al.* also link their suggestion to an interface model by assuming that the net displacement will be away from the interface, giving effectively rows of vacancies on the twin side of the interface, and they further assume that this applies at both interfaces of a thin enclosed twin, thus requiring a very small increase of volume. However, the structure of the twin interface cannot be settled by considering only possible shuffle and shear displacements since a lower energy might correspond to an atomic configuration in which the two crystals are given an additional relative translation.

Examination of the results for non-cubic superlattices shows that only one of the six variant pairs is a pseudo mode for the orthorhombic (Pt_2Mo) superlattice, whereas there are three pseudo modes in the two monoclinic structures and in the rhombohedral ($L1_1$) structure. The remaining four superlattices are tetragonal; three of them have four pseudo modes, but the Ni_4Mo structure has only two. Thus we might expect twinning to be most inhibited in tetragonal structures and least in orthorhombic structures.

Experimental results appear to have been reported for the $L1_0$, Pt_2Mo, $D0_{22}$ and Dla structures. Krasevec *et al.* [27] found that the NiMn phase with the $L1_0$ structure deforms by twinning on $\{111\}^c$ planes, and that the structure is unchanged by this twinning, which was presumably confined to the true, combined modes. The many results on the deformation behaviour of the CuAu I superlattice are complicated by the fact that the microstructure usually contains a large number of {101} type order twins [10, 28–30] and the propagation of dislocations or deformation twins across these boundaries has to be considered. Contrary to the conclusions of Syutkina and Yakovleva [29], Pashley *et al.* [30] found that {111} twinning is very important in the deformation of this superlattice, and they speculate that the structure may be changed in some of the twins. Some electron diffraction evidence was obtained in support of the hypothesis that pseudo twins are formed, although the authors are properly cautious about claiming that this has been established. Their conclusion "should this be confirmed, it represents an unusual (and novel) observation of a structure created solely by mechanical deformation" is interesting in showing that the concept of stress-induced phase transformation has not been widely recognised until recently (and indeed may still be unfamiliar) except to specialists in martensitic transformations.

The most complete investigation of twinning in a $L1_0$ structure to date was made by Schectman *et al.* [31] for an equiatomic titanium–aluminium alloy. They identified the specific variants of the $\{111\}^c$ $\langle 112 \rangle^c$ twins which were formed during deformation, and showed that these were the variants which lead to true (combined) twins. [The variants they list correspond to the two true mode pairs in 4(i) above.] Finally, and very importantly, they were able to measure the shear magnitude in the deformation twins and this was found to be $2^{-1/2}$ as expected from the 2.2 mode. Thus it appears that in TiAl under the conditions investigated, only true twinning is observed.

Hansson and Barnes [10] first pointed out that the structure produced by pseudo twinning of $L1_0$ has a single set of $\{111\}^c$ planes alternately occupied by A and B atoms and hence is effectively that of $L1_1$ (CuPt type), and this was also recognised by Pashley *et al.* It follows that the reverse is also true; the pseudo mode of $L1_1$ gives the $L1_0$ structure and these relations can be seen by comparing Fig. 11(a) and (b). The number of predicted variants which correspond to these transitions is interesting. According to the table in Section 4(i), there are four variant pairs which give pseudo modes of $L1_0$ and these correspond to the four possible orientations of the unique axis of $L1_1$. On the other hand, there are only three variant pairs which give pseudo modes for a given $L1_1$ orientation [see 4(ii)], and these correspond to the three possible orientations of the c axis in the resulting $L1_0$ structure. This example also shows why statement (iii) at the end of Section 1 is misleading. Although a general shear always leads to a lowering of symmetry corresponding to a sub-group of the original structure and the shear, Cahn [5] points out that super-groups may form at special values of the shear magnitude, thus effectively increasing the symmetry.

Deformation twinning has also been reported for three other of the non-cubic superlattice structures considered in Section 4, namely Pt_2Mo type, $D0_{22}$ and Dla. An orthorhombic Pt_2Mo type superlattice forms in certain nickel–molybdenum–chromium alloys (known commercially as Hastelloy alloys *S*, C-4 and C-276) and Tawancy [32] found deformation to be largely by twinning. The twinning shear was not measured and it is also not clear whether there was any preference for combined, type I or type II twins.

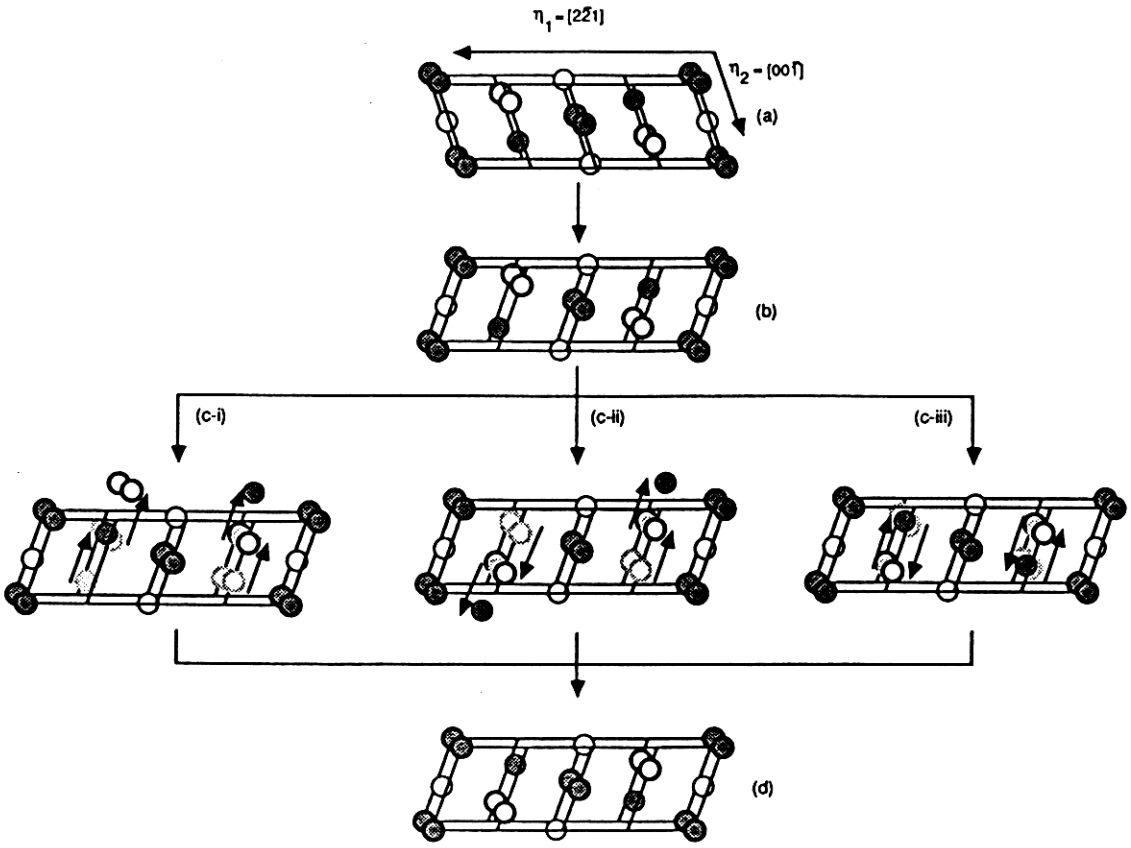


Fig. 12. To illustrate {114} (2.3^T) shuffle mode in B2 structure. Symbols as in Fig. 3. (a) Parent structure. (b) Sheared structure. (c) (i), (ii) and (iii) show alternative possible shuffles. (d) (Combined orientation) twin.

The author notes, in agreement with the table in 4(iv), that only two of the 12 normal twinning systems are unfavourable in the superlattice, and he speculates that this is why twinning is preferred to slip.

Vanderschaere and Sarrazin [33] studied deformation twinning in a Ni_3V alloy with the $D0_{22}$ structure. By careful dark field microscopy, they demonstrated that the twinned regions of the deformed alloy had the same crystal structure as the untwinned regions. In an interesting discussion, they consider the possibility of twinning produced by partial dislocations of type $\frac{1}{6}\langle 112\rangle$ or $\frac{1}{3}\langle 112\rangle$ of the disordered structure, corresponding to modes derived from the usual cubic mode 2.2 and the "anti-mode" 1.3. The majority of the twins were stopped at antiphase boundaries and examination of the Burgers vectors of the twinning dislocations confirmed that these were of the types required to produce true twins either according to our table in 4(iv), or by twice the opposite shear (i.e. the true twin derived from mode 1.3). The stacking relations discussed by Vanderschaere and Sarrazin can be inferred from our figures; Fig. 1 of their paper corresponds to Fig. 8(g) and the six plane stacking of the {111} planes (K_1 and K_2) can be seen in Fig. 11(e). In the normal mode pseudo twin, this becomes a 12 plane stacking of K_1 and in the alternative pseudo twin with the opposite shear of $2^{1/2}$, it becomes a three plane stacking, as also can be seen from Fig. 11(e). Some of the twins were observed to be continuous across antiphase boundaries, and the authors speculate that these involve still larger twinning dislocations of type $\frac{2}{3}\langle 112\rangle$, in order that no faults are produced. This formally implies a twin derived from mode 1.9 with a shear of $8^{1/2}$ which seems very improbable.

Finally, Nesbit and Laughlin [34] have investigated slip and deformation twinning in the Dla structure of a fully ordered Ni_4Mo alloy. Superdislocations were not observed, but wide intrinsic stacking faults and deformation twins were a pronounced feature of the deformation. The results were interpreted as indicating that the faults were of low energy produced by the passage of Shockley partials which do not change the number of each kind of first neighbour atom pairs, and that the twins were true twins which may be regarded as an assembly of such faults, but no direct evidence for this or for the shear magnitude was obtained. In discussing the twinning mechanism, η_1 is chosen in the $\langle\bar{1}2\bar{1}\rangle$ direction in which the Mo atoms are closest together [Fig. 8(j)] and the orientation relation is described as a reflection in the twinning plane *and* the $(\bar{1}2\bar{1})$ plane. In fact, as our table in 4(vii) shows, this choice of η_1 leads to a type II orientation relation, but it is equally possible by a

different choice of η_1 to obtain true twins with a type I relation.

There is no work of which we are aware on twinning in the remaining non-cubic structures considered above, and indeed there do not appear to be any known examples of the two monoclinic superlattices. However, the copper–platinum system displays a wide range of ordering reactions, and it would be interesting to investigate further the early suggestion [35] that at the composition Pt_7Cu, a cubic superlattice with symmetry $Fm\bar{3}m$ forms, as predicted and illustrated by Khachaturyan [9, 36]. This structure which is also reported for Ca_7Ge [37] should be able, in principle, to form true twins without shuffles in all variants of the usual f.c.c. mode.

We note, in conclusion, that there are many intermetallic compounds with structures which are not obtained by ordering and some of these are known to undergo deformation twinning. In general, true twinning in these structures will require atomic shuffling so that the tendency to avoid shuffling of the lattice points is no longer so important in the choice of twinning mode. An interesting example is the tetragonal compound Cu_2Sb recently studied by Paxton and Entwisle [38].

6. CONCLUSIONS

1. With rare exceptions, cubic superlattice structures cannot form true twins in modes derived from those of the disordered b.c.c. or f.c.c. structures.

2. True twins without shuffles can always be formed (geometrically) by choosing a mode of higher shear magnitude, but many such modes are implausible. There is some indirect evidence for the formation of true twins in $L1_2$ in this way, but the B2 structure either forms pseudo twins or true twins in a new mode which requires atomic (but not displacement) shuffles.

3. Non-cubic superlattices may, in principle, form pseudo twins in some variants of the usual disordered mode and true twins in others. There is good experimental evidence for the formation of true twins in several of these structures.

Acknowledgements—This work began during the tenure by DEL of an SERC Visiting Fellowship at Oxford and was also partly supported by NSF Grant DMR-8413155. The assistance of Mr Jeff Simmons and Mr Gary Pierini in producing the figures is gratefully acknowledged.

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