Deformation twinning in intermetallic compounds—the dilemma of shears vs. shuffles

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Abstract

In this paper the geometric description and general theory of mechanical twinning are reviewed, the twins in general lattices and superlattices are summarized, and the kinematic process by which mechanical twins form is revisited. A case study of mechanical twinning of $HfV_2 + Nb$, a C15 (cubic) Laves phase, is presented and the synchroshear of selected atomic layers is proposed to explain the physical process of twin formation. If the twins form in this way, then long shear vectors and/or atomic shuffles are not really necessary.

1. Introduction

In the development of intermetallic compounds as structural materials, an alternative method for obtaining ductility and toughness is to consider non-dislocation deformation modes, e.g. mechanical twinning [1, 2]. Mechanical twinning can be the dominant deformation and toughening mode at low temperatures in some intermetallic compound-based alloys, e.g. TiAl-based alloys [3].

1.1. Twinning

When a crystal contains two regions which are specially oriented with respect to one another, the crystal is said to be twinned. The most frequently occurring special orientation is with the crystal structure of one part the mirror image of the other part, with the so-called twinning plane as the mirror plane. Twinned crystals are often produced during growth, recrystallization and plastic deformation. Mechanical twinning is a common mechanism of plastic deformation, particularly when straining is carried out at low temperatures and/or at high speed. Like slip, mechanical twinning enables a crystal to undergo a permanent change in shape with a negligible change in volume, but unlike slip, mechanical twinning involves shear by a fixed magnitude, characteristic of the crystal structure.

If we accept for the moment that a mechanical twin may be formed by a simple shear (we modify this assumption later), a deformation twin can be geometrically described by six parameters K_1, η_1, K_2, η_2, S and g, which are called the twinning elements, as illustrated in Fig. 1. All points of the lattice on the upper side of a plane K_1 are displaced in the direction η_1 by an

amount which is proportional to their distance above K_1. The proportionality constant g is the strength of the simple shear. The plane containing η_1 and the normal to K_1 is called the plane of shear S. It can be seen that a vector parallel to η_2 in S will be the same length before and after shear if the angle α which it makes with the normal to K_1 is given by $g = 2 \tan \alpha$. Evidently all vectors in that plane through η_2, which is normal to S, are unchanged in length, although rotated. This plane, AOB in Fig. 1, is conventionally labeled K_2 and is called the second undistorted plane. K_1 is neither rotated nor distorted and is called the twin plane, or first undistorted plane.

Neglecting some exceptions, based on the rationality of the twinning elements, two types of twinning can be distinguished. For type I twins, K_1 and η_2 have rational indices. The orientation changes involved may be achieved hypothetically by reflection in the K_1 plane or by a rotation of π about the normal to K_1. For type II twins, K_2 and η_1 have rational indices, the orientation relationship being a rotation of π about η_1 or a reflection in the plane normal to η_1. In crystals of high symmetry type I and II twins are equivalent. Such twins
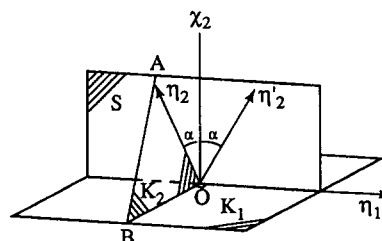

Fig. 1. The twinning elements.

are said to be compound or degenerate, and all elements are rational. All twins in cubic materials are degenerate, and since in the balance of this paper we will consider only cubic materials, we will not distinguish type I and type II twins.

In the more complex twinning modes, most frequently occurring in superlattices, a simple homogeneous shear displaces only a fraction of the atoms of the crystal directly to positions appropriate to the twinned structure, and therefore "shuffles" of the remaining atoms are hypothetically required to restore the original crystal structure [4]. In this case, another element, the percentage of atoms undergoing this shuffling, is needed to describe completely the twinning process. Generally speaking, twins in some simple metals (particularly b.c.c. metals) and most complex superlattices involve long shear vectors, and/or atomic shuffling, if the shear is assumed to be homogeneous, as it is in the usual treatment.

It is worth noting that the geometric description of twinning does not necessarily apply to the real physical process of the formation of deformation twins. Two questions exist: (1) what is the real physical process by which mechanical twins form, and (2) are long shear vectors and/or shuffles really necessary in the formation of deformation twins in intermetallic compounds? In this paper, these issues are investigated using deformation twinning in a C15 (cubic) Laves phase, $HfV_2 + Nb$, as an example.

In Sections 1.2 and 1.3, we briefly review deformation twinning, twinning modes in general lattices and superlattices and experimental techniques. We then report on our study of mechanical twinning in the cubic C15 Laves phase $HfV_2 + Nb$ in Sections 2 and 3. In Section 4, we focus on the mechanism of C15 twinning in which synchroshear of selected layers is proposed to explain the physical process by which twins form. We then discuss the formation of mechanical twinning in f.c.c. $L1_2$, A4 and C15 structures using different models and demonstrate that the model presented here is more physically reasonable since long shear vectors and/or shuffles are not required for deformation twinning to occur in some intermetallic compounds. The conclusions are drawn in Section 5.

1.2. Review of deformation twinning

Twinning elements can be identified by several methods. For macroscopic twins, the method of Greninger and Troiano [5] can be used to measure the changes in the surface topography caused by twinning. If a macroscopic twin is introduced into a rectangular-shaped single crystal then in general the faces of the crystal in the twinned region become tilted relative to the matrix, and the boundaries between the twin and matrix make traces on the sides of the crystal. The

angles between these traces and the edges of the crystal and the tilt of the lateral surfaces in the twinned region may be measured optically. Using this information combined with stereographic projections, all six twin elements can be deduced [6]. It is important to realize that the magnitude of the twinning shear can only be deduced if the actual motion of the lateral surfaces can be measured. If such measurements cannot be made, as for example in a small twin totally contained within a polycrystalline matrix, then the shear magnitude is unknown (although the direction is known).

In most cases, some of the twinning elements are determined from diffraction patterns using a proper zone axis in a transmission electron microscope (TEM) [7]. When the twin plane K_1 lies parallel to the electron beam, the twin axis is then parallel to the reciprocal lattice corresponding to the diffraction pattern, and the twin diffraction pattern is immediately obtained by a simple rotation. A rotation of 180° about the twin axis corresponds to a mirror image of the matrix diffraction pattern across the twin axis. This is demonstrated in Fig. 2 for the case of a [110] diffraction pattern and a $(1\bar{1}1)$ twin plane in f.c.c. crystals. It should be noted that using this method only some of the twin elements can be identified. For example, the f.c.c. twin in Fig. 2 could have occurred by a motion of $1/6[\bar{1}\bar{1}2]$ or by $2/6[1\bar{2}1]$ on each {111} plane parallel to the composition plane, since these two differ by $1/2[1\bar{1}0]$, a lattice translation vector. This mechanism is closely related to the Christian mechanism [4]. Thus the strength of the simple shear remains unknown if only the diffraction patterns and relative orientations are known. In the case of an f.c.c. crystal, there is no reason to expect the shear vector to exceed $1/6\langle112\rangle$ so this is universally assumed, even in the absence of macroscopic shear data. Several attempts have been made to account for the observed twinning elements in terms of the crystal structure involved. These theories, for example the theory of Bevis and Crocker [8], examine the geometry of the shear and shuffles that would be required by various hypothetical twinning modes in order to obtain
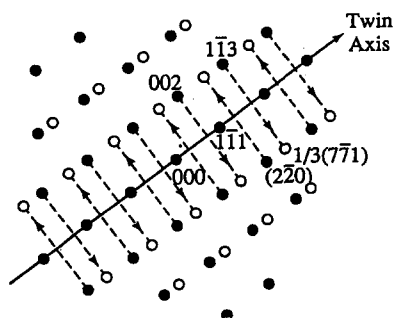

Fig. 2. The [110] diffraction pattern for a {111}⟨11$\bar{2}$⟩ twin in the f.c.c. structure: ● matrix spots, ○ twin spots.

the observed twins. All these theories have difficulty in deciding which of the possible twinning systems will operate in practice [9]. The atomistic structure of the twin–matrix interface can be observed using high resolution electron microscopy.

Using these methods, twin elements in some lattices, e.g. b.c.c. and f.c.c., have been identified. For example, for b.c.c. lattices K_1, η_1, K_2, η_2 and g are given by (112), $[\bar{1}\bar{1}1]$, $(11\bar{2})$, $[111]$ and 0.707 respectively, and for f.c.c. lattices by (111), $[11\bar{2}]$, $(11\bar{1})$, $[112]$ and 0.707. For these twins in the f.c.c. and b.c.c. lattices, only short shear vectors and no shuffles are required and in these cases it is physically reasonable to assume that the formation of twins is due to a homogeneous shear of every atomic plane along η_1 on the K_1 plane, since all planes are compositionally and structurally identical.

Twin structures in some superlattices have also been identified. Some possible corresponding twinning elements for various superlattices are listed in Table 1 [4, 10]. For these twins, long shear vectors and/or shuffles are commonly used in the description, but this does not mean that such long shears and complex shuffles actually occur. For example, in C15 intermetalic compounds the shuffling of a large number of atoms in this topologically closed-packed structure at low temperatures is probably physically unreasonable. It is probable that neither of the twinning modes listed in Table 1 for the C15 twin actually operates in practice. This is the main subject of the balance of this paper.

1.3. Deformation twinning in C15 HfV₂ + Nb

Although most previous studies of mechanical deformation in intermetallic compounds have been made on structures that are ordered forms of f.c.c., b.c.c. and h.c.p., most intermetallics have more complex structures. Laves phases comprise the largest class of such compounds.

Inoue *et al.* [11, 12] have reported that Hf–V–Nb alloys with substantial volume fractions of the HfV₂-based Laves phase can be rolled without cracking at room temperature. Livingston and Hall [13] found that the major deformation mode in the C15 Laves phase is $\{111\}\langle11\bar{2}\rangle$ twinning, typical of those seen in the deformation of f.c.c. materials. Based on these reports, we decided to study the deformation of this HfV₂ + Nb ternary C15 Laves phase.

2. Experimental procedures

Arc-melted buttons were prepared using elemental Hf, V, and Nb with nominal purities 99.99%, 99.6% and 99.7% respectively. The buttons were homogenized at 1000 °C for 100 h and then quenched into water. Compression specimens of dimension $3 \times 3 \times 5$ mm³ were cut using electrical discharge machining (EDM) and mechanically polished. Before mechanical testing polished sections of these samples were examined in an optical microscope after etching with a reagent consisting 30 ml HNO₃, 30 ml lactic acid, 2 ml HF and a few drops of water. Compression tests were performed in an Instron machine at different strain rates ranging from 4.2×10^{-4} s⁻¹ to 8.5×10^{-3} s⁻¹.

Samples were prepared for transmission electron microscopy from the deformed samples by EDM cutting, mechanical grinding to a thickness of about

TABLE 1. Possible twinning elements in various superlattices

Material	Lattice	K_1	η_1	K_2	η_2	f	Shuffle (%)
CsCl, NiAl	B2	$\bar{1}12$	$1\bar{1}1$	112	$\bar{1}11$	0.707	0[a]
		$\bar{1}12$	$1\bar{1}\bar{1}$	$\bar{1}10$	001	1.414	0
		$\bar{1}12$	$1\bar{1}1$	001	$\bar{1}10$	2.828	0
		$1\bar{1}4$	$2\bar{2}1$	$1\bar{1}0$	$00\bar{1}$	0.707	50
Ni₃Al, Al₃Ti + Fe	L1₂	$1\bar{1}\bar{1}$	$1\bar{1}2$	$\bar{1}11$	$1\bar{1}2$	0.707	0[a]
		$1\bar{1}\bar{1}$	$1\bar{1}2$	$\bar{1}11$	$1\bar{1}2$	0.707	33.0
		$1\bar{1}\bar{1}$	$\bar{1}12$	001	$1\bar{1}0$	1.414	0
		$1\bar{1}\bar{1}$	$1\bar{1}2$	$1\bar{1}0$	001	2.828	0
Al₃Ti	DO₂₂	$1\bar{1}1$	$\bar{1}12$	001	$1\bar{1}0$	1.414	0
		$1\bar{1}1$	$1\bar{1}2$	$1\bar{1}0$	001	2.828	0
TiAl	L1₀	$1\bar{1}\bar{1}$	$\bar{1}12$	001	$1\bar{1}0$	1.414	0
		$1\bar{1}\bar{1}$	$1\bar{1}2$	$1\bar{1}0$	001	2.828	0
HfV₂ + Nb	C15	$1\bar{1}\bar{1}$	$1\bar{1}2$	$\bar{1}11$	$1\bar{1}2$	0.707	83.3
		$1\bar{1}\bar{1}$	$1\bar{1}2$	$1\bar{1}0$	001	2.828	33.0

[a]Pseudo-twinning, *i.e.* there is a compositional disorder across the interface.

70 μm and ion milling using a liquid nitrogen cold stage on a Gatan ion milling machine. The samples were viewed in a Phillips 400T TEM operating at 120 kV.

X-ray powder diffraction combined with computer simulation was employed to examine the substitution of Nb in HfV_2. A powder specimen was prepared with a particle size of approximately 40–60 μm using a Spex mixer/milling machine. Diffraction experiments were conducted on a Rigaku diffractometer using Cu $K\alpha$ radiation ($\lambda = 1.5406$ Å) and Bragg angles in the range 20°–140°. The theoretical X-ray powder diffraction pattern was obtained using the Lazy/Pulverix program.

3. Results

The single-phase C15 alloy prepared in the course of determining the phase diagram [14] showed substantially different degrees of brittleness as indicated by sensitivity to thermal shock and handling stress. Those alloys in the region of [V]/[Hf] > 2 and with substantial ternary Nb additions are less brittle than those for which [V]/[Hf] < 2. With this qualitative result in mind we performed mechanical tests on two-phase C15 alloys consisting of a matrix of C15 Laves phase with [V]/[Hf] > 2 surrounding the V-rich b.c.c. solid solution. A microstructure of an $Hf_{14}V_{64}Nb_{22}$ alloy is shown in Fig. 3.

Compression stress–strain curves from tests performed between room temperature and 1000 °C in a 10^{-5}–10^{-6} Torr vacuum are shown in Fig. 4. Note the loss in ductility at intermediate temperatures.

TEM examination of the sample tested at room temperature showed that the major deformation mode in the ternary C15 Laves phase is mechanical twinning, as shown in Fig. 5(a). The diffraction pattern using a $\langle 110 \rangle$ zone axis, as demonstrated in Fig. 5(b), unambiguously identifies it as the $\{111\}\langle 11\bar{2} \rangle$ twin, the twin commonly seen in f.c.c. materials. Note, however, that this does not define the strength of the simple shear. TEM observations of the samples plastically deformed above 800 °C showed that the major deformation mode in the C15 phase at high temperatures is $b = 1/2\langle 110 \rangle$ dislocation slip, as shown in Fig. 6. The slip plane was not determined.

An experimental X-ray powder diffraction pattern from a single-phase C15 alloy, $Hf_{25}V_{60}Nb_{15}$, is shown in Fig. 7(a). Based on the assumption that there are no antisite defects and Nb randomly occupies both Hf and V sites in a ratio that satisfies stoichiometry (i.e. the atomic fraction of Hf + Nb atoms on Hf sites is 1/3 and that of V + Nb atoms on V sites is 2/3), we calculated
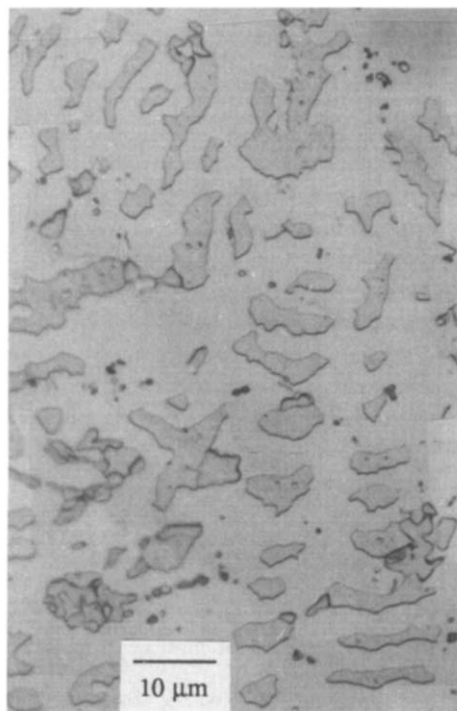

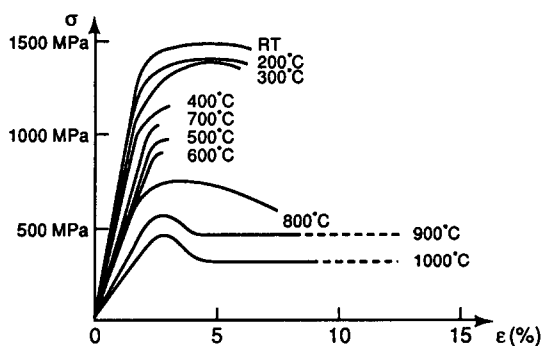Fig. 3. Microstructure of an $Hf_{14}V_{64}Nb_{22}$ alloy. The matrix is C15, the second phase is b.c.c. solid solution.

Fig. 4. Compressive stress–strain curves of an $Hf_{14}V_{64}Nb_{22}$ alloy at various temperatures.

the theoretical X-ray powder diffraction pattern shown in Fig. 7(b).

4. Discussion

4.1. C15 structure

In order to understand the mechanical properties of C15 intermetallic compounds, it is crucial to understand the crystal structure. The C15 structure of composition AB_2 is cubic with eight formula units per cell, as shown in Fig. 8, and belongs to the space group $Fd3m(227)$. There are eight A atoms in positions (a):
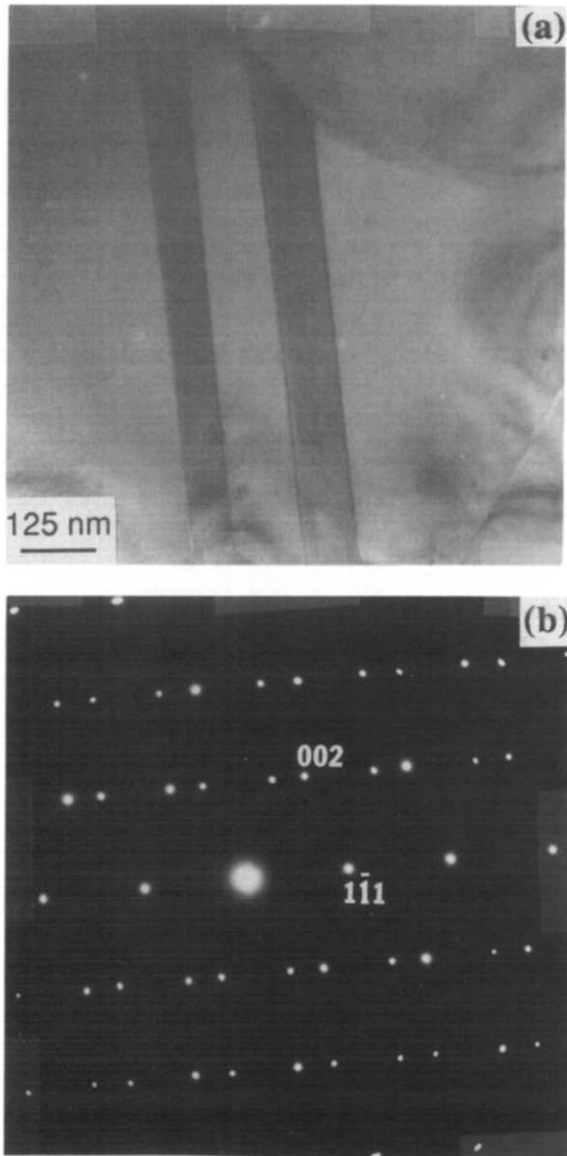
Fig. 5. (a) Microstructure of a plastically deformed C15 alloy. The zone axis is [110]; the twin interface is $(1\bar{1}1)$. (b) $[1\bar{1}0]$ diffraction pattern of $\{111\}\langle11\bar{2}\rangle$ twin in this alloy.

Fig. 6. Dislocations in the plastically deformed C15 alloy.

$(0\ 0\ 0,\ 0\ 1/2\ 1/2;\ \bigcirc)+0\ 0\ 0,\ 1/4\ 1/4\ 1/4$. There are 16 B atoms in positions (d): $(0\ 0\ 0,\ 0\ 1/2\ 1/2;\ \bigcirc)+$ 5/8 5/8 5/8, 5/8 7/8 7/8; $\bigcirc$. The structure can be regarded as being made up of two interpenetrating lattices of A and B atoms, as illustrated in Fig. 9, where the larger atom A is indicated by Greek letters and the smaller B atom occupies those indicated by Roman letters.

The main characteristic of the C15 structure, a type of topologically close-packed structure similar to geometrically close-packed metals, is the specific stacking sequence along the [111] direction. The C15 structure is constructed by an ...abcabc... stacking seqence
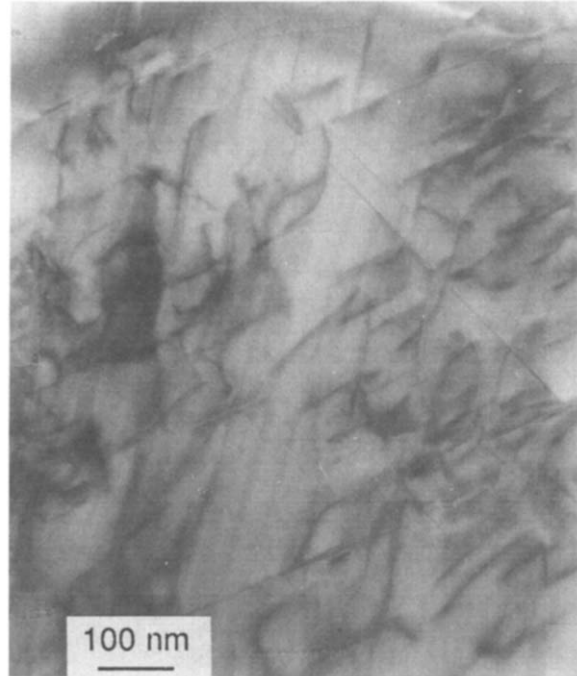
owing to the interpenetration of A and B lattices shown in Fig. 6, which is similar to the f.c.c. structure but different in the sense that each of these symbols represents a four-layer group. In detail, the stacking sequence of (111) planes in the C15 structure is given by:

$$...\alpha A a c\beta B \beta a \gamma C \gamma b...$$

Two different kinds of sandwiches occur in the stacking sequence, $\alpha A a(\beta B\beta$ and $\gamma C\gamma)$ and $ac\beta(\beta a\gamma$ and $\gamma b a)$, as demonstrated in Fig. 10. Note that each (111) layer contains only one kind of atom. Likewise the C14 structure is produced by an ...abab... stacking sequence and the C36 structure by an ...abacabac... sequence.

4.2. Synchroshear of selected layers: a new mechanism of C15 twinning

The synchroshear mechanism was proposed to explain basal slip and twinning of sapphire, a complex hexagonal structure. In order to shear, two adjacent layers undergo cooperative shears in different directions. The layers move synchronously, but the vectors over which the large and small atoms move are different. This mechanism was termed synchroshear by Kronberg [15, 16]. Based on TEM observations of stacking faults in Laves phases, Allen et al. [17] proposed that synchroshear occurs in the C15 structure, and is the mechanism for twinning which we propose here.
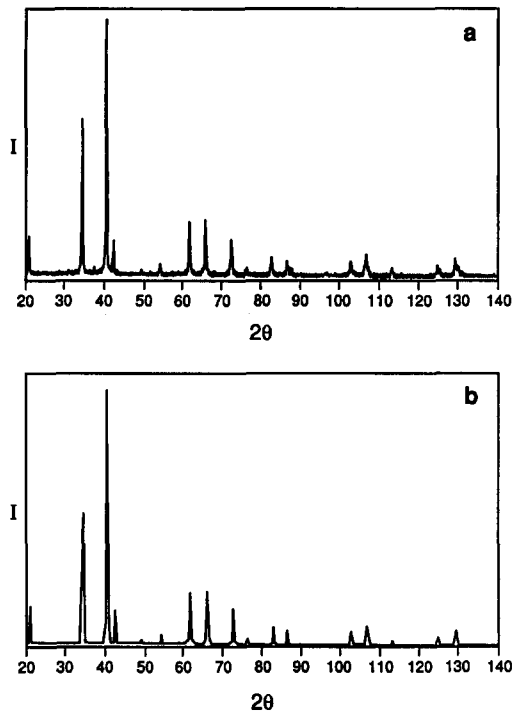
Fig. 7. (a) Experimental X-ray powder diffraction pattern of $Hf_{25}V_{60}Nb_{15}$; (b) theoretical X-ray powder diffraction pattern of $Hf_{25}V_{60}Nb_{15}$.

Fig. 9. The two interpenetrating lattices of A and B atoms. The plane of the layers is (111).

Fig. 8. The C15 crystal structure AB_2.

Fig. 10. The two types of sandwich in the C15 stacking sequence along [111]: the rigid $\alpha A\alpha$ type, and the more deformable $ac\beta$ type.

Considering an $\alpha A\alpha$ type sandwich shown in Fig. 10, if glide takes place, the original stacking sequence becomes

$$... \gamma C \gamma b a A \beta a \gamma C \gamma b a A a ...$$

or

$$... \gamma C \gamma b a A \gamma b a A a c \beta B \beta ...$$

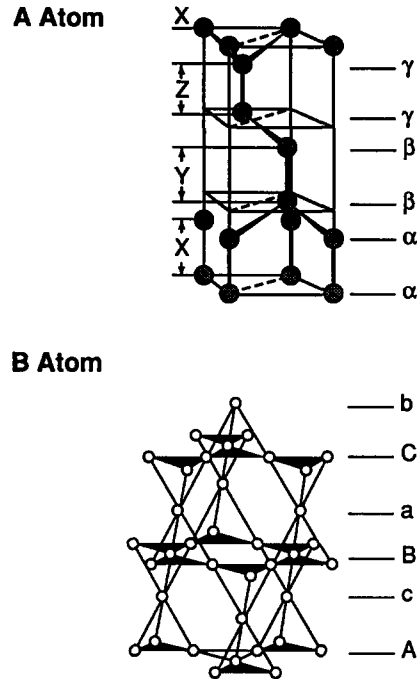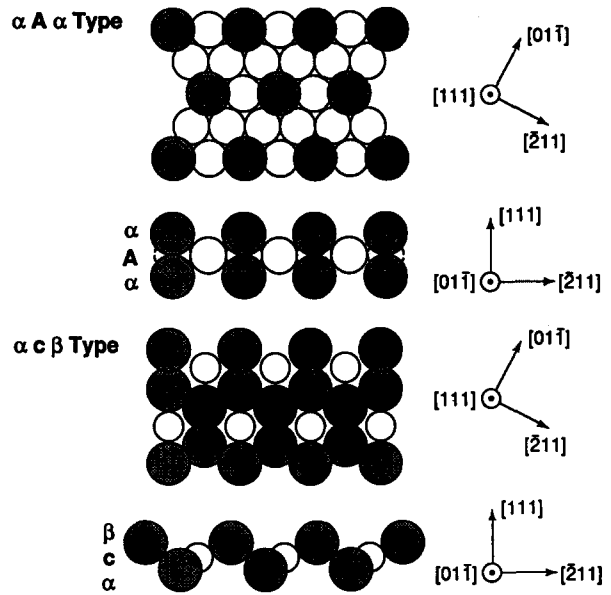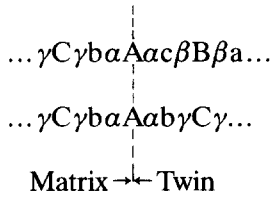The corresponding displacement vector is

$$R = 1/6[11\bar{2}] + 1/12[111]$$

or
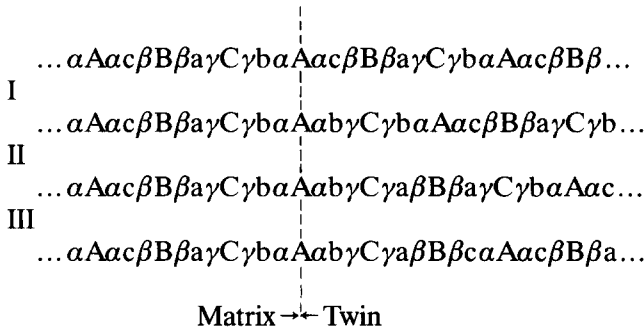
$$R = 1/6[\bar{2}11] + 1/12[111]$$

Note that the total displacement is a sum of shear along $\langle 112 \rangle$ in the plane of shear, and a displacement along [111] perpendicular to the plane of shear. Because of

the longer shear vector and the directional bonding along [111] between a-a atoms, this glide is very unlikely. Thus, an aAa type sandwich is a rigid group. However, the $ac\beta$ type sandwich is more deformable as long as synchroshear is operative within the sandwich. In this process, the smaller atoms shear by $1/6[\bar{2}11]$, the larger atoms move synchronously but with a shear displacement of $1/6[11\bar{2}]$, as shown in Fig. 11. The net result is that the upper block moves by $1/6[\bar{1}2\bar{1}]$ on the (111) plane relative to the lower block, thereby producing the following stacking sequence, which obviously produces a $\{111\}\langle11\bar{2}\rangle$ twin:

$$\ldots \gamma C\gamma ba\overset{|}{A}ac\beta B\beta a\ldots$$

$$\ldots \gamma C\gamma ba\overset{|}{A}ab\gamma C\gamma\ldots$$

$$\text{Matrix}\rightarrow\!\!\leftarrow\text{Twin}$$

A detailed examination of the three-dimensional lattice shows that consecutive synchroshears in the order I, II and III below do yield a $\{111\}\langle11\bar{2}\rangle$ twin in the C15 structure in the following way:

$$\ldots \alpha A ac\beta B\beta a\gamma C\gamma ba\overset{|}{A}ac\beta B\beta a\gamma C\gamma ba A ac\beta B\beta\ldots$$
I
$$\ldots \alpha A ac\beta B\beta a\gamma C\gamma ba\overset{|}{A}ab\gamma C\gamma ba A ac\beta B\beta a\gamma C\gamma b\ldots$$
II
$$\ldots \alpha A ac\beta B\beta a\gamma C\gamma ba\overset{|}{A}ab\gamma C\gamma a\beta B\beta a\gamma C\gamma ba A ac\ldots$$
III
$$\ldots \alpha A ac\beta B\beta a\gamma C\gamma ba\overset{|}{A}ab\gamma C\gamma a\beta B\beta ca A ac\beta B\beta a\ldots$$

$$\text{Matrix}\rightarrow\!\!\leftarrow\text{Twin}$$

The reason for increased twinning with Nb additions can be partially understood based on Fig. 7 and the fact that Nb substitutes both for Hf and V. There is a relatively high density of Hf atoms but a low density of V atoms in the $ac\beta$ type sandwiches (Fig. 10). Thus when Nb atoms substitute for Hf and V, free volume is produced in the $ac\beta$ type sandwiches since more Nb atoms are on Hf sites than on V sites in these layers (remember $R_{Hf} > R_{Nb} > R_V$ and since [V]/[Hf] > 2 more Nb atoms go to Hf sites than to V sites). Consequently, the additional free volume in the $ac\beta$ type sandwiches
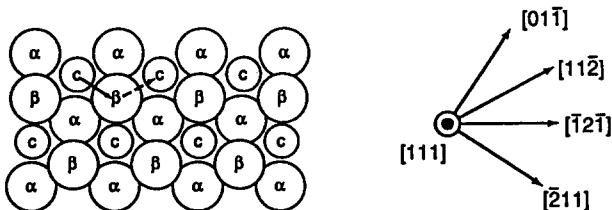
leads to easier synchroshear and, therefore, easier twinning.

A similar idea has been also suggested by Livingston and Hall [13]. We believe that the selected layer synchroshear mechanism proposed here is more physically plausible than the homogeneous shear–shuffle model for the twinning because it involves shorter shear vectors and no atomic shuffling.

Synchroshear could also be accomplished by the motion of synchro-Shockley partials and zonal dislocations [15, 16, 18, 19].

4.3. Discussion: mechanical twinning in f.c.c., LI_2, A4 and C15 structures

Generally speaking, the experimentally observed mechanical twinning mode in f.c.c. based structures, e.g. f.c.c., LI_2, A4 (diamond cubic) and C15, is $\{111\}\langle11\bar{2}\rangle$. Here we briefly compare the conventional twinning mechanism in the f.c.c. and LI_2 structures with the selected layer synchroshear mechanism in the diamond cubic and C15 structures. The possible kinematics of the formation of these twins are as follows.

F.c.c. During twinning, the atoms on each layer shear along the $[11\bar{2}]$ direction with a shear, $g = 0.707$, without atomic shuffles, as demonstrated in Fig. 12.

LI_2. Here, the atoms on each layer glide along the $[11\bar{2}]$ direction with a shear, $g = 1.414$, without atomic shuffling, as shown in Fig. 13. The same scheme can also be employed to explain the mechanical twinning in LI_0 and DO_{22} structures. A shear of 0.707 produces a pseudo-twin or requires shuffles involving interchanges between some A and B atoms.

A4. In the A4 (diamond cubic) structure the stacking sequence is $\ldots aa\beta\beta\gamma\gamma\ldots$ along the [111] direction, the same sequence as for the A atoms in an AB_2 C15 Laves phase. As in the analysis of C15 twinning, the aa type layers ($\beta\beta$ and $\gamma\gamma$) are considered to be rigid because of the long shear vector required and directional bonding. The $a\beta$ type layers ($\beta\gamma$ and γa),

Fig. 11. The synchroshear within the $ac\beta$ type sandwich.
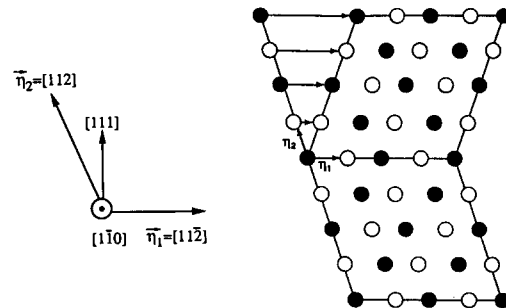

Fig. 12. The formation of a $\{111\}\langle11\bar{2}\rangle$ twin in the f.c.c. structure.
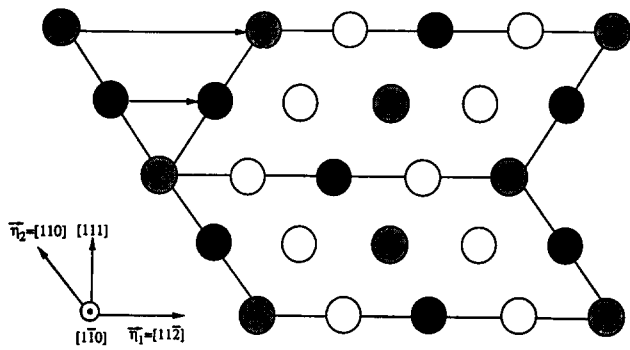
Fig. 13. The formation of a $\{111\}\langle11\bar{2}\rangle$ twin in the $L1_2$ structure A_3B. Black and white circles are A, the others are B.
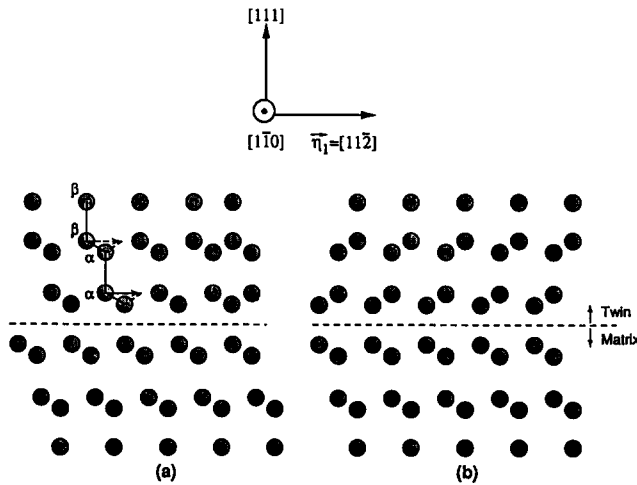

Fig. 14. The formation of a $\{111\}\langle11\bar{2}\rangle$ twin in the A4 structure: (a) twinning process, (b) twinned structure.
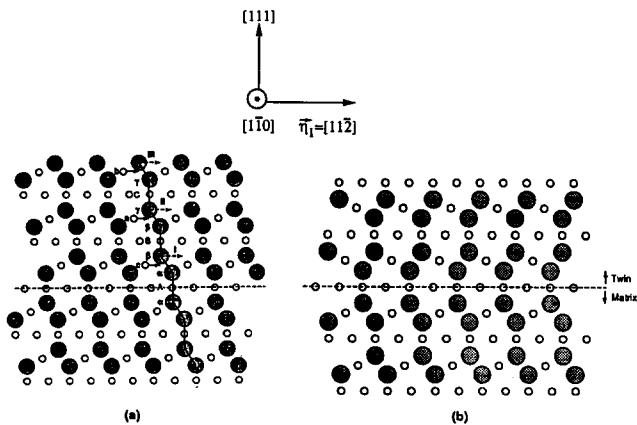

Fig. 15. The formation of a $\{111\}\langle11\bar{2}\rangle$ twin in the C15 structure: (a) twinning process, (b) twinned structure.

however, are more deformable via $1/6\langle11\bar{2}\rangle$ glide. In the formation of a twin, the $\alpha\alpha$ layers shear by $1/6[\bar{2}11]$, then the $\beta\beta$ layers move by $1/6[11\bar{2}]$, and as a net result the upper block moves along the $[\bar{1}2\bar{1}]$

direction on the (111) plane without atomic shuffling, thereby forming the $\{111\}\langle11\bar{2}\rangle$ twin in the cubic diamond structure, as shown in Fig. 14. The same scheme can also be used to describe pseudo-twinning of the B3 (cubic ZnS) structure.

C15. The physical process for the formation of a $\{111\}\langle11\bar{2}\rangle$ twin is demonstrated in Fig. 15 using the proposed mechanism of synchroshear of selected layers. Since the C14 and C36 structures are related to the C15 simply by variations in stacking sequence, the synchroshear mechanism applies to those structures, as well.

5. Conclusions

(1) Twinning is the major mode of plastic deformation at low temperatures in C15 Hf–V–Nb alloys based on HfV_2.

(2) The twinning occurs on $\{111\}$ planes by a shear in the $\langle112\rangle$ directions.

(3) This twinning mode can be accomplished, via the synchroshear mechanism, by shear on selected $\{111\}$ planes, *i.e.* the shear is inhomogeneous.

(4) This synchroshear involves only short displacements, $1/6\langle112\rangle$, and requires no atomic shuffles.

(5) The substitution of Nb into HfV_2 appears to facilitate twinning by increasing the free volume in the planes undergoing synchroshear.

(6) Such a mechanism is also applicable to the C14 and C36 structures, since they are produced by variations of the same stacking sequence as in C15.

(7) It is possible that twinning may occur by inhomogeneous shear in other compounds with complex atomic arrangements, rather than by combinations of long shears and/or shuffles.

Acknowledgments

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