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Atom positions in the R-phase unit cell in TiNi shape memory alloy

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A crystallographic analysis of the atom positions in the unit cell of the R-phase of the TiNi shape memory alloy has been performed. In addition to a homogeneous shape change the atoms are found to shuffle in the $[111]_{B2}$ and $\langle\text{-}211\rangle_{B2}$ directions during the B2 to R-phase transformation. The origin of these shuffles is found to be a complex interaction between $\langle 110\rangle\langle 1\text{-}10\rangle$ transverse acoustic and $\langle 111\rangle$ longitudinal acoustic soft phonon modes.

1. Introduction

It is known that the austenite (B2 structure with $a = 0.302$ nm) to R-phase transformation in the TiNi shape memory alloy is a first-order displacive transformation [1–5], and that a soft mode is involved in this transition [4, 6–13]. Before the R-phase appears, $\{111\}_{B2}$ diffuse planes are observed and an incommensurate phase forms by a second-order transformation. At this point 1/3(01-1) and 1/3(111) supperlattice reflections appear in X-ray and electron diffraction patterns, these superlattice reflections will be the 1/3 positions when the commensurate R-phase forms [2–6, 11, 14, 15].

Based on X-ray diffraction data taken on the incommensurate phase several attempts have been made to explain the structure of the incommensurate phase and the R-phase [4, 11–13]. However none of these proposals have generated a three-dimensional model that can be compared with the full range of experimental data. Although the R-phase and the incommensurate phase have quite similar diffraction patterns, they may have a different structure and a different symmetry. The structure of the commensurate R-phase should be simpler than that of the incommensurate phase. Therefore, a simple and direct approach to the problem is to start from the R-phase.

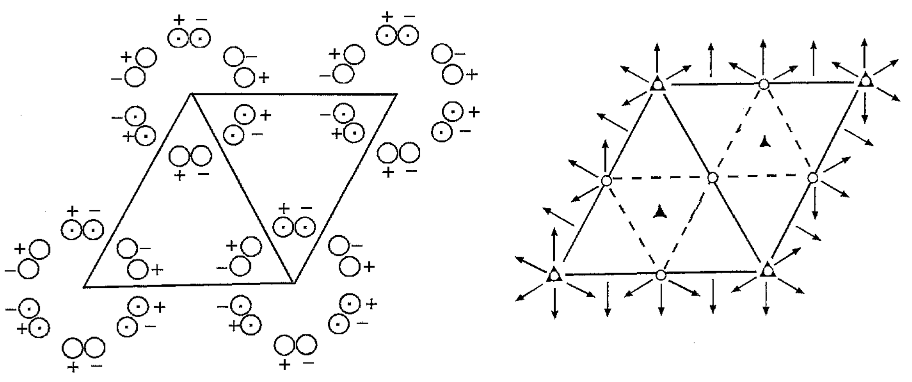
It is agreed that the rhombohedral R-phase [1–4, 14] has a hexagonal unit cell with $a = 0.738$ nm, $c = 0.532$ nm [5]. There are nine Ti atoms and nine Ni atoms in one unit cell of the R-phase. The orientation relationship between the R-phase and the B2 phase is $(0001)_R//(111)_{B2}$, $\langle 2\text{-}1\text{-}10\rangle_R//\langle\text{-}211\rangle_{B2}$ [5]. The reciprocal lattice of a single R-phase has been studied and the shuffle during the transition is proposed to be along $\langle 112\rangle_{B2}$ directions on $\{111\}_{B2}$ planes [16, 17]. However these shuffles cannot generate the 1/3(111) diffraction spots [18]. A convergent beam electron diffraction (CBED) study shows that the R-phase has a space group of *P*-3*lm* [5]. While the results of a comparison between kinematically calculated intensities and observed electron diffraction patterns show that the crystal structure of the R-phase belongs to the space group *P*3 [19]. It is well accepted that there is an antiphase-like boundary in a single R-phase variant and that the micro domain size of the R-phase is about 30–150 nm [2, 3, 20, 21]. However the electron diffraction pattern obtained in an electron microscope definitely comes from an area larger than 500 nm. As a result, the *P*3 space group suggested from analysing electron diffraction patterns is an average of many R-phase micro domains, and this symmetry may be lower than the symmetry of one R-phase domain. On the other hand, the CBED technique is a good one for the study of micro structure since it can give the space group from a small sample area on the order of several nm. One potential error in this study is that the beam might have been focused on the antiphase-like boundaries of the R-phase so that the symmetry obtained might be lowered. According to group theory [22], the ordering (or the displacive) transformation is usually accompanied by a decrease in symmetry in such a way that the point group of the ordered structure is a subgroup of the point group of the disordered structure. Whilst the *P*-3*lm* space group is the maximal subgroup of *Pm*-3*m* space group (that for B2 matrix) containing a three fold axis. Therefore, a *P*-3*lm* space group is believed to be the space group of a single R-phase domain.

Based on all these experimental data a crystallographic analysis of the problem will be attempted with the objective of finding the atom positions in the R-phase unit cell.

2. Method description

From a crystallographic viewpoint, the symmetry or the space group of a structure is defined by all the atoms and their positions in the structure. Atoms in a structure can only locate at certain positions defined by the space group. The permitted positions for

$P\bar{3}lm$ No. 162 $P\bar{3}l2/m$ $\bar{3}m$ Trigonal
D^1_{3d}



Origin at centre ($\bar{3}lm$)

Number of positions Wyckoff notation and point symmetry			Co-ordinates of equivalent positions					Conditions limiting possible reflections
12	l	1	$x,y,z;$ $\bar{x},\bar{y},\bar{z};$ $y,x,z;$ $\bar{y},\bar{x},\bar{z};$	$\bar{y},x-y,z;$ $\bar{y},y-x,\bar{z};$ $\bar{x},y-x,z;$ $x,x-y,\bar{z};$	$y-x,\bar{x},z;$ $x-y,x,\bar{z};$ $x-y,\bar{y},z;$ $y-x,y,\bar{z};$			General: No conditions
6	k	m	$x,0,z$:	$0,x,z;$	$\bar{x},\bar{x},z;$ $\bar{x},0,\bar{z};$	$0,\bar{x},\bar{z};$	$x,x,\bar{z};$	Special No conditions
6	j	2	$x,\bar{x},\frac{1}{2};$ $\bar{x},x,\frac{1}{2}$	$x,2x,\frac{1}{2};$ $\bar{x},2\bar{x},\frac{1}{2};$	$2\bar{x},\bar{x},\frac{1}{2}$ $2x,x,\frac{1}{2}$			
6	i	2	$x,\bar{x},0;$ $\bar{x},x,0$	$x,2x,0;$ $\bar{x},2\bar{x},0;$	$2\bar{x},\bar{x},0$ $2x,x,0$			
4	h	3	$\frac{1}{3},\frac{2}{3},z;$	$\frac{1}{3},\frac{2}{3},z;$	$\frac{2}{3},\frac{1}{3},z;$ $\frac{2}{3},\frac{1}{3},z.$			
3	g	$2/m$	$\frac{1}{2},0,\frac{1}{2};$	$0,\frac{1}{2},\frac{1}{2};$	$\frac{1}{2},\frac{1}{2},\frac{1}{2};$			
3	f	$2/m$	$\frac{1}{2},0,0;$	$0,\frac{1}{2},0;$	$\frac{1}{2},\frac{1}{2},0.$			
2	e	$3m$	$0,0,z;$	$0,0,\bar{z}$				
2	d	32	$\frac{1}{3},\frac{2}{3},\frac{1}{2};$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$				
2	c	32	$\frac{1}{3},\frac{2}{3},0;$	$\frac{2}{3},\frac{1}{4},0.$				
1	b	$\bar{3}m$	$0,0,\frac{1}{2},$					
1	a	$\bar{3}m$	$0,0,0.$					

Figure 1

a structure with a P-$3lm$ space group are shown in Fig. 1 [23]. Atoms in the R-phase unit cell should locate at some of these positions.

It is well known that there are two kinds of atom movements involved in a displacive transformation, (a) homogeneous shape change and (b) shuffle. Homogeneous shape change will change primary vectors (including direction and length) of the unit cell, but will not change the atom co-ordinates in the unit cell. So that the homogeneous shape change can be mathematically expressed by co-ordinate transformations. Whilst a shuffle is a relative movement between atoms and it will change atom co-ordinates. However during the displacive transformation, the atom arrangements will not change and usually the amount of shuffle is smaller than that of the homogeneous shape change. Therefore, the atom positions after a homogeneous shape change (called position M in this paper) are the approximate positions in the produced phase (called position R here). Remember that the position R must be included in positions allowed in the space group of the product phase (position S). Comparison between position M and position S will give position R, and the shuffle during the transformation can also be found.

3. Atom positions in the R-phase unit cell and the shuffle during the transformation

Based on the currently available data on the R-phase unit cell and the orientation relationship between B2 and R-phases [5], it can be found that:

$[100]_R \sim= [\text{-}211]_{B2}$
$[010]_R \sim= [1\text{-}21]_{B2}$
$[001]_R \sim= [111]_{B2}$

TABLE I Atom positions and shuffles

Ti atom positions and shuffles

No.	1	2	3	4	5	6	7	8	9
position in B2	000	$0\bar{1}1$	$\bar{1}01$	100	010	001	$\bar{1}00$	$0\bar{1}0$	$00\bar{1}$
position M	000	$\frac{1}{3}\frac{2}{3}0$	$\frac{2}{3}\frac{1}{3}0$	$\frac{\bar{1}}{3}0\frac{1}{3}$	$0\frac{\bar{1}}{3}\frac{1}{3}$	$\frac{1}{3}\frac{1}{3}\frac{1}{3}$	$\frac{1}{3}0\frac{\bar{1}}{3}$	$0\frac{1}{3}\frac{\bar{1}}{3}$	$\frac{\bar{1}}{3}\frac{\bar{1}}{3}\frac{\bar{1}}{3}$
position R	000	$\frac{1}{3}\frac{2}{3}0$	$\frac{2}{3}\frac{1}{3}0$	$X0Z$	$0XZ$	$\bar{X}\bar{X}Z$	$\bar{X}0\bar{Z}$	$0\bar{X}\bar{Z}$	$XX\bar{Z}$
shuffle	0	0	0	A0B	0AB	$\bar{\mathrm{A}}\bar{\mathrm{A}}$ B	$\bar{\mathrm{A}}0\bar{\mathrm{B}}$	$0\bar{\mathrm{A}}\bar{\mathrm{B}}$	$\mathrm{AA}\bar{\mathrm{B}}$

Ni atom positions and shuffles

No.	1	2	3	4	5	6	7	8	9
position in B2	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}\frac{\bar{1}}{2}\frac{3}{2}$	$\frac{\bar{1}}{2}\frac{1}{2}\frac{3}{2}$	$\frac{1}{2}\frac{\bar{1}}{2}\frac{\bar{1}}{2}$	$\frac{\bar{1}}{2}\frac{1}{2}\frac{\bar{1}}{2}$	$\frac{\bar{1}}{2}\frac{\bar{1}}{2}\frac{1}{2}$	$\frac{\bar{1}}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}\frac{\bar{1}}{2}\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{\bar{1}}{2}$
position M	$00\frac{1}{2}$	$\frac{1}{3}\frac{2}{3}\frac{1}{2}$	$\frac{2}{3}\frac{1}{3}\frac{1}{2}$	$\frac{\bar{1}}{3}0\frac{\bar{1}}{6}$	$0\frac{\bar{1}}{3}\frac{\bar{1}}{6}$	$\frac{1}{3}\frac{1}{3}\frac{\bar{1}}{6}$	$\frac{1}{3}0\frac{1}{6}$	$0\frac{1}{3}\frac{1}{6}$	$\frac{\bar{1}}{3}\frac{\bar{1}}{3}\frac{1}{6}$
position R	$00\frac{1}{2}$	$\frac{1}{3}\frac{2}{3}\frac{1}{2}$	$\frac{2}{3}\frac{1}{3}\frac{1}{2}$	$X'0Z'$	$0X'Z'$	$\bar{X}'\bar{X}'Z'$	$\bar{X}'0\bar{Z}'$	$0\bar{X}'\bar{Z}'$	$X'X'\bar{Z}'$
shuffle	0	0	0	C 0 D	0 C D	$\bar{\mathrm{C}}\ \bar{\mathrm{C}}$ D	$\bar{\mathrm{C}}$ 0 $\bar{\mathrm{D}}$	0 $\bar{\mathrm{C}}\bar{\mathrm{D}}$	C C $\bar{\mathrm{D}}$

TABLE II

Ti atom	shuffle
$[1, 0, 0]_{B2}$	$[A, 0, B]_R = A[-2, 1, 1]_{B2} + B[1, 1, 1]_{B2}$
$[0, 1, 0]_{B2}$	$[0, A, B]_R = A[1, -2, 1]_{B2} + B[1, 1, 1]_{B2}$
$[0, 0, 1]_{B2}$	$[-A, -A, B]_R = A[1, 1, -2]_{B2} + B[1, 1, 1]_{B2}$
$[-1, 0, 0]_{B2}$	$[-A, 0, -B]_R = -A[-2, 1, 1]_{B2} - B[1, 1, 1]_{B2}$
$[0, -1, 0]_{B2}$	$[0, -A, -B]_R = -A[1, -2, 1]_{B2} - B[1, 1, 1]_{B2}$
$[0, 0, -1]_{B2}$	$[A, A, -B]_R = -A[1, 1, -2]_{B2} - B[1, 1, 1]_{B2}$

Ni atom	shuffle
$[1/2, -1/2, -1/2]_{B2}$	$[C, 0, D]_R = C[-2, 1, 1]_{B2} + D[1, 1, 1]_{B2}$
$[-1/2, 1/2, -1/2]_{B2}$	$[0, C, D]_R = C[1, -2, 1]_{B2} + D[1, 1, 1]_{B2}$
$[-1/2, -1/2, 1/2]_{B2}$	$[-C, -C, D]_R = C[1, 1, -2]_{B2} + D[1, 1, 1]_{B2}$
$[-1/2, 1/2, 1/2]_{B2}$	$[-C, 0, -D]_R = -C[-2, 1, 1]_{B2} - D[1, 1, 1]_{B2}$
$[1/2, -1/2, 1/2]_{B2}$	$[0, -C, -D]_R = -C[1, -2, 1]_{B2} - D[1, 1, 1]_{B2}$
$[1/2, 1/2, -1/2]_{B2}$	$[C, C, -D]_R = -C[1, 1, -2]_{B2} - D[1, 1, 1]_{B2}$

where the R-phase co-ordinates are the three-digit indices.

The transformation matrices can also be calculated:

$$M = \begin{bmatrix} -1/3 & 0 & 1/3 \\ 0 & -1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \end{bmatrix} \quad m = \begin{bmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

Any vector or position co-ordinate can be translated between the B2 phase co-ordinate system and the R-phase co-ordinate system by using:

$$\begin{bmatrix} u' \\ v' \\ w' \end{bmatrix}_R = M \begin{bmatrix} u \\ v \\ w \end{bmatrix}_{B2} \quad \text{(I)} \qquad \begin{bmatrix} u \\ v \\ w \end{bmatrix}_{B2} = m \begin{bmatrix} u' \\ v' \\ w' \end{bmatrix}_R \quad \text{(II)}$$

If a Ti atom is chosen to be at the origin of the co-ordinate system, then the initial positions of atoms, which are later in the R-phase unit cell after the transformation, can be written for the B2 phase co-ordinate system as listed in the second line in Table I. By using Equation I, the atom positions after homogeneous shape change (position M) can be found out for the R-phase co-ordinate system (shown in the third line in Table 1). The real atom positions in the R-phase unit cell (position R) will be given by comparing the permitted co-ordinates in *P*-3*lm* (see Fig. 1) and position M. The results are shown below and also listed in Table I. The nine Ti atoms in the R-phase unit cell:

a	$-3m$	0, 0, 0
c	32	1/3, 2/3, 0; 2/3, 1/3, 0
k	*m*	$x, 0, z$; $0, x, z$; $-x, -x, z$; $-x, 0, -z$; $0, -x, -z$; $x, x, -z$

The nine Ni atoms in the R-phase unit cell:

b	$-3m$	0, 0, 1/2
d	32	1/3, 2/3, 1/2; 2/3, 1/3, 1/2
k	*m*	$x', 0, z'$; $0, x', z'$; $-x', -x', z'$; $-x', 0, -z'$; $0, -x', -z'$; $x', x', -z'$

here, x' and z' are used for the Ni atom since they do not have the same co-ordinate as Ti atoms.

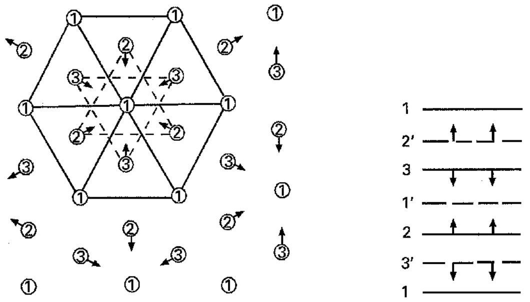


Figure 2 (a) Atomic shuffle viewed down the $[1\,1\,1]_{B2}$ direction. The atoms with the same number are in the same plane perpendicular to $[1\,1\,1]_{B2}$. (b) The stacking sequence of the planes parallel to $[1\,1\,1]_{B2}$ and atomic shuffle parallel to $[1\,1\,1]_{B2}$.

It is through a shuffle during the transformation that atoms move from position M to position R, thus the amount of shuffle could be found in the R-phase co-ordinate system as is shown in Table I, where $A = x + 1/3$, $B = z - 1/3$, $C = x' + 1/3$, and $D = z' + 1/6$. By using Equation II the shuffle can be expressed in items of the B2 co-ordinate system, (see Table II). Fig. 2a shows the atom positions and atomic shuffle projected on to the $(111)_{\rm B2}$ plane and Fig. 2b shows the stacking of the planes along $[111]_{\rm B2}$ and the atomic shuffle parallel to $[111]_{\rm B2}$. It can be seen clearly that shuffles in the $[111]_{\rm B2}$ direction change the plane period in $(111)_{\rm B2}$ and as a result the 1/3 $(111)_{\rm B2}$ diffraction spot appears. The $1/3(01\text{-}1)_{\rm B2}$ diffraction spot is introduced by shuffles inside $(111)_{\rm B2}$, which are in $\langle -211\rangle_{\rm B2}$ directions.

Since there is no reason to think that a different structure would be given if a Ni atom instead of a Ti atom is chosen to be at the origin of the co-ordinate system, then it must be true that $A = C$ and $B = D$. Also, to ensure that $1/3(111)_{\rm B2}$ and $1/3(01\text{-}1)_{\rm B2}$ exist, neither A (or C) nor B (or D) can be equal to zero.

4. Soft mode origin

It has been confirmed that $\langle 110\rangle\langle 1\text{-}10\rangle$ transverse acoustic phonon modes (TA2) as well as $\langle 111\rangle$ longitudinal acoustic phonon modes (LA) become soft before the R-phase transformation by neutron scattering [6, 7, 10], ultrasonic velocity and attenuation [9], and electron diffraction [8] investigations. The TA2 soft mode before the R-phase transformation is suggested to be expressed as:

$$\vec{q}_{\rm I}^{\,(1)} = \frac{1}{3}(1,\bar{1},0), \quad \vec{e}_1 \parallel [110],$$

$$\vec{q}_{\rm I}^{\,(2)} = \frac{1}{3}(0,1,\bar{1}), \quad \vec{e}_2 \parallel [011],$$

$$\vec{q}_{\rm I}^{\,(3)} = \frac{1}{3}(\bar{1},0,1), \quad \vec{e}_3 \parallel [101],$$

while the LA phonon modes are [11]:

$$\vec{q}_{II}^{\,(1)} = \frac{1}{3}(\bar{1},\bar{1},2), \quad \vec{e} \parallel [111],$$

$$\vec{q}_{II}^{\,(2)} = \frac{1}{3}(2,\bar{1},\bar{1}), \quad \vec{e} \parallel [111],$$

$$\vec{q}_{II}^{\,(3)} = \frac{1}{3}(\bar{1},2,\bar{1}), \quad \vec{e} \parallel [111].$$

The simple linear combination of the three $\vec{q}_{\rm I}$ will give *P*3*lm* or *P*-3 symmetry depending on the choice of the cosine function or sine function as the phase factor. Similarly, the simple linear combination of the three $\vec{q}_{\rm II}$ will give *P*3*ml* or *P*-3*ml* [11]. Neither of these four symmetries fits the observed R-phase symmetry. Since both TA2 and LA phonon modes become soft before the R-phase transformation then the structure of the R-phase should be constructed from both of these soft modes. We introduce the following combination of TA2 and LA soft modes to construct the displacement

TABLE III Atom shuffle

atom position (in B2)	soft mode results	crystallographic results
0, 0, 0	0	0
1, 1, 1	0	0
0, −1, 1	0	0
1, 0, −1	0	0
1, 0, 0	$-(3^{1/2}/4)\,a[-2,1,1] - (3.3^{1/2}/2)\,b[1,1,1]$	$A[-2,1,1] + B[1,1,1]$
0, 1, 0	$-(3^{1/2}/4)\,a[1,-2,1] - (3.3^{1/2}/2)\,b[1,1,1]$	$A[1,-2,1] + B[1,1,1]$
0, 0, 1	$-(3^{1/2}/4)\,a[1,1,-2] - (3.3^{1/2}/2)\,b[1,1,1]$	$A[1,1,-2] + B[1,1,1]$
−1, 0, 0	$(3^{1/2}/4)\,a[-2,1,1] + (3.3^{1/2}/2)\,b[1,1,1]$	$-A[-2,1,1] - B[1,1,1]$
0, −1, 0	$(3^{1/2}/4)\,a[1,-2,1] + (3.3^{1/2}/2)\,b[1,1,1]$	$-A[1,-2,1] - B[1,1,1]$
0, 0, −1	$(3^{1/2}/4)\,a[1,1,-2] + (3.3^{1/2}/2)\,b[1,1,1]$	$-A[1,1,-2] - B[1,1,1]$
1/2, 1/2, 1/2	0	0
1/2, −1/2, 3/2	0	0
−1/2, 1/2, 3/2	0	0
1/2, −1/2, −1/2	$-(3^{1/2}/4)\,a[-2,1,1] - (3.3^{1/2}/2)\,b[1,1,1]$	$A[-2,1,1] + B[1,1,1]$
−1/2, 1/2, −1/2	$-(3^{1/2}/4)\,a[1,-2,1] - (3.3^{1/2}/2)\,b[1,1,1]$	$A[1,-2,1] + B[1,1,1]$
−1/2, −1/2, 1/2	$-(3^{1/2}/4)\,a[1,1,-2] - (3.3^{1/2}/2)\,b[1,1,1]$	$A[1,1,-2] + B[1,1,1]$
−1/2, 1/2, 1/2	$(3^{1/2}/4)\,a[-2,1,1] + (3.3^{1/2}/2)\,b[1,1,1]$	$-A[-2,1,1] - B[1,1,1]$
1/2, −1/2, 1/2	$(3^{1/2}/4)\,a[1,-2,1] + (3.3^{1/2}/2)\,b[1,1,1]$	$-A[1,-2,1] - B[1,1,1]$
1/2, 1/2, −1/2	$(3^{1/2}/4)\,a[1,1,-2] + (3.3^{1/2}/2)\,b[1,1,1]$	$-A[1,1,-2] - B[1,1,1]$

of the *K*th atom:

$$\vec{U}_{\mathrm{K}} = a\left[\mathrm{SIN}\left(\frac{4\pi}{3}[111]\cdot\vec{r}_{\mathrm{K}}\right)\right]\sum_i \vec{e}_i\,\mathrm{COS}(\vec{q}_I^{(i)}\cdot\vec{r}_{\mathrm{K}})$$

$$+\,b\sum_i \vec{e}\,\mathrm{SIN}(\vec{q}_{II}^{(i)}\cdot\vec{r}_{\mathrm{K}})$$

where *a* and *b* are parameters not equal to zero. The second term is simply a linear combination of the ⟨111⟩ LA soft modes. The first term is a simple linear combination of the ⟨110⟩⟨1-10⟩TA but with its amplitude modified by the wave function of the [111] LA soft mode. Such defined atom displacements of the atoms in the R-phase unit cell are calculated and compared in Table III with the atom shuffles obtained earlier in this paper. We observe a very close agreement.

*P*3*lm* or *P*-3 have been suggested to be the symmetry of the incommensurate phase [11]. Interestingly, these two space groups are subgroups of the R-phase space group *P*-3*lm*. It is possible that the ⟨111⟩LA and ⟨110⟩⟨1-10⟩TA do not harmonize in the incommensurate phase so that the symmetry there is lowered and the lock in process is just a process in which these two kinds of soft mode become harmonized.

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References

1. H. C. LING and R. KAPLOW, *Metall. Trans.* **11A** (1980) 77.
2. C. M. HWANG, M. MEICHLE, M. B. SALMON and C. M. WAYMAN, *Phil. Mag. A* **47** (1983) 9.
3. *Idem., Ibid.* **47** (1983) 31.
4. M. B. SALMON, M. E. MEICHLE and C. M. WAYMAN, *Phys. Rev. B* **31** (1985) 7306.
5. E. GOO and R. SINCLAIR, *Acta Metall.* **33** (1985) 1717.
6. A. I. LOTKOV, *et al.*, Proceedings of the International Symposium on Shape Memory Alloys, Guilin, China (1986) 153.
7. M. MULLNER, H. TIETZE, G. ECKOLD and W. ASSMUS, Proceedings of the International Conference on Martensitic Transformations (Japan Institute of Metals, Sendai, 1986) 159.
8. D. Y. LI, X. F. WU and T. KO, *Phil. Mag. A* **63** (1991) 585.
9. LI MANOSA, D. PIOS-JARA, J. ORTIN, A. PLANES and X. BHIGAS, *J. Phys. Condens. Matter* **4** (1992) 7059.
10. R. KUENTZLER, *Solid State Communications* **82** (1992) 989.
11. S. M. SHAPIRO, Y. NODA, Y. FUJII and Y. YAMADA, *Phys. Rev. B* **30** (1984) 4314.
12. Y. YAMADA, Y. NODA and M. TAKIMOTO, *Solid State Communications* **55** (1985) 1003.
13. I. FOLKINS and M. B. WALKER, *Phys. Rev. B* **40** (1989) 1.
14. D. P. DAUTOVICH and G. R. PURDY, *Canadian Metallurgical Quarterly* **4** (1965) 129.
15. F. E. WANG, W. J. BUEHLER and S. J. PICKART, *J. Appl. Phys.* **36** (1965) 3232.
16. S. K. WU and C. M. WAYMAN, *Acta Metall.* **37** (1989) 2805.
17. *Idem, Scripta Metall.* **27** (1992) 245.
18. W. BUHRER, M. ZOLLIKER and R. GOTTHARDT, *Ibid* **26** (1992) 1149.
19. T. HARA, T. OHBA, S. NENNO and K. OTSUKA, in Proceedings of the 3rd IUMRS International Conference on Advanced Materials (1993) HP(B)-7.
20. E. GOO and R. SINCLAIR, *Scripta Metall* **19** (1985) 1257.
21. Q. CHEN, X. F. WU and C. J. HUMPHREYS, *Acta Metall. Sinica* (*English Letters*) **9(3)** (1996) 157.
22. G. VAN TENDELOO and S. AMLIMCKX, *Acta Cryst.* **A30** (1974) 431.
23. International Tables for X-ray Crystallography, Vol. 1, (Birmingham Kynoch Press, 1952).

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