Transactions of the Materials Research Society of Japan 28 [3] 759-762 (2003)

FORMATION OF A PITSCH-RELATED B.C.C. CRYSTAL AT AN INTERSECTION OF <112>{111} SHEARS IN A F.C.C. CRYSTAL

T. Inamura, K. Takashima* and Y. Higo*

Graduate student, Precision and Intelligence Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta-cho, Midori-ku, Yokohama, 226-8503, Japan

Fax: +81-45-924-5631, e-mail: tinamura@ames.pi.titech.ac.jp

*Precision and Intelligence Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta-cho, Midori-ku, Yokohama, 226-8503, Japan

Resultant orientation relationship (OR) between parent f.c.c. crystal and produced b.c.c. crystal in the lattice deformation model of Bogers and Burgers was examined numerically. Vector analysis has been carried out and found that the OR of the product b.c.c. lattice formed at <112>{111}f shears is not the Kurdjumov-Sachs (KS) OR, but the Pitsch OR. On the other hand, ORs of α'-martensites (b.c.c.) formed at intersections of <112>{111}f shear-bands have been investigated by transmission electron microscopy (TEM) in an austenitic stainless steel (f.c.c., 5% compressed at 77 K) and found that ORs of α'-martensites formed at intersections of <112>{111}f shear-bands were almost close to Pitsch OR even when the size of the product is a few nm. Lattice deformation (f.c.c.-b.c.c.) toward the formation of the Pitsch related b.c.c. lattice is discussed.

Keywords: Lattice deformation, orientation relationship, martensitic transformation

1. INTRODUCTION

Bain proposed a plausible lattice deformation model for f.c.c.-b.c.t. (or b.c.c.) transformations [1]. This lattice deformation has been well known as 'Bain deformation' and has been regarded as the essential mechanism of α'-martensitic transformation (f.c.c.→ b.c.t. or b.c.c.) in ferrous alloys [2].

In the actual α'-martensitic transformation in ferrous alloys, orientation relationships (ORs) between α'-martensite (b.c.c., b.c.t) and austenite (f.c.c.) become Kurdjumov-Sachs (K-S) OR, Nishiyama-Wassermann (N-W) OR or Greninger-Troiano (G-T) OR in common [3-7]. In these three major ORs, there exists one set of $\{110\}_b$ plane and $\{111\}_f$ plane which are parallel or almost parallel (~1°) each other. Here, subscripts f and b denote parent austenite lattice and martensite lattice, respectively. However, pure Bain deformation gives no such $\{110\}_b$ and $\{111\}_f$ planes. Kurdjumov and Sachs [3] proposed a lattice deformation model to account for the formation of K-S oriented b.c.c. crystal, using 1/12 $\langle 112\rangle\{111\}_f$ shear-displacements and small shear-displacements on $\{242\}_f$ plane, based on the Bain correspondence. Nishiyama [4-5] also has proposed a lattice deformation model to explain formation of N-W oriented b.c.c. crystal by 1/12$\langle 112\rangle\{111\}_f$ shears and small dilatation along $\langle 110\rangle_f$.

On the contrary, Bogers and Burgers attempted to simulate the Bain deformation by combinations of common slip systems in f.c.c. crystal. They found that the Bain deformation can be approximately simulated by successive operation of particular $\langle 112\rangle\{111\}_f$ shear-displacements in a f.c.c. crystal which was formed by 'hard-spheres' [8-9]. However, as suggested by Olson and Cohen, common parallel closest packed plane does not appear in the Bogers-Burgers model [10]. This means that the product of the lattice deformation of Bogers-Burgers holds neither K-S OR nor N-W OR. However, the OR of the product crystal in the model of Bogers and Burgers has not been examined in detail. In this study, the OR of b.c.c. crystal formed by the original Bogers-Burgers model has been examined numerically and transmission electron microscopy (TEM) observations of α'-martensite formed at intersections of $\langle 112\rangle\{111\}_f$ shear-bands have been carried out to examine the validity of the model.

2. ANALYSIS OF BOGERS-BURGERS MODEL

2.1 Transformational strain

The orientation relationship between parent f.c.c. crystal and the produced b.c.c. crystal in the model of Bogers and Burgers was firstly examined. According to Bogers and Burgers [8-9], one of a pair of $\langle 112\rangle\{111\}_f$ shear-displacements to complete f.c.c. →b.c.c. transformation is αB (for 1st shear) and δC (for 2nd shear) in Thompson's notation. The second shear is, strictly to say, slightly away from δC because the first shear on α-plane inclines and distorts δ-plane. Figure 1(a) shows Thompson's tetrahedron with indication of the two shears used in the analysis. Arrows indicate the shift of material outside the tetrahedron, relative to inside of that. It is known that $\langle 112\rangle\{111\}_f$ shear in f.c.c. lattice is unidirectional.

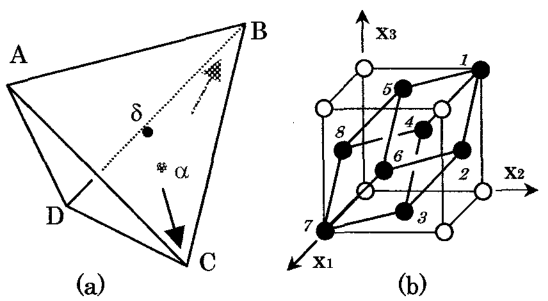

Figure 1: Indication of (a) the shear displacements and (b) f.c.c. coordinate system

The shear directions of 'Greek-Roman' type are the possible directions. Unit cell of f.c.c. in Fig. 1(b) has a lattice parameter of unity. Each atom (each filled circle) is numbered by italic number. The position vector of atom *i* is termed $\mathbf{r}_i$, hereafter.

The displacement vectors for the two shears were calculated referred to the coordinate system described in Fig. 1(b) as follows, with the assumption that atoms are 'hard-spheres' of $\sqrt{2}/4$ in radius.

$$\mathbf{u}_{\mathrm{I}} = \left[\frac{1}{18}(5-2\sqrt{10}) \quad \frac{1}{18}(2\sqrt{10}-5) \quad \frac{1}{9}(4-\sqrt{10})\right]_{\mathrm{f}}$$

$$\mathbf{u}_{\mathrm{II}} = \left[0.0644553 \quad 0.0810419 \quad -0.102211\right]_{\mathrm{f}} \qquad (1)$$

Here, $\mathbf{u}_{\mathrm{I}}$ and $\mathbf{u}_{\mathrm{II}}$ are the relative displacements between successive $\{111\}_f$ planes on which the 1st and the 2nd shears were operated, respectively. Displacement vector of $\mathbf{u}_{\mathrm{I}}$ (αB shear) was firstly added to $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$ and $\mathbf{r}_4$, and then displacement of $\mathbf{u}_{\mathrm{II}}$ (~δC shear) was added to $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_5$ and $\mathbf{r}_6$. Transformational matrix **S** was formed as follows, using $\mathbf{a}_1 = \mathbf{r}_6 - \mathbf{r}_4$, $\mathbf{a}_2 = \mathbf{r}_2 - \mathbf{r}_8$ and $\mathbf{a}_3 = \mathbf{r}_5 - \mathbf{r}_3$ after the operation of the two shear displacements.

$$\mathbf{S} = \left(\mathbf{a}_1 \ \mathbf{a}_2 \ \mathbf{a}_3\right)$$

$$= \begin{pmatrix} 1.13804 & -0.00913111 & 0.138042 \\ 0.00745552 & 1.154630 & 0.00745552 \\ -0.195292 & -0.00913111 & 0.804708 \end{pmatrix}$$

$$= \begin{pmatrix} 0.985573 & -0.00790777 & 0.169066 \\ 0.00645667 & 0.999937 & 0.00913111 \\ -0.169128 & -0.00790777 & 0.985562 \end{pmatrix} \cdot \begin{pmatrix} 1.15470 & & \\ & 1.15470 & \\ & & 0.816497 \end{pmatrix} \qquad (2)$$

Lattice parameter ratio (a_f/a_b) of the parent f.c.c. lattice and the produced b.c.c. lattice is found to be 1/0.816497 = 1.22474. a_f/a_b of α'-martensite (b.c.c.) in ferrous alloys are about 1.25 and is larger than that calculated in the Bogers-Burgers model. This is due to that the atoms in the model of Bogers and Burgers are treated as simple hard spheres. Uniform contraction of the produced b.c.c. crystal is required to simulate the principal strain of actual f.c.c.-b.c.c. transformation in ferrous alloys.

2.2 Orientation relationship

Angles between some low indexed directions (and plane normals) were calculated using eq.(2) and summarized as;

$[\bar{1}01]_f$	//	$[\bar{1}\bar{1}1]_b$	
$[010]_f$	0.64°	$[\bar{1}10]_b$	
$(101)_f$	0.64°	$(112)_b$	
$(1\bar{1}1)_f$	5.91°	$(101)_b$	(the 1st shear plane)
$(111)_f$	4.62°	$(011)_b$	(the 2nd shear plane)

Here, following Bain correspondence (from f.c.c. to b.c.c.) matrices were used.

Direscions(column vector) Plane normals (row vector)

$$\mathbf{C}_d = \begin{pmatrix} 1\,\bar{1}\,0 \\ 1\,1\,0 \\ 0\,0\,1 \end{pmatrix} \quad (3) \qquad \mathbf{C}_p = \frac{1}{2}\begin{pmatrix} 1\,1\,0 \\ \bar{1}\,1\,0 \\ 0\,0\,2 \end{pmatrix} \quad (4)$$

There is no common parallel closest packed plane in the calculated OR as Olson and Cohen pointed out [10]. Therefore, the obtained OR is neither K-S nor N-W OR. One can realize that obtained OR is close to Pitsch OR [11] (inverse N-W, $[010]_f // [\bar{1}10]_b$, $[\bar{1}01]_f // [\bar{1}\bar{1}1]_b$) and that the Bogers-Burgers model transforms a f.c.c. lattice into an almost Pitsch related b.c.c. lattice in case that two $<112>\{111\}_f$ shears were operated. Pitsch and K-S are related by ±5.3° rotations around the common parallel close packed direction [12]. Deviation from the exact Pitsch OR is rotation of 0.64° around $[\bar{1}01]_f$ // $[\bar{1}\bar{1}1]_b$ (intersecting line of the two shear displacements) in the above OR.

The effect of reversing the order of the shears on OR has been examined. The sense of small deviation from the exact Pitsch OR (0.64° rotation around $[\bar{1}01]_f$ // $[\bar{1}\bar{1}1]_b$) becomes opposite signed one by reversing the order of the two shears. It was confirmed that the same Pitsch variant is essentially produced independent of the order of the shears, once the shear systems to be operated are given.

3. PITSCH-RELATED α'-MARTENSITE IN AN AUSTENITIC STAINLESS STEEL

3.1 α'-Martensite in austenitic stainless steels

It has been well known that ε-martensites were formed during deformation or cooling, in austenitic stainless steels [13-17]. ε-Martensite has h.c.p. structure, and is generated by the propagation of Shockley partials on every two layer of $\{111\}_f$ plane. Intersections of $<112>\{111\}_f$ shear-bands (including ε-martensite) are known to produce nucleation sites for α'-martensite[14, 16-17]. α'-Martensite in austenitic stainless steels holds K-S OR with respect to the parent austenite in general [13-14]. However, some researchers reported that α'-martensites formed at intersections of $<112>\{111\}_f$ shears held N-W OR [17]. On the other hand, according to the calculation presented above, Pitsch OR is expected to be a reasonable OR at intersections of $<112>\{111\}_f$ shear-displacements.

In this section, orientation relationships of α'-martensite, including very early stage of the transformation, formed at intersections of <112>{111}$_f$ shear bands have been re-examined using TEM.

3.2 Experimental procedures

The material used was a commercially available 304-type austenitic stainless steel. The material was annealed at 1473K for 100 min and quenched into water. Grain size was about 200μm or less. Specimen of 7x3.5x3.5mm was cut from the material and compressive loading of 5% was applied in a liquid nitrogen bath, using 1.35kg hand-hammer. The specimens were immediately taken out from the liquid nitrogen bath after the compressive loading and warmed in laboratory air. Thin foil specimens for TEM observation were prepared using twin-jet polishing technique. Polishing was continued until perforation, but buckling of the foils were not confirmed in the observed areas. TEM observation was carried out using Philips CM200 operated at 200kV.

It is convenient to set the electron beam direction parallel to the common closest packed direction to distinguish K-S and Pitsch OR. Figure 2 depicts indexed diffraction pattern of austenite (f.c.c.) and α'-martensite (b.c.c.) taken from the common parallel closest packed direction of K-S OR. Angle between reflections of $0\bar{2}0_f$ and $1\bar{1}0_b$ is termed θ, hereafter. θ is 5.3° for exact K-S OR, and 0° for exact Pitsch OR.

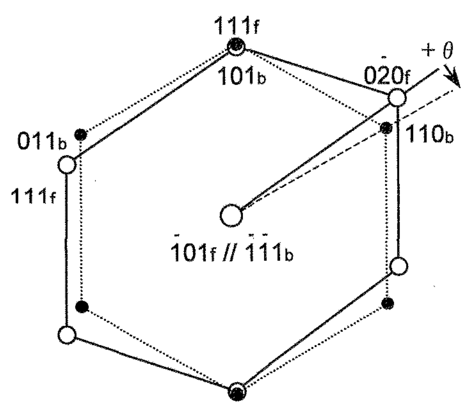

Figure 2: Schematic illustration of SAD

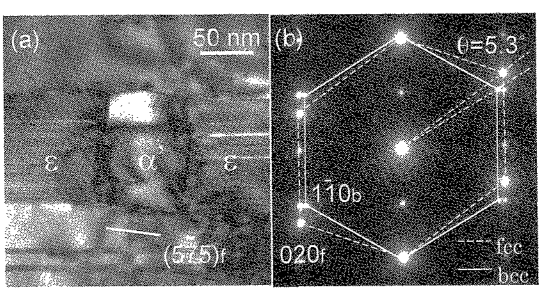

Figure 3: TEM images of α'-martensite formed in banded ε-martensites of single habit plane (a) Bright field image and (b)Corresponding SAD

Forty α'-martensites were observed in the same austenite grain and θ was measured on selected area diffraction pattern (SAD) in each α'-martensite.

3.3 Results of TEM observation

Figure 3(a) shows TEM bright field image of α'-martensite formed in banded ε-martensites of single habit plane of $(1\bar{1}1)_f$, taken with zone axis of $[\bar{1}01]_f$ // $[\bar{1}\bar{1}1]_b$, and Fig. 3(b) shows corresponding SAD. θ is 5.3° for this α'-martensite. This α'-martensite held almost exact K-S OR. Shape of this α'-martensite was rod-shaped along the electron beam direction, and habit plane was found to be $(5\bar{7}5)_f$ by a single trace analysis. More than 90% of the α'-martensites observed in banded ε-martensites on $(1\bar{1}1)_f$ held K-S OR within 0.5°, judging from the value of θ. This result well agrees with that obtained by other researchers [13].

On the other hand, α'-martensites formed at intersections of ε-martensites or <112>{111}$_f$ shear-bands exhibited different crystallographic features. Figure 4(a) shows an intersection of ε-martensite on $(1\bar{1}1)_f$ plane and shear-band on $(111)_f$ plane. Electron beam direction was parallel to $[\bar{1}01]_f$ // $[\bar{1}\bar{1}1]_b$. Needle-shaped α'-martensite of $[\bar{1}01]_f$-needle axis was formed at the intersection. Figure 4(b) and 4(c) show lattice image of the α'-martensite and a diffractogram taken from 4(b), respectively. Cross sectional diameter of this α'-martensite was about 15 nm. It was found that θ is 0° for this α'-martensite by analyzing the diffractogram and SAD of this area. This indicates that the α'-martensite in Fig. 4(b) held Pitsch OR with respect to the surrounding austenite. Major habit plane was found to be $(4\bar{1}4)_f$, and was different from that of K-S related α'-martensites. As far as judging from Fig. 4(b), matching of layer of atoms were not good across the habit plane and highly distorted.

More than 20 α'-martensites at intersections of <112>{111}$_f$ shears were examined in detail in this austenite grain. Habit plane was found to be $(4\bar{1}4)_f$ ~$(101)_f$. It was further found that θ of α'-martensite formed at intersections of <112>{111}$_f$ shears ranged from 0° to 5°, but more than half had θ of less than 2°. According to that α'-martensites formed in banded ε-martensites did not exhibit such deviation from K-S OR in the same austenite grain, appearance of Pitsch OR at intersections of <112>{111}$_f$ shears is considered to be originated by neither chance nor thin-foil effects. The α'-martensite in Fig. 4 is the smallest one which was observed at an intersection of <112>{111}$_f$ shears in this austenite grain. It should be noted that α'-martensites formed at intersections of <112>{111}$_f$ shears hold Pitsch OR even in this early stage of the transformation, and habit plane is highly distorted.

4. Discussion

Venables [14] suggested that fine needle shaped α'-martensite formed at intersections of ε-martensite grows into plate-shaped α'-martensite of K-S OR with {252}$_f$-type habit plane, in an austenitic stainless steel. However, it has been demonstrated that α'-martensite formed at intersections of <112>{111}$_f$ shear tends to hold Pitsch OR. It is apparent that lattice deformation

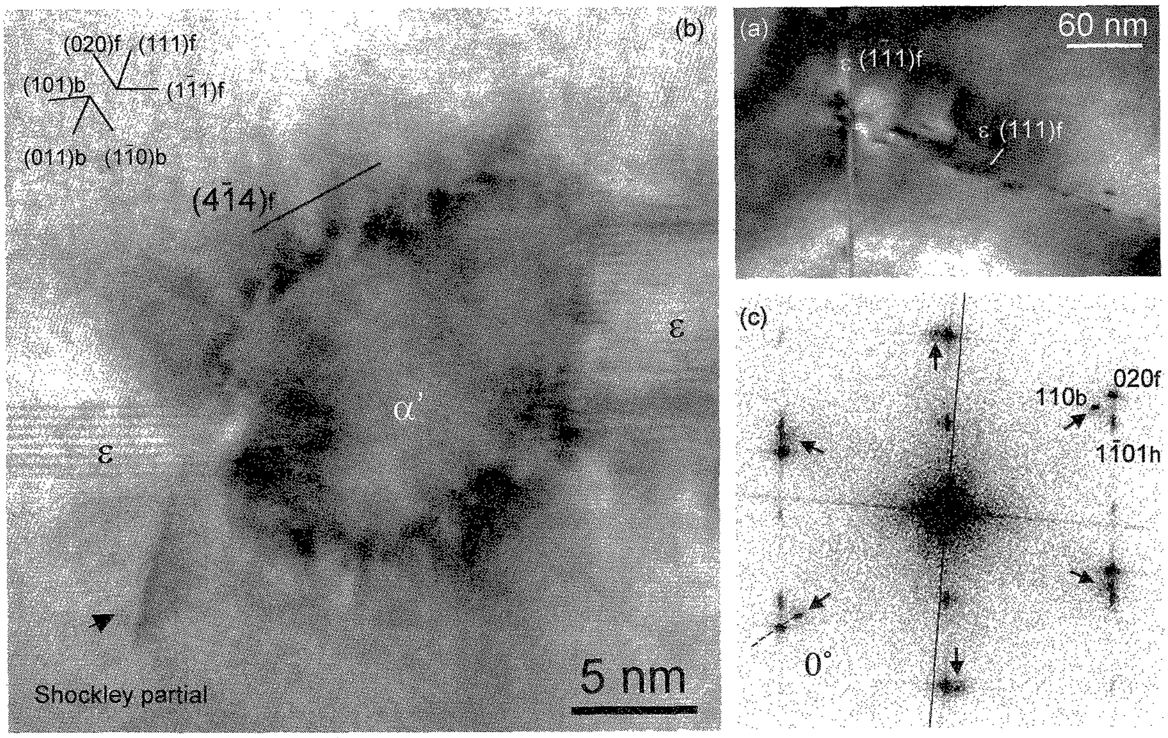

Figure 4: α'-martensite formed at intersection of <112>{111} f shears (a)Bright field image, (b)Lattice image and (c) Diffractogram taken from (b). Orientation relationship between α'-martensite and surrounding austenite is Pitsch OR and major habit plane was (4$\bar{1}$4)f.

models of Kurdjumov and Sachs [3], Nishiyama [4-5] and Venables [14] cannot simply explain the formation of Pitsch-related α'-martensite at intersection of <112>{111}f shears, because these models were developed to explain K-S or N-W OR. Pitsch [12] has proposed a lattice deformation model to account for the formation of Pitsch OR. However, intersecting shear displacements of <112>{111}f are not used in Pitsch's model. The model of Bogers and Burgers is suggested to be one of the most plausible mechanism to explain the formation of Pitsch-related α'-martensite at intersections of <112>{111} f shears.

5. CONCLUSIONS

The model of Bogers and Burgers transforms f.c.c. crystal into b.c.c. crystal with almost Pitsch OR as follows, in case that the transformation is expressed by a combination of two <112>{111}f shears.

$[\bar{1}01]_f$	//	$[\bar{1}\bar{1}1]_b$	
$[010]_f$	0.64°	$[\bar{1}10]_b$	
$(101)_f$	0.64°	$(112)_b$	
$(1\bar{1}1)_f$	5.91°	$(101)_b$	(the 1st shear plane)
$(111)_f$	4.62°	$(011)_b$	(the 2nd shear plane)

Deformation induced α'-martensite formed at intersections of <112>{111}f shears tends to hold Pitsch OR in 304-type austenitic stainless steel. The Bogers-Burgers mechanism is considered to be one of the most plausible model to account for the formation of Pitsch-related α'-martensite at intersections of <112>{111}f shears.

REFERENCES

[1] E. C. Bain, *Trans. AIME*, **70**, 25 (1924).
[2] Z. Nishiyama, "Martensitic Transformation", Academic Press, New York (1978).
[3] G. Kurdjumov and G. Sachs, *Zeits. Phys.*, **64**, 325 (1930).
[4] Z. Nishiyama, *Sci. Rep. Tohoku Univ.*, **23**, 637 (1934).
[5] Z. Nishiyama, *Sci. Rep. Tohoku Univ.*, **25**, 79 (1936).
[6] G. Wassermann, *K-W-I Eisenf.*, **17**, 149 (1935).
[7]A. B. Greninger and A. R. Troiano, *Trans. AIME*, **145**, 289 (1941).
[8] A. J. Bogers and W. G. Burgers, *Acta metall.*, **12**, 255 (1964).
[9] W. G. Burgers, *Acta metall.*, **13**, 568 (1965).
[10] G. B. Olson and M. Cohen, *Metall. Trans. A*, **7A**, 1905 (1976).
[11] W. Pitsch, *J. Inst. Metals*, **87**, 444 (1959).
[12] U. Dahmen, *Acta metall.*, **30**, 63 (1982).
[13] J. Dash and H. M. Otte, *Acta metall.*, **11**, 1169 (1963).
[14] J. A. Venables, *Phil. Mag.*, **7**, 35 (1962).
[15] T. Suzuki, H. Kojima, K. Suzuki, T. Hashimoto and M. Ichihara, *Acta metall.*, **25**, 1151 (1977).
[16] K. P. Staudhammer, L. E. Murr and S. S. Hecker, *Acta metall.*, **31**, 267 (1983).
[17] P. L. Mangonon, JR and G. Thomas, *Metall. Trans.*, **1**, 1577 (1970).

(Received Febuary 20, 2003; Accepted March 19, 2003)