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Double shear mechanism and orientation relationships in austenite/ferrite steels

Patricia Donnadiou ⁽¹⁾ and Michel Duneau ⁽²⁾

⁽¹⁾ Laboratoire d'Etude des microstructures (*), BP 72, 92322 Châtillon Cedex, France

⁽²⁾ Centre de Physique Théorique (**), Ecole Polytechnique, 91128 Palaiseau Cedex, France

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Abstract. — We propose a new approach of structural transformation between lattices by means of simple bounded transformations composed of two « fractional shears ». The strength point of this double shear mechanism in lattice transformations is to specify particular orientation relationships. Though the basis of the model concerns the general 3D diffusionless transformation, the case of 2D lattices is presented in detail. When applied to the transformation of fcc (111) plane into the bcc (110) plane, the model is able to predict precise orientation relationships close to those observed in metallurgy (Kurdjumov-Sachs or Nishiyama-Wasserman relationships). This 2D model seems to be particularly relevant for materials such as the duplex steels.

1. Introduction.

In previous studies, the problem of mapping two different lattices onto each other by *bounded* transformations has been considered in the most general cases (n -dimensional lattices) [1, 2]. It was shown that any n -dimensional lattice can be mapped onto another lattice by a sequence of at most $n + 1$ shear transformations provided that the two lattices have the same density of nodes. This property is preserved when *fractional* shears, *bounded* versions of the linear shear transformations, are considered. These bounded transformations define globally the displacement of each lattice point. Still, using the fractional shear transformation imposes that the shear vectors belong to the lattice.

Moreover, it was demonstrated that in some cases, less than $n + 1$ shear operations are sufficient. In particular, two successive shears might be enough to map a lattice onto another one in 3D. The general case of $n + 1$ shears is met when the two lattices have no particular orientation relationship. On the contrary, the transformation can be achieved by less than $n + 1$ shears provided that the lattices exhibit particular orientation relationships.

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These bounded transformations are then meeting the main features of the martensitic transformations [3] : structural transformations between lattices without diffusion and existence of definite orientation relationships. We thus propose to examine in more detail the two-dimensional case and consider whether it might describe some known metallurgical situation. We must underline first that double shear mechanisms have already been proposed for martensitic transformations but these models are macroscopic or phenomenological. In the present case by means of an exact model, we predict a set of orientation relationships which are in agreement with the observations.

In section 2, before specifying the two-dimensional (2D) case, we will recall some basic features concerning fractional shears and the double shear restriction is examined in section 3. In section 4, the orientation relationships between 2D-lattices will be derived as function of the shear vectors. We give explicit solutions of the double shear mechanism which transform the $(110)_{bcc}$ 2D-lattice into a $(111)_{fcc}$ 2D lattice in section 5. The non-equivalent shear vectors (direction and amplitude) are given together with the corresponding orientation relationship. In section 6, the predicted orientations will be compared with that encountered in martensitic transformations. The case of duplex steels will be considered with special interest since these materials might justify 2D model.

2. Shears and fractional shears.

This section recalls the geometrical definition of shear transformations and of fractional shears, their bounded versions. The latter transformation is of crucial importance. Without this bounded version the double shear mechanism developed in this paper would have no physical interest in the description of diffusionless transformations.

A shear is a linear mapping which transforms points by translations of fixed given direction. Using the notation of Dirac's brackets a 3D shear has the following form :

$$S = I + |s\rangle \langle \sigma| = \begin{bmatrix} 1 + s_1 \sigma_1 & s_1 \sigma_2 & s_1 \sigma_3 \\ s_2 \sigma_1 & 1 + s_2 \sigma_2 & s_2 \sigma_3 \\ s_3 \sigma_1 & s_3 \sigma_2 & 1 + s_3 \sigma_3 \end{bmatrix}$$

so that the transformation reads :

$$S(x) = x + \langle \sigma | x \rangle s .$$

The vector s determines the direction of the displacement. The vector σ , in reciprocal space, specifies the amplitude of the transformation and defines the invariant plane of the shear for $S(x) = x$ is equivalent to $\langle \sigma | x \rangle = 0$. We shall consider shears of unit determinant, a condition equivalent to $\langle \sigma | s \rangle = 0$ (the shear direction lies in the invariant plane and s is invariant). In this case the inverse S^{-1} is also a shear transformation given by :

$$S^{-1} = I - |s\rangle \langle \sigma|$$

A shear transformation maps any lattice L onto a new lattice $L' = S(L)$. The mapping S is linear and therefore unbounded in the sense that $S(x) - x$ diverges when x runs over L . In other words, the atomic displacements are not bounded so that this transformation is not a convenient model for a global diffusionless transformation between two lattices. However, if s is a lattice vector of L , and only in this case, the above shear transformation has a bounded version, called a fractional shear [1, 2], which also transforms L into L' . If $S = I + |s\rangle \langle \sigma|$ is the linear shear, the associated fractional shear Σ is defined by :

$$\Sigma(x) = x + \text{Frac} [\langle \sigma | x \rangle] s$$

where $\text{Frac } [t]$ denotes the fractional part of the real number t , between $-1/2$ and $1/2$, so that $t = \text{Round } [t] + \text{Frac } [t]$ and $\text{Round } [t]$ denotes the nearest integer.

The displacement field $u(x) = \Sigma(x) - x = \text{Frac } [\langle \sigma | x \rangle] s$ is now bounded by $\|s\|/2$ so that Σ is a bounded transformation. This field has the structure of a periodic modulation of wave vector σ , though the amplitude is not the usual Cosine or Sine function but the Frac function (see Fig. 1). Actually, $u(x)$ has the following Fourier expansion

$$u(x) = \sum_{n \neq 0} \frac{(-1)^{n+1}}{2 \pi n} \sin(2 \pi n \langle \sigma | x \rangle) s.$$

Fig. 1. — The linear shear S has the lattice shear vector $a_1 = b_1$ which belongs to both lattices. The displacements $S(x) - x$ diverge when x goes to infinity. The fractional shear Σ performs the same global mapping but only involves bounded displacements.

The property of Σ to map L onto $L' = S(L)$ is due to the fundamental requirement that s is an irreducible vector of L . In this case, $s = S(s)$ is also an irreducible vector of L' so that L and L' share a 1D sublattice spanned by s . We conclude that the fractional shear Σ also maps L onto L' because $\Sigma(x)$ differs from $S(x)$ by $\text{Round } [\langle \sigma | x \rangle] s$, which is a common lattice vector. Actually Σ maps any point x of L onto the nearest point of L' lying on the common lattice line parallel to s . Finally, the inverse transformation of Σ has the same general form and is given by $\Sigma^{-1}(x) = x - \text{Frac } [\langle \sigma | x \rangle] s$.

It is proved in [4] that such fractional shears are the most simple bounded one-to-one mappings between lattices of equal density which involve a 1D displacement field.

3. The double shear condition.

If L_a and L_b are any two lattices of equal density, they cannot in general be related by one unique shear $S = I + |s\rangle \langle \sigma|$, where s should be a common lattice vector: the intersection of

the two lattices $L_a \cap L_b$ usually reduces to the origin $\{0\}$. Even if L_b is rotated by some rotation R , standing for a particular orientation relationship, L_a and $R L_b$ will not, in general, share any 1D sublattice and both lie on a bundle of lattice lines parallel to some lattice vector s .

The minimal number of successive shears required to map L_a onto $R L_b$ is well defined. This number depends on the rotation R and was proved in [1, 2] to be at most and generically four in 3D and three in 2D. This property can be easily expected on the basis of dimension arguments. Actually, the set of 3D lattices of given density can be labelled by 8 continuous variables necessary to build all 3 by 3 matrices of unit determinant. On the other hand, a 3D shear with a lattice direction depends on the *discrete* parameter s and on 2 *continuous* variables which specify σ as a wave vector orthogonal to s . Therefore 4 shears are required to account for the 8 parameters in 3D. The same argument suggests that 3 shears are generically required to map a 2D lattice onto another 2D lattice of equal density.

However, for particular pairs of lattices and for particular rotations, only two shears may be enough to map the first lattice onto the second one. In 2D this double shear condition can always be satisfied provided the lattices have a *particular* relative orientation which we believe to be physically significant. In this situation, an intermediate A lattice is naturally involved : L_a and A are related by a first shear of lattice vector s_a , which belongs to them. A second shear maps A onto $R L_b$ with a shear vector $R s_b$. The corresponding geometry is now investigated in more detail.

4. Determination of the 2D shears in the general case.

Let L_a and L_b denote two lattices in 3D with respective unit cells of volume Ω_a and Ω_b . We assume that there exist a lattice plane P_a of L_a and a lattice plane P_b of L_b such that the 2D lattices $A_a = L_a \cap P_a$ and $A_b = L_b \cap P_b$ have the same density of nodes (their 2D unit cells have the same area). If P_a and P_b are orthogonal to the primitive reciprocal vectors q_a and q_b , the equality of the 2D areas reads $\Omega_a |q_a| = \Omega_b |q_b|$. The 2D shears S_a and S_b will be specified in order that the transformed lattices $S_a(A_a)$ and $S_b(A_b)$ are related by a simple rotation. In other words, we look for a virtual 2D intermediate lattice A and a rotation R such that

$$A = S_a(A_a) = R S_b(A_b).$$

The rotation R is partially settled by the requirement that it transforms P_b into P_a so that the 2D lattices A_a and $R(A_b)$ are coplanar. R will be eventually completely specified by the double shear condition. The shears have the following form

$$\begin{aligned} S_a &:= I + |s_a\rangle \langle \sigma_a| \\ S_b &:= I + |s_b\rangle \langle \sigma_b| \end{aligned}$$

where s_a and s_b are irreducible lattice vectors in A_a and A_b respectively. The covectors σ_a and σ_b will specify the invariant planes of the shears.

Since s_a and s_b are invariant by the shears S_a and S_b respectively, s_a and $R s_b$ will belong to the 2D intermediate lattice A . We shall assume that these two vectors actually span this lattice. Now it is convenient to use adapted bases of the 2D lattices, $\{s_a, t_a\}$ for A_a and $\{t_b, s_b\}$ for A_b , such that $\{s_a, t_a\}$ and $\{t_b, s_b\}$ have the same orientation. After possibly changing s_b into $-s_b$ and t_b into $-t_b$, we can also assume that the basis $\{s_a, R s_b\}$ has also the same orientation. Consequently $\{s_a, R s_b\}$ is the image by S_a of some basis of A_a of the form $\{s_a, t_a + m s_a\}$, where m is an integer. Similarly, the same basis rotated by R^{-1} , $\{R^{-1} s_a, s_b\}$, is the image by S_b of a basis of A_b of the form $\{t_b + n s_b, s_b\}$ (see Fig. 2 where

Fig. 2. — The shears S_a and S_b transform the 2D lattices $L_a \cap P_a$ and $L_b \cap P_b$ into the same 2D lattice Λ , up to a rotation R which specifies the orientation relationship. The 2D intermediate lattice Λ has a basis $\{s_a, R s_b\}$ which is the image of the basis $\{s_a, t_a\}$ by the shear S_a , and of the basis $\{s_b, t_b\}$ by the shear S_b , followed by the rotation R .

m and n are assumed to vanish). Different 2D shears are solutions of this problem but the integers m and n will be chosen in order to get the smallest shear parameters.

With this notation, the 2D shear transformations read

$$\begin{aligned} S_a(s_a) &= s_a \\ S_a(t_a + m s_a) &= t_a + [\langle \sigma_a | t_a \rangle + m] s_a \\ S_b(t_b + n s_b) &= t_b + [\langle \sigma_b | t_b \rangle + n] s_b \\ S_b(s_b) &= s_b. \end{aligned}$$

The basis $\{s_a, R s_b\}$ of the intermediate lattice Λ is related to $\{s_a, t_a\}$ and $\{t_b, s_b\}$ by the following :

$$\begin{aligned} s_a &= R S_b(t_b + n s_b) = R t_b + [\langle \sigma_b | t_b \rangle + n] R s_b \\ R s_b &= S_a(t_a + m s_a) = t_a + [\langle \sigma_a | t_a \rangle + m] s_a. \end{aligned}$$

Since the shears have unit determinant we have

$$s_a \times R s_b = \Omega_a q_a = \Omega_b R q_b.$$

This cross product specifies the area of the unit cell of Λ , so that the angle θ between s_a and $R s_b$ can be deduced from

$$|s_a| |s_b| \sin(\theta) = \pm \Omega_a |q_a| = \pm \Omega_b |q_b|$$

A necessary condition for a solution to exist is that $|s_a| |s_b| \geq \Omega_a |q_a|$, or equivalently, $|s_a| |s_b| \geq \Omega_b |q_b|$. In this case, two possible rotations R are now completely determined by the conditions $R q_b = q_a$ and $(s_a, R s_b) = \pm \theta$.

The parameters of the shears can be partially determined by computing the scalar product of the above intermediate basis vectors by Rs_b and s_a respectively

$$\frac{|s_a| |s_b| \cos(\theta) - (s_b, t_b)}{s_b^2} = \langle \sigma_b, t_b \rangle + n$$

and

$$\frac{|s_a| |s_b| \cos(\theta) - (s_a, t_a)}{s_a^2} = \langle \sigma_a, t_a \rangle + m.$$

Different values of $\langle \sigma_a | t_a \rangle$ and $\langle \sigma_b | t_b \rangle$ are obtained depending on m and n . They actually give the same geometry so that we may choose the smallest shear parameters

$$\begin{aligned} \langle \sigma_a | t_a \rangle &= \text{Frac} \left[\frac{|s_a| |s_b| \cos(\theta) - (s_a, t_a)}{s_a^2} \right] \\ \langle \sigma_b | t_b \rangle &= \text{Frac} \left[\frac{|s_a| |s_b| \cos(\theta) - (s_b, t_b)}{s_b^2} \right] \end{aligned}$$

and

$$\begin{aligned} m &= \text{Round} \left[\frac{|s_a| |s_b| \cos(\theta) - (s_a, t_a)}{s_a^2} \right] \\ n &= \text{Round} \left[\frac{|s_a| |s_b| \cos(\theta) - (s_b, t_b)}{s_b^2} \right]. \end{aligned}$$

Finally, we see that the shear parameters are derived by the above formula and only depend on the choice of the shear vectors s_a and s_b .

5. Application to BCC and FCC lattices.

The previous model is now applied to the 2D lattices provided by the (111) plane in the fcc lattice and the (110) plane of the bcc lattice (see Fig. 3). The $(111)_{\text{fcc}}$ lattice plane is spanned by $v_{\text{fcc}} = [1/2, -1/2, 0]_{\text{fcc}}$ and $w_{\text{fcc}} = [1/2, 0, -1/2]_{\text{fcc}}$. The unit cell is a rhombus with angles 60° and 120° . Since the shear vector s_{fcc} controls the bound on the displacements induced by the fractional shear we shall only consider the two smallest cases (up to symmetry): $s_{\text{fcc}} = v_{\text{fcc}}$ and $s_{\text{fcc}} = v_{\text{fcc}} + w_{\text{fcc}}$. The $(110)_{\text{bcc}}$ lattice plane is spanned by $v_{\text{bcc}} = [1/2, -1/2, 1/2]_{\text{bcc}}$ and $w_{\text{bcc}} = [1/2, -1/2, -1/2]_{\text{bcc}}$. The unit cell is a rhombus with angles $\approx 70.53^\circ$ and 109.47° . Similarly, we shall assume that the shear vector s_{bcc} is of type v_{bcc} or $v_{\text{bcc}} \pm w_{\text{bcc}}$.

The application of the previous model requires that the 2D-lattice has the same density. In other words the unit cell areas must be equal. This condition leads to a simple consequence on the cell parameters: $a_{\text{bcc}}/a_{\text{fcc}} = (3/8)^{1/4} \approx 0.7825$.

The table I lists the first five non-equivalent solutions of the double shear geometry. Each column gives the principal parameters of the shears. The orientation relationship is characterized in the last three lines by the angle between a simple fcc direction and a simple bcc direction.

Figure 4a illustrates the solution corresponding to the smallest angle (0.6287°) between $[-2, 1, 1]_{\text{fcc}}$ and $[-1, 0, 1]_{\text{bcc}}$. Figure 4b gives the solution corresponding to the smallest

Table I.

$\angle (v_{FCC}, v_{BCC})$	-5.8931	61.4460	-1.6619	-111.5949	-13.7705
s_{FCC}	[1-1 0]	[2-1-1]	[1-1 0]	[2-1-1]	[-1 0 1]
σ_{FCC}	(0.0, -0.146)	(0.039, -0.068)	(0.0, -0.321)	(-0.099, 0.171)	(0.267, -0.154)
$\langle \sigma_{FCC} v_{FCC} \rangle$	0.0	0.0279	0.0	-0.0700	0.1890
$\langle \sigma_{FCC} w_{FCC} \rangle$	-0.0894	-0.0279	-0.1964	0.0700	0.0
s_{BCC}	[1-1-1]	[1 1-1]	[1 0-1]	[0 1 0]	[0 1 0]
σ_{BCC}	(0.168, -0.059)	(0.0, 0.195)	(0.048, -0.067)	(0.153, 0.108)	(-0.092, -0.065)
$\langle \sigma_{BCC} v_{BCC} \rangle$	0.1136	0.0	0.0322	0.1038	-0.0626
$\langle \sigma_{BCC} w_{BCC} \rangle$	0.0	0.1249	-0.0322	0.1038	-0.0626
u_{FCC}	[-2 1 1]	[-1 0 1]	[-1 1 0]	[-1 1 0]	[-1 0 1]
u_{BCC}	[-1 0 1]	[-1-1 1]	[-1-1 1]	[1-1-1]	[-1 1 1]
$\angle (u_{FCC}, u_{BCC})$	0.6287	1.4460	1.6679	2.1237	3.2417

Fig. 3. — The unit cells of the fcc lattice and of the bcc lattice. The interface plane is $[111]_{fcc} = [110]_{bcc}$. In the case of the duplex steel under consideration, the areas of the 2D unit cells in the common lattice plane are equal.

angle (1.4460°) between $[-1, 0, 1]_{fcc}$ and $[-1, -1, 1]_{bcc}$. The displacement field indicated in figures 4 results from the combination of the two fractional shears.

This particular case exemplifies clearly how the present model realizes a global transformation of the lattice by site displacement on the microscopic scale. The only requirement of the

Fig. 4. — White squares belong to the $(111)_{fcc}$ plane and black circles belong to the $(111)_{bcc}$ plane. a) The shear vectors are $[1 - 10]_{fcc}$ and $[1 - 1 - 1]_{bcc}$. The relative orientation is specified by the angle 0.6287° between $[-211]_{fcc}$ and $[-101]_{bcc}$. This solution is close to N-W orientation relationship. b) The shear vectors are $[2 - 1 - 1]_{fcc}$ and $[11 - 1]_{bcc}$ and the relative orientation is specified by the angle 1.4460° between $[-101]_{fcc}$ and $[-1 - 11]_{bcc}$ which is close to K-S.

2D model is that the planar site density is unchanged. Therefore this model is a reasonable candidate to account for displacive transformations such as the martensitic transformation. Martensitic transformations are non-diffusive lattice transformations commonly encountered in metallurgy (for a review see [5]). The most classical one concerns the iron system in which austenite, solid solution of fcc iron transforms without diffusion in a centered tetragonal crystal close to ferrite ($c/a = 1.05$).

It is remarkable that the sets of orientation relationships listed in table I are reminiscent of those martensite relating to its parent phase : the first column in table I recalls the Nishiyama-Wasserman (N-W) orientation relationship, while the other solutions are closer to the Kurdjumov-Sachs (K-S) case. We recall that both experimental orientations set the $(111)_{\text{fcc}}$ plane parallel to the $(110)_{\text{bcc}}$ plane but in the K-S case : $[1 - 110]_{\text{fcc}} // [1 - 11]_{\text{bcc}}$ when with the N-W relation : $[-211]_{\text{fcc}} // [01 - 1]_{\text{bcc}}$ (equivalent to $[10 - 1]_{\text{fcc}} // [001]_{\text{bcc}}$).

Finally it should be noted that the conditions on the equality of lattice density provide a very simple criterion for the cell parameters of both lattices. For example, as far as bcc and fcc lattices are concerned, a 3D double shear mechanism requires equal volumes : i.e. $a_{\text{bcc}}/a_{\text{fcc}} = 2^{-1/3} (= 0.7937)$. A 1D mechanism needs equal interplanar spacing between some planes of both lattices. In other words each mechanism is characterized by a particular cell parameter ratio. Incidentally we do not expect that the 2D model is relevant for all the martensitic transformations but only for some cases.

The following discussion will focus on the predictions deriving of the 2D version of the double shear mechanism and the features encountered in some metallurgical cases.

6. Discussion.

A martensitic transformation is characterized by two main features : the orientation relationships and the interface plane (usually called habit plane) between both phases. As mentioned previously the model predicts orientation relationships which are close to those encountered in steels. A habit plane is also predicted by our model : in the 2D restriction of the double shear mechanism the habit plane is the transformation plane. For the fcc/bcc transformation previously achieved, the habit plane is the $(111)_{\text{fcc}}$ plane ($= 110)_{\text{bcc}}$).

Experimentally, this habit plane is encountered (for example in low carbon steels) but not as a general case (habit planes oriented $(225)_{\text{fcc}}$ and $(259)_{\text{fcc}}$ are frequently observed [6]. Anyhow these habit planes are not the most relevant for comparison with our model since the product of the martensitic transformation is martensite, a centered tetragonal structure, not ferrite, the body centered cubic crystal. A bibliographical survey has brought to our knowledge duplex steels which seem to justify the present model.

Duplex steels consist in a two-phase microstructure : ferrite (bcc) labelled α or δ , and austenite (fcc) labelled γ . They provide a wide spectrum of structures : from dispersion of small austenite grains in a ferritic matrix to the opposite case of ferrite grains in austenite. These particular microstructure are obtained owing to appropriate high temperature heat treatments (600 °C to 1 300 °C) and to the addition of numerous solute elements (Ni, Cr, Mo, Mn, N...). At room temperature these solute elements are shared unequally between both phases (for an introduction to duplex steels see [7]). The two-phase microstructure results from martensitic transformation as well as diffusion. The martensitic stage is revealed by the existence of the K-S or N-W orientation relationships between the austenite and ferrite with $(111)_{\text{fcc}}$ habit plane. These typical features are encountered in two frequent microstructures of duplex steels : the growth of austenite particles within ferrite grains and the Widmanstätten ferrite laths.

In the former microstructure, Transmission Electron Microscopy and in-situ chemical analysis have revealed the typical martensitic morphology of the austenite platelets (orientation

relationships and habit planes) but that the chemical composition of the austenite particles might differ or not from the one of the ferrite matrix ([8, 9]. Widmanstätten laths consist of side plates of ferrite nucleating at the austenite grain boundaries but growing in the matrix among well defined planes ($(111)_{\text{fcc}}$ plane in duplex steels [7, 8, 10]).

Though these duplex steels provide microstructures in good agreement with our 2D model, it is not possible to test with accuracy whether they obey the primary requirement of our approach : a constant site density in the transformation plane. As mentioned previously, this condition is expressed by a particular cell parameter ratio. Unfortunately cell parameters are known only at room temperature and their values at high temperatures are not only modified by dilation but also by the partition of a large amount of solute elements between austenite and ferrite, solute elements which are known to modify the cell parameters [11, 12]. Since, to our knowledge, no high temperature cell parameters have been measured, the evolution of the cell parameter ratio with temperature is badly known. Taking only the dilation effect into account, figure 5 compares the evolution with temperature of the cell parameter ratio in a duplex steel (CF8M, $a_{\text{bcc}} = 0.285 \text{ nm}$, $a_{\text{fcc}} = 0.3598 \text{ nm}$ [13]) with some remarkable values relative to the site density conservation. The usual dilation coefficients of austenite and ferrite have been here used (Austenite : $\alpha_{\text{fcc}} = 23 \times 10^{-6} \text{ K}^{-1}$, Ferrite : $\alpha_{\text{bcc}} = 14 \times 10^{-6} \text{ K}^{-1}$). At high temperature the cell parameter ratio tends to meet the value required by the present 2D model. This is in agreement with the necessity of high temperature treatment to develop the previously mentioned microstructures. However because of the unknown compositional effect the comparison with experimental data should not be further developed.

Actually the point is that our requirement on cell parameter ratio meets well known features of the martensitic transformation : the relation between the cell parameter ratio, habit planes and orientation relationships. This dependence, earlier noticed in carbon steels [6], has been emphasized by a large survey of the experimental data [14]. Such a phenomenon is interpreted with the metallurgical models in use to describe the martensitic transformation. These models, which are first all macroscopic, are based on the assumption that the martensitic transformation involves shears and keeps invariant some atomic line. Therefore, after a shear deformation,

Fig. 5. — The dependence of the lattice parameters for a duplex steel (CF8M) [13] as a function of temperature. The horizontal lines specify the three different ratios $a_{\text{fcc}}/a_{\text{bcc}}$ corresponding to the equality of atomic volumes, planar spacing along $[111]_{\text{fcc}} // [110]_{\text{bcc}}$ or 2D cell areas. For the CF8M duplex steel, the room temperature data are $a_{\text{bcc}} = 0.285 \text{ nm}$, $a_{\text{fcc}} = 0.3598 \text{ nm}$).

some rigid body rotation generating a particular orientation relationship is necessary to get an invariant line. This approach is phenomenological since the invariant line hypothesis is only derived from the observations. Our model also predicts a strong dependence of orientation relationship and habit planes since the mechanism will depend on the site density. The strength point is that, in our work, this dependence is derived from the most basic principle : the conservation of the lattice density. This very conservation indicates which shear mechanism is « mathematically » allowed : 1D, 2D or 3D.

7. Conclusion.

To our knowledge the present model, though restricted to the 2-dimensional case, is the first to achieve a global as well as a microscopic transformation which, when applied to the fcc/bcc lattices predicts the observed orientation relationships. It is worth noting that the experimentally noticed dependence of the mechanism on the cell parameter ratio is also accounted for by our approach. Because of the present 2D restriction, the model cannot be considered as relevant for the most general case of transformation, still a class of materials (the duplex steels) provides experimental features in this 2D frame.

In the present model the site displacement results from the combination of two shear transformations. This double shear is sufficient to generate the observed orientation relationship between the lattices. This remarkable property is one of the most general ones of the transformation between the lattices of equal density. Therefore the double shear mechanism appears as the most natural basis for displacive transformations, however it should be stressed that a fractional double shear should be used in order to have physically meaningful site displacements.

As mentioned in the discussion the observed (225), (259) habit planes cannot be supported by the present 2D approach. In general this 2D-model is not likely to be relevant for all martensitic transformation but only in those cases where some lattice planes of both phases have the same density of nodes. Therefore with the same basic ideas (fractional double shears), we will examine the 1D on 3D cases further on : i.e. lattices exhibiting either a direction with constant atomic spacing or a constant atomic volume.

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