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APPLICATION OF TRIPLE-SHEAR MODEL TO MARTENSITIC TRANSFORMATIONS IN Fe-Ni-C ALLOYS

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ABSTRACT

Although double-shear theories of martensite crystallography were considered more successful than the classical theories, still it is not possible to explain the complete nature of the transformations especially in Fe alloys with $\{225\}_f$ and $\{259\}_f$ habit planes. Since the double-shear theories give better results than the classical theories and more than two simple shear elements were observed by electron microscope observations in these transformations, it is concluded that the number of the simple shears used in these theories should be increased. The triple-shear model which was based on the above mentioned results was found to be in good agreement with the observations in some Fe alloys with $\{225\}_f$ habits. The same model was also applied to the Fe-Ni-C alloys with $\{259\}_f$ habits and gave succesful results.

INTRODUCTION

The first crystallographic martensite theories were developed by Wechsler, Lieberman and Read (1953) and Bowles and Mackenzie (1954). These phenomenologic theories, later were shown by Christian as to be be mathematically equivalent and were only able to predict the relations between parent and product phases, but could not explain how the atoms have gone to their last positions during the transformation. They considered the Bain strain (1924) as the base of the macroscopic shape change after the transformation. The invariant nature of an interface plane between parent and product phases which was called "the habit plane" of new phase was explained by these theories with an existance of a lattice invariant shear. The both theories consider the lattice invariant shear as slip or twinning type lattice imperfections. Although these early theories were very successful to explain the whole nature of martensite crystallography in the phase transformations with $\{3\ 10\ 15\}_F$ habits, the same success could not be obtained in especially Fe alloys with $\{225\}_F$ and $\{259\}_F$ habit planes. The "dilatation parameter" consept of the Bowles Mackenzie theory could also not be able to overcome this discrepancy.

The macroscopic shape change produced by a homogeneous strain is given in these theories as,

$$F = R\ P\ S$$

where, F, R, P and S are matrices with 3x3 type and represent the total shape strain, rigid body rotation, Bain strain and simple shear respectively.

In general, an invariant plane strain is given by,

$$B_{ij} = \delta_{ij} + m\, d_i\, p_j, \ (i, j = 1,2,3)$$

where, δ_{ij} is Kronecker delta, P_j the unit normal of invariant plane and d_i and m are the unit vector along the displacement direction and the magnitude of displacement respectively. If the condition, $\vec{p} \cdot \vec{d} = 0$, is satisfied, the invariant plane strain then becomes a simple shear or lattice invariant strain.

Acton and Bevis (1969) and Ross and Crocker (1970) suggested new double lattice invariant shear models to overcome the discrepancies between the results given by the classical theories and the observations. Undoubtedly, the doubleshear theories are more flexible than the previous descriptions but even these theories are not very successful in predicting all the crystallographic parameters of those transformations which do not fit the standart theories.

Since the double-shear theories give more successful results than the classical theories and the presence of more than two shears dedected by Wayman, Hanefee and Read (1961), Shimizu and Nishiyama (1972), Durlu (1978), the total shape strain producing the macroscopic shape change was given by Wayman (1972) as,

$$F = R\ P\ S_n \ldots S_2\ S_1$$

In the multiple-shear model, the most prominent difficulty is the application order of the simple shears.

The case of triple-shear was studied by Dikici and Durlu (1978) and shown that the triple-shear model is more convenient than the early theories in explaining the observed discrepancies.

The aim of the present study is to apply the tripleshear model to the martensitic transformations with $\{259\}_F$ habits in some Fe alloys.

II. DETERMINATION OF THE CRYSTALLOGRAPHIC PARAMETERS

In the crystallographic martensite model with tripleshear, the homogeneous strain giving the macroscopic shape change is given as,

$$F = R\ P\ T\ S\ K \tag{1}$$

where, T, S and K are complementary shears. The habit plane change caused by Bain strain can be restored with the opposite effects of these three shears and the rigid body rotation, R, also satisfies the condition that the undistorted habit plane does not rotate. All these matrices are 3x3 types.

The planes and directions of T, S and K have been chosen from the shear elements which can be observed experimentally and elements of P matrix could easily be determined by using lattice parameters of both austenite and martensite crystals. Therefore, we need to determine the F and R matrices, and the magnitudes of simple shear. Firstly, the magnitudes of simple shears were limited in such a way that F is an invariant plane strain, and then the strain F was found. Secondly, the rigid body rotation, R, was determined from Equation 1.

II. 1 Boundary Condition for the Magnitudes of Simple Shears

If a homogeneous strain keeps the habit plane undistorted and also unrotated, this strain should not change any $\vec{x}$ vector on the habit plane. This can be shown in the matrix representation as $Fx = x$. Since the length of this vector is not changed during the transformation, this may be written as the form,

$$x'\,x = x'\,F'\,F\,x \tag{2}$$

where, the exponent (′) shows the transpose of the matrix. The Equation 2 gives the condition for an undistorted habit plane, and represents the cone of lines remained unchanged in length during the transformation. Since $\vec{x}$ is on the habit plane, the unit normal of this plane fits to the condition, $\vec{h} \cdot \vec{x} = 0$, which indicates the existence of two perpendicular lines. By using F′F matrix multiplication in the Equation 2 and $R' = R^{-1}$, we find,

$$Z = K' S' T' P' P T S K$$

and Equation 2 becomes,

$$x' (Z - I) x = 0$$

to find nonsingular solutions to this Equation, following condition is to be satisfied,

$$\text{Det } (Z - I) = 0 \tag{3}$$

this gives a limitation to the magnitudes of simple shears for which the homogeneous strain F is an invariant plane strain.

If we describe invariant plane strain matrices F, T, S and K in the orthonormal austenite base, then the Z matrix is obtained as,

$$Z_{ij} = \delta_{ij} + \gamma^2 u_i h_j + \gamma (u_i h_j + h_i u_j), \ (i, j = 1,2,3) \tag{4}$$

F strain also keep the habit plane normal $\vec{h}$ invariant. This can also be describe in the matrix form as $hF^{-1} = h$. The condition for undistorted $\vec{h}$ vector after the transformation is,

$$h h' = (h F^{-1}) (h F^{-1})' \tag{5}$$

If $Z^{-1} = F^{-1} (F^{-1})'$, then, by describing the determinant of F as D,

$$Z_{ij}^{-1} = \delta_{ij} + \gamma^2 D^{-2} i_i u_j - \gamma D^{-1}(u_i h_j + h_i u_j), \ (u,j = 1,2,3) \tag{6}$$

is obtained.

The determinant of F is,

$$D = 1 + \gamma_i h_i = n_1 n_2 n_3, \ (i = 1,2,3) \tag{7}$$

where, n_1, n_2 and n_3 represent the Bain strains.
If the traces of the matrices, elements of which are given by Equations 4 and 6, and Equation 7 were used together we obtain,

$$Z_{ii} - n_1^2 n_2^2 n_3^2 Z_{ii}^{-1} = 1 - n^2{}_1 b^2{}_2 n^2{}_3, \ (i = 1,2,3) \tag{8}$$

This equation does not include the values connected with F strain. Thus, a limitation was emposed on the magnitudes of T, S and K simple shears in such a way that F is undistorted plane strain.

II. 2 Determination of the Crystallographic Parameters

The magnitude of the macroscopic displacement can be determined by using the Equation 4 and 7 as,

$$\gamma^2 = Z_{ii} - 2 n_1 n_2 n_3 - 1, \ (i = 1,2,3) \tag{9}$$

If, $i = \alpha$ and $j = \beta$, the then habit plane normal is obtained from Equation 4,

$$h^2_\beta\,(Z_{\alpha\alpha} - 1) - 2h_\alpha h_\beta Z_{\alpha\beta} - h^2_\alpha\,(Z_{\beta\beta} - 1) = 0 \quad (10)$$

By repeting the same procedure, the direction of macroscopic strain can also be found from Equation 6 and 7,

$$u^2_\beta\,(Z_{\alpha\alpha}^{-1} - 1) - 2u_\alpha u_\beta Z^{-1}{}_{\alpha\beta} - u^2_\alpha\,(Z_{\beta\beta}{}^{-1} - 1) = 0 \quad (11)$$

Since the other parameters were determined earlier, the rigid body rotation, R, is the only unknown in Equation 1 and can be obtained as,

$$R = F\,K^{-1}\,S^{-1}\,T^{-1}\,P^{-1} \quad (12)$$

III. CALCULATION OF THE CRYSTALLOGRAPHIC VALUES

III. 1 Determination of the Simple Shear Elements

In the Fe-Cr-C martensites with $\{225\}_F$ habits, the twinning plane was found as the $(112)_M$ plane of new phase by Shimizu and Nishiyama (1972) and same as in some Fe alloys with $\{3, 10\ 15\}_F$ habits. It was also shown in the same alloys that there were $(011)_M$ twins, and $(\bar{1}12)_M$ slip traces which cross the $(112)_M$ twinning systems. Therefore, as being different from $(112)_M$ twins, $(011)_M$ twins and $(\bar{1}12)_M$ slip traces can be special for the $\{225\}_F$ martensites. Since the $(011)_M$ twins were also observed in the $\{259\}_F$ martensites of Fe-1.8 % C alloys, the existence of $(011)_M$ twinning systems depends on the tetragonality of martensite structure rather than the type of habit planes. $(\bar{1}12)_M$ slips have not been observed in $\{3\ 10\ 15\}_F$ martensites yet as indicated by Shimizu and Nishiyama (1972).

In the application of the triple-shear model to $\{259\}_F$ martensites observed by Durlu in some Fe-Ni-C alloys (1978, 1979) were also taken into account, in addition to above mentioned shear elements.

III. 2 Calculation of the Crystallographic Values

The crystallographic value needed to test the triple shear model in some Fe alloys with $\{259\}_F$ habits were obtained from the systems in Section III.1 by using a computer programme.

Firstly, t, s and k magnitudes of complementary shears were determined by using Equation 8. In finding the third parameter, the first two parameters were changed with 0.10 and 0.005 steps. The change of γ were then studied. It was shown that the minimum values of γ changed with the composition of alloys and the planes, directions and magnitudes of simple shears, and the application order of complementary shears. After the determination of t, s and k values, these were used in finding the macroscopic strain elements and also in finding the orientation relationships. The results are given in Table 1 and 2, where $\varnothing$, θ and ψ values illustrate the angles corresponding to the rotations of the $(111)_F$ plane and the $[\bar{1}01]_F$ and $[\bar{1}\bar{1}2]_F$ directions respectively. The martensite habit plane normals of Fe-22 % Ni-0.8 % C steel is given in Figure 1. Examination of this stereographic projection in conjunction with the computer outputs revealed that the habit plane normals changed on the lines between $(3, 10\ 15)_F$, $(252)_F$ and $(10\ 15\ 3)_F$ poles as depending on the magnitudes of simple shears, and between $(010)_F$ and $(111)_F$ poles as depending on the application order of simple shears.

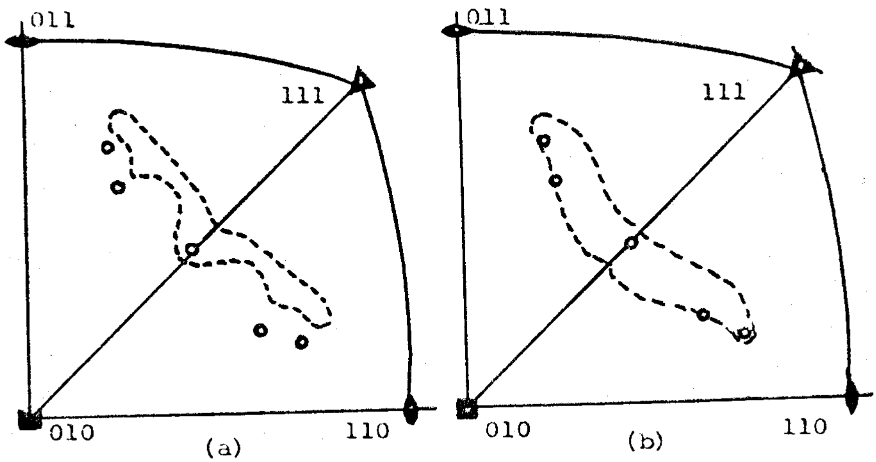

Figure 1 Austenite stereographic projections showing tbe martensite habit plane normals; (a) For the shear comnination af $(\bar{1}01)$ $[101]_f$, (011) $[0\bar{1}1]_f$ and (111) $[\bar{1}01]_f$. (b) For the shear combination of (011) $[0\bar{1}1]_f$, (101) $[\bar{1}01]_f$ and (111) $[\bar{1}01]_f$.
(The full rounds show the common habit plane poles of Fe alloys and tbe broken lines indicate the regions for possible habit plane normals).

IV. DISCUSSION OF THE RESULTS

The crystallographic parameters of austenite-martensite phase transmations were calculated for Fe-22 % Ni-0.8 % C and Fe-17.1 % Ni-0.81 % C steels by using the triple-shear model and the results were compared with those of prior experiments.

For the cases 7-13 listed in Table 1, The habit plane normals and the macroscopic shear directions were compared with the experimental results of Greninger and Troiano (1949). and it was shown that the results obtained by using the triple shear model are in good agreement with the observations, and they are better than those of given by classical theories. The results listed in Table 2 and the cases 1-6 in Table 1 show that

	Shear elements	t	s	k	γ	h	u	∅	θ	Ψ
1	(101) [$\bar{1}$01], (111) [0$\bar{1}$1], (011) [0$\bar{1}$1]	0,21	0,06	0,13	0,07	[0,857 −0,480 0,185]	[0,100 −0,979 0,178]	1,34	3,31	1,44
2	(101) [$\bar{1}$01], (011) [0$\bar{1}$1], (11$\bar{1}$) [110]	0,33	0,14	−0,09	0,09	[0,450 −0,211 0,867]	[−0,561 −0,435 0,705]	0,60	3,04	1,70
3	(111) [$\bar{1}$01], (011) [0$\bar{1}$1], (101) [$\bar{1}$01]	0,04	0,07	0,21	0,12	[0,200 0,851 0,485]	[−0.374 0,758 −0,535]	0,24	3,27	1,39
4	(011) [0$\bar{1}$1], (101) [$\bar{1}$01], (111) [0$\bar{1}$1]	0,05	0,22	0,13	0,07	[0,853 −0,489 0,180]	[0,010 −0.958 0,287]	1,43	3,24	1,52
5	(101) [$\bar{1}$01], (111) [132], (011) [11$\bar{1}$]	0,22	0,25	−0,04	0,15	[0,857 0,171 0,487]	[0,321 −0,902 0,290]	1,06	2,84	1,94
		0,26	0,26	−0,02	0,15	[0,833 0,157 0,531]	[0,172 −0,861 0,478]	0,68	2,10	2,61
6	(011) [1$\bar{1}$1], (101) [101], (111) [1$\bar{3}$2]	0,11	0,12	0,17	0,18	[0,548 0,91 0,813]	[0,895 −0,372 −0,247]	1,33	2,12	2,71
		0,04	0,31	0,18	0,11	[0,854 −0.198 0,482]	[−0,174 −0,557 0,812]	0,59	2,35	2,36
7	(101) [$\bar{1}$01], (011) [011], (111) [$\bar{1}$01]	0,21	0,93	0,03	0,16	[0,167 0,807 0,567]	[−0,293 0,706 −0,580]	0,24	3,41	1,25
8	(111) [$\bar{1}$01], (011) [0$\bar{1}$1], (101) [$\bar{1}$01]	0,03	0,04	0,21	0,15	[0,166 0,822 0,545]	[−0,285 0,755 −0,591]	0,25	3,38	1,28
9	(011) [0$\bar{1}$1], (101) [$\bar{1}$01], (111) [0$\bar{1}$1]	0,29	0,26	−0,27	0,21	[0,823 0,544 0,162]	[−0,108 0,713 −0,693]	0,26	2,52	2,16
10	(011) [0$\bar{1}$1], (101) [$\bar{1}$01], (111) [$\bar{1}$01]	0,04	0,21	0,03	0,15	[0,167 0,822 0,546]	[−0,287 0,754 0,591]	0,25	3,20	1,26
11	(111) [1$\bar{3}$2], (011) [11$\bar{1}$], (101) [$\bar{1}$01]	0,10	0,12	0,30	0,20	[0,163 −0,825 −0,542]	[−0,295 −0,711 −0,639]	0,76	2,49	2,20
12	(011) [1$\bar{1}$1], (101) [$\bar{1}$01 , (111) [1$\bar{3}$2]	0,10	0,13	0,18	0,17	[0,548 0,165 0,820]	[0,888 −0,394 −0,237]	1,23	1,80	3,01
13	(011) [11$\bar{1}$], (111) [1$\bar{3}$2], (101) [$\bar{1}$01]	0,11	0,10	0,29	0,19	[0,165 −0,824 −0,542]	[−0,258 −0,718 0,647]	0,63	2,53	2,16

Table 2 Crystallographic predictions of the triple shear model for Fe-17.1 % Ni-0.81 % C steel.

	Shear elements	t	s	k	γ	h	u	Ø	θ	Ψ
1	(111) $[0\bar{1}\bar{1}]$, (101) $[\bar{1}01]$, (011) $[0\bar{1}\bar{1}]$	0,11	0,19	0,11	0,05	[0,840; −0,191; 0,508]	[0,346; −0,934; −0,093]	0,87	3,39	1,31
2	(111) $[\bar{1}01]$, (011) $[0\bar{1}\bar{1}]$, (101) $[\bar{1}01]$	0,00	0,06	0,22	0,14	[0,212; 0,821; 0,529]	[−0,225; 0,698; −0,680]	0,36	3,26	1,41
		0,02	0,10	0,25	0,09	[0,482; 0,850; 0,212]	[−0,574; 0,730; −0,420]	0,40	1,59	3,12
3	(011) $[0\bar{1}\bar{1}]$, (101) $[\bar{1}01]$, (111) $[0\bar{1}\bar{1}]$	0,12	0,26	−0,14	0,09	[0,552; 0,814; 0,181]	[−0,450; 0,708; −0,544]	0,40	1,71	3,00
4	(011) $[0\bar{1}\bar{1}]$, (101) $[\bar{1}01]$, (111) $[\bar{1}01]$	0,09	0,20	0,06	0,11	[0,215; 0,869; 0,446]	[−0,481; 0,744; −0,464]	0,30	3,37	1,34
5	(011) $[0\bar{1}\bar{1}]$, (111) [011], $(\bar{1}01)$ $[\bar{1}01]$	0,30	0,70	0,24	0,19	[0,203; 0,494; 0,846]	[−0,027; −0,746; 0,666]	0,31	3,50	1,26
		0,32	0,07	0,24	0,21	[0,190; 0,512; 0,838]	[0,016; 0,746; 0,665]	0,31	3,49	1,26
6	(101) $[\bar{1}01]$, (111) $[1\bar{3}2]$, (011) $[\bar{1}\bar{1}1]$	0,24	0,11	−0,03	0,14	[0,194; −0,846; −0,496]	[0,320; −0,647; 0,693]	0,86	2,85	1,91
		0,27	0,15	0,04	0,07	[0,820; −0,530; 0,215]	[−0,023; −0,681; 0,731]	0,48	2,67	2,09
7	(101) $[\bar{1}01]$, (111) $[1\bar{3}2]$, (011) $[1\bar{1}\bar{1}]$	0,26	0,03	−0,04	0,14	[0,236; 0,862; 0,449]	[−0,459; 0,705; −0,541]	0,38	1,78	2,96
8	(111) $[1\bar{3}2]$, (101) $[\bar{1}01]$, (011) $[1\bar{1}\bar{1}]$	0,25	0,20	−0,07	0,17	[0,834; 0,220; 0,505]	[0,455; −0,888; 0,069]	1,47	3,14	1,81
		0,03	0,26	−0,03	0,14	[0,223; 0,859; 0,460]	[0,421; 0,708; −0,568]	0,35	1,87	2,84
		0,04	0,26	−0,03	0,13	[0,194; 0,872; 0,449]	[0,427; 0,670; −0,574]	0,39	1,90	2,83
9	(111) $[1\bar{3}2]$, (011) $[1\bar{1}\bar{1}]$, (101) $[\bar{1}01]$	0,11	0,12	0,31	0,19	[0,199; −0,828; −0,525]	[0,312; −0,704; 0,639]	0,82	2,40	2,34
10	(011) $[\bar{1}\bar{1}1]$, (101) $[\bar{1}01]$, (111) $[1\bar{3}2]$	0,26	0,21	0,16	0,24	[0,219; 0,484 ...	[0,821; −0,511 ...	1,42	1,90	2,92

the habit plane normals concentrated about the $\{259\}_F$ poles. The G-T orientation relationships were also ensured for these two alloys, although the angle values show a small difference of 0.10°–0.25° with the early experimental measurements, but this can be explained in terms of statistical measurement errors.

As mentioned by Wayman (1972) the parameters of martensitic transformation are very sensitive to the application order of simple shears. The habit plane normals displace from the $\{3\ 10\ 15\}_F$ poles to the $\{259\}_F$ or $\{225\}_F$ as depending on the numbers, orders and magnitudes of simple shears.

The triple shear model applied to the $\{259\}_F$ transformations is more convanient than the early theoretical models to explain the crystallography of martensitic transformation.

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