The Crystallography of the Martensitic Transformation in (225) Steels

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The crystallography of the martensitic transformation in (225) steels is described by a combination of a $\{110\}_M \langle 1\bar{1}1\rangle_M$ secondary shear and a twin shear on a $\{112\}_M \langle 11\bar{1}\rangle_M$ of the martensite lattice. It is shown that good agreement exists between the theory and the observations.

Die Kristallographie der Martensittransformation in (225) Stählen

Es wird gezeigt, daß die Martensitumwandlung in (225) Stählen durch eine inhomogene Scherung auf einem $\{110\}_M \langle 1\bar{1}1\rangle_M$ Schersystem und einem $\{112\}_M \langle 11\bar{1}\rangle_M$ Zwillingssystem der Martensitphase in guter Übereinstimmung mit den Beobachtungen beschrieben werden kann.

In spite of considerable effort it has not yet been possible to predict the observed features of the (225) transformation in steels. Whereas the (259) habit can be explained by an inhomogeneous secondary shear on a $\{112\}_M$ plane in the martensitic body centered phase, no single secondary shear can account for the (225) habit. Wechsler, Read and Liebermann [1]) discussed the possibility that the change from the (259) to the (225) martensite is due to a change from a $\{112\}_M$ to a $\{110\}_M$ secondary shear plane. One of the habit plane normals $\mathbf{p}_1'$ they calculated lies near the observed habit but still 6° outside of the scatter of the experimentally determined values. Moreover the predicted amount of the macroscopic shear $m_1 \approx 0.28$ is higher than the observed magnitude of 0.21. In subsequent papers more complex transformation mechanisms were discussed [2]) to [5]) and are reviewed by Dunne and Wayman [6]). However none of them is in agreement with the existing experimental results [6]).

In this paper it will be shown that the crystallography of the (225) martensite can satisfactorily be explained on the basis of a secondary shear system of type $\{110\}_M < 1\bar{1}1 >_M$ as proposed by Wechsler, Read and Liebermann [1]), if an additional twin shear on a $\{112\}_M < \bar{1}11 >_M$ is taken into account.

Formulation of the theory

In the Wechsler-Liebermann-Read phenomenological theory [7]), the transformation is decomposed into a Bain distortion, an inhomogeneous deformation and a rigid rotation. In our model the inhomogeneous deformation is further decomposed into two shears on different systems. We adopt the following sequence of operations: a) a homogeneous Bain distortion to a bcc structure with the same interatomic distance as the original austenitic fcc phase, described by the matrix B_1, b) a shear on a $\{110\}_M < 1\bar{1}1 >_M$ system in the martensite phase, denoted by P_1, c) an additional inhomogeneous twin shear on a $\{112\}_M < 11\bar{1} >_M$ system, denoted by P_2, d) a final homogeneous distortion B_2 to adjust to the observed lattice parameters, e) a rigid rotation R. The total shape deformation therefore is given by the matrix product $RB_2P_2P_1B_1$. (A decomposition into two shears first, followed by the Bain distortion and a rigid rotation would have been an equivalent possibility.) The amount g_1 of secondary shear on $\{110\}_M < 1\bar{1}1 >_M$ is chosen as a parameter, and the amount g_2 of the $\{112\}_M < 11\bar{1} >_M$ twin shear is calculated from the condition that an undistorted habit plane exists. ($g_2 = 0$ corresponds to a shear on $\{110\}_M < 1\bar{1}1 >_M$ only). In addition the habit plane normal $\mathbf{p}_1'$, the amount of macroscopic shear m_1 and the direction $\mathbf{d}_1'$ are calculated as a function of g_1. Several combinations of shear variants have been considered but the only combination that yields results in agreement with the observations are the systems $(011)_M$ $[\bar{1}1\bar{1}]_M$ and $(12\bar{1})_M$ $[\bar{1}11]_M$. (See fig. 1.) The numerical calculations were made using as input lattice parameters those for an Fe–7.9 Cr – 1.1 C alloy which was studied by Morton and Wayman [8]) (a_0 = 3.169 Å, a = 2.860 Å, c = 2.983 Å). The results show that solutions exist only if g_2 is smaller than 0.1286 and that for $g_2 < 0$ the resulting m_1 is larger than the m_1 for $g_2 = 0$.

The crystallographic data were computed for different values of g_1 as parameter, corresponding to g_2 between zero and 0.1286. In fig. 1 are shown the

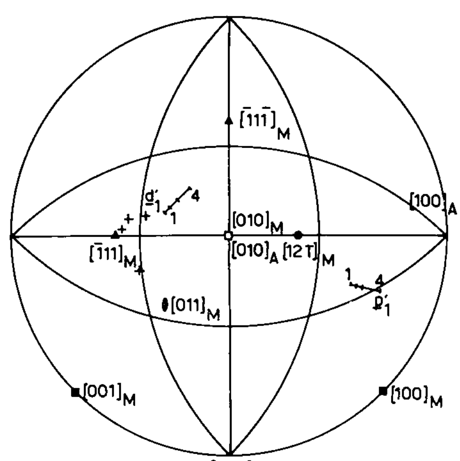

Fig. 1 Stereographic projection showing the calculated habit plane normal $\mathbf{p}_1'$, the calculated and observed (+) macroscopic shear directions $\mathbf{d}_1'$. The index A and M refer to the fcc austenitic and the bcc martensitic lattice, respectively. The two shear systems are $(011)_M$ $[\bar{1}1\bar{1}]_M$ and $(12\bar{1})_M$ $[\bar{1}11]_M$. By the numbers 1 to 4 are denoted the calculated values for $g_2 = 0$; 0.0349; 0.0735 and 0.1286.

habit plane normal $\mathbf{p}_1'$ and the macroscopic shear direction $\mathbf{d}_1'$ for $g_2 = 0$; 0.0349; 0.0735 and 0.1286 (denoted by numbers 1 to 4). In fig. 2 the $\mathbf{p}_1'$ are compared with the experimental results of Morton and Wayman for the Fe − 7.9 Cr − 1.1 C alloys [8]. In fig. 3 the amount of macroscopic shear m_1 and g_1 as a function of the twin shear g_2 is plotted. In table 1 are listed the predictions for $g_2 = 0$; 0.0735; 0.1286 and the experimentally determined quantities.

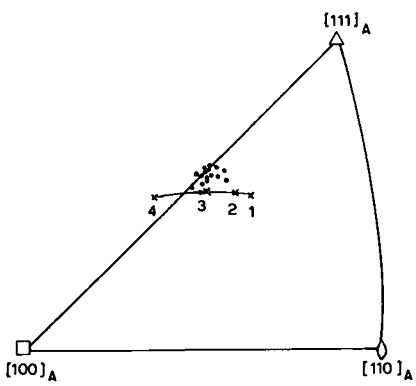

Fig. 2. Calculated and observed habit planes $\mathbf{p}_1'$. (The notation is the same as in fig. 1).

Discussion

Figure 3 shows that the amount of macroscopic shear can be reduced considerably by an additional twin

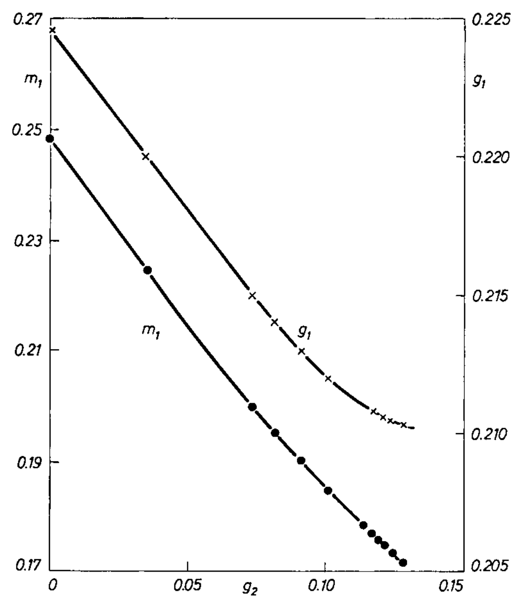

Fig. 3. The amount of macroscopic shear m_1 and of the shear g_1 on the $(011)_M$ plane as a function of the twin shear g_2.

Table 1. Calculated and experimental transformation parameters

	$g_2 = 0.1286$	$g_2 = 0.0735$	$g_2 = 0$	observed [8]
Habit plane $\mathbf{p}_1'$	$\begin{pmatrix}0.8986\\0.2891\\0.3299\end{pmatrix}_A$	$\begin{pmatrix}0.8545\\0.3906\\0.3424\end{pmatrix}_A$	$\begin{pmatrix}0.8177\\0.4734\\0.3273\end{pmatrix}_A$	$\begin{pmatrix}0.850\\0.387\\0.356\end{pmatrix}_A$
Macroscopic shear direction $\mathbf{d}_1'$	$\begin{pmatrix}-0.3181\\0.8594\\-0.4002\end{pmatrix}_A$	$\begin{pmatrix}-0.4425\\0.8486\\-0.2900\end{pmatrix}_A$	$\begin{pmatrix}-0.5460\\0.8182\\-0.1799\end{pmatrix}_A$	$\begin{pmatrix}-.0.72\\0.67\\-0.02\end{pmatrix}_A$
m_1	0.1719	0.2003	0.2485	0.183; 0.206; 0.216; 0.254.
g_1	0.21049	0.2150	0.22461	–
Orientation relationship: $[100]_A \rightarrow [10\bar{1}]_M$ =	$\begin{pmatrix}0.9953\\-0.0930\\-0.0279\end{pmatrix}_A$	$\begin{pmatrix}0.9959\\-0.0816\\-0.3800\end{pmatrix}_A$	$\begin{pmatrix}0.9964\\-0.0702\\-0.0485\end{pmatrix}_A$	–
$[010]_A \rightarrow [010]_M$ =	$\begin{pmatrix}0.0957\\0.9882\\0.1194\end{pmatrix}_A$	$\begin{pmatrix}0.0858\\0.9881\\0.1278\end{pmatrix}_A$	$\begin{pmatrix}0.0762\\0.9877\\0.1364\end{pmatrix}_A$	–
$[001]_A \rightarrow [101]_M$ =	$\begin{pmatrix}0.0166\\-0.1215\\0.9924\end{pmatrix}_A$	$\begin{pmatrix}0.0271\\-0.1305\\0.9911\end{pmatrix}_A$	$\begin{pmatrix}0.0384\\-0.1395\\0.9895\end{pmatrix}_A$	–
$(111)_A \rightarrow (110)_M$ =	$\begin{pmatrix}0.5826\\0.5744\\0.5749\end{pmatrix}_A$	$\begin{pmatrix}0.5816\\0.5755\\0.5749\end{pmatrix}_A$	$\begin{pmatrix}0.5809\\0.5765\\0.5746\end{pmatrix}_A$	–
Angle between planes $(111)_A$ and $(110)_M$	0.40°	0.35°	0.35°	0.45°
Angle between directions $[01\bar{1}]_A$ and $[\bar{1}1\bar{1}]_M$	3.1°	2.1°	1,1°	0.53°
Angle between directions $[\bar{1}10]_A$ and $[\bar{1}11]_M$	6.3°	7.3°	8.3°	10.1°
Angle between directions $[10\bar{1}]_A$ and $[00\bar{1}]_M$	1.8°	2.7°	3.7°	4.65°

shear, the reduction rate being largest for small g_2; g_1 is affected only little, it varies by about 7 % in the whole range between $0 \leq g_2 \leq 0.1286$. The habit plane normal $\mathbf{p}'_1$ moves 12° for the same variation in g_2. The $\mathbf{p}'_1$ for $g_2 = 0$ lies outside the experimental values, as already shown by Wechsler, Read and Liebermann[1]). The habit corresponding to the smallest m_1 does not agree either with the observations. Best agreement with the observed $\mathbf{p}'_1$ is obtained for an intermediate g_2 near 0.0735. For this reason the calculations were made also for this value. The calculated $\mathbf{d}'_1$ lie slightly outside the experimental data. Since the scatter of the measured $\mathbf{d}'_1$ is quite large, the deviations are not considered serious. The measured m_1 scatter considerably but lie within the range given by $g_2 = 0$ and 0.1286, the average value being consistent with $g_2 = 0.0735$. The observed orientation relationship is in good agreement with the calculations for $g_2 = 0$, but the deviations increase with increasing twin shear. As has been pointed out by Morton and Wayman[8]), the $(111)_A$ plane of the austenite phase nearest to the habit plane $(522)_A$ is transformed into a $(110)_M$ plane whose pole lies between $(111)_A$ and $(522)_A$. This observation is in agreement with the calculations. Additional information on the orientation of the observed twin plane variant with respect to the habit plane comes from the studies of Jana and Wayman[9]). They made a trace analysis of the habit and the twin plane. In one case (their fig. 10) the observed twin plane variant is the same as predicted by the present model. In the other case (their fig. 8) two different habit plane variants are consistent with the trace analysis, the $(\bar{5}\bar{2}2)_F$ variant which they plotted in their figure and a $(\bar{2}\bar{2}5)_F$ variant which they do not mention. If the second choice is taken agreement with our predictions is obtained.

Thus the contribution of the $(12\bar{1})_M$ twin shear can explain the observed habit orientation $\mathbf{p}'_1, m_1$ and to a lesser degree $\mathbf{d}'_1$, but it fails to account correctly for the orientation relationship. This failure and the good agreement for $g_2 = 0$ instead can be explained if the internal structure of the martensite plates is taken into account: It has been observed by transmission electron microscopy that the martensite plates contain twins on one side of the martensite-austenite interface only[8])[10]). This implies that a change in lattice orientation exists between the twinned and the untwinned region, provided the total twin shear is not taken up by shears on other systems. In the present model there is however no need for this to occur since the elimination of the twin shear requires only a small adjustment of g_1 in order to conserve an undistorted habit plane. The sharpest X-ray reflections are likely to result from the untwinned part, therefore it is not surprising that the measured orientation relationship agrees with the calculations for $g_2 = 0$ and not for $g_2 > 0$.

A further consequence of the composite martensite structure is that the habit planes on both sides of the piate should no longer be parallel if both remained undistorted. The question arises why the measured habit planes are those corresponding to an intermediate g_2 and not to $g_2 = 0$. The following argument is presented which also serves to give a reason for the existence of the composite martensite. It has been observed by transmission electron microscopy that in β-copper-zinc the martensitic transformation occurs in two steps[11]), first by the growth of thin platelets which subsequently thicken, both having the same (2, 11, 12) habit that is also observed for martensite in bulk. There is considerable evidence that the martensite in steels grows in the same way[12]). In the initial stage of the transformation thin platelets have been observed by transmission electron microscopy[10]). These plates have the same (225) habit as the fully grown thicker plates. (The thin plates are associated with faults on (111) planes which are thought to be the nucleation sites of the martensite[13]).) In the thin platelets the surrounding matrix exerts constraining forces which are reduced by lowering the amount of macroscopic shear m_1. But the introduction of twins increases the free energy of the martensite. Therefore g_2 is determined by the distortion energy and the total twin boundary energy and not by m_1 alone. For this reason the amount of the twin shear can be smaller than 0.1286, which would be required if m_1 had the smallest possible value. When the thin platelets thicken during the second stage of the martensite growth, the matrix constraints become less important and by eliminating the twin interfaces the driving force for the growth can be increased since the free energy is lowered. A martensite plate that stops growing after it has reached a constant thickness has its austenite-martensite interfaces parallel to the habit plane of the initial twinned platelet. If the elimination of the twin shear is not compensated for by the small change in g_1 the resulting orientation relationship may differ from that calculated for $g_2 = 0$. This effect may be responsible for the small deviations from the observed values (see table 1).

In conclusion, it has been shown that the crystallography of the (225) martensite in steels can be explained satisfactorily by a composite shear on a $(011)_M$ $[\bar{1}1\bar{1}]_M$ and a $(12\bar{1})_M$ $[\bar{1}11]_M$ system. The change from a (259) to a (225) martensite is essentially due to a change of the secondary shear plane from a $\{112\}_M$ to a $\{110\}_M$ plane. The additional twin shear serves only to reduce the amount of the macroscopic shear.

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Literature

1) M. S. WECHSLER, T. A. READ and D. S. LIEBERMAN, Trans. AIME **218** (1960) 202.
2) D. S. LIEBERMAN, Acta Met. **14** (1966) 1723.
3) J. S. BOWLES and D. P. DUNNE, Acta Met. **17** (1969) 677.
4) A. F. ACTON and M. BEVIS, Mater. Sci. Eng. **5** (1969/70) 19.
5) N. H. D. ROSS and A. G. CROCKER, Acta Met. **18** (1970) 405.
6) D. P. DUNNE and C. M. WAYMAN, Met. Trans. **2** (1971) 2327.
7) M. S. WECHSLER, D. S. LIEBERMAN and T. A. READ, Trans. AIME **197** (1953) 1503.

8) A. J. MORTON and C. M. WAYMAN, Acta Met. **14** (1966) 1567.
9) S. JANA and C. M. WAYMAN, Met. Trans. **1** (1970) 2825.
10) K. SHIMIZU and Z. NISHIYAMA, Met. Trans. **3** (1972) 1055.
11) R. RAPACIOLI and M. AHLERS, Scripta Met. **7** (1973) 977.
12) R. L. PATTERSON and C. M. WAYMAN, Acta Met. **14** (1966) 347.
13) M. AHLERS, to be published.

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