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Formation of α-Martensite Crystals with Habits (*hhl*) in Cryston Model

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Abstract. The mechanisms of formation of martensite with habit planes of the {*hhl*}-type are discussed for Fe-based alloys which undergo a γ-α (fcc-bcc) martensitic transformation. The relaxation of the lattice is interpreted in the framework of the "cryston" model. A "cryston" is the combination of dislocations of one or two slip systems which play the role of quasiparticles among the dislocation association on the mesoscale level. A number of cryston models of simple shear are presented. A possibility of the limiting transition to the cryston wave model is noted. Using the lath martensite as an example, it has been shown that using the cryston model allows to interpret morphological features of separated martensite crystals such as non-equivalence of parallel faces of lath crystals, deflection of orientation relationships from the ideal ones, the high residual density of dislocations. It is emphasized that the choice of prismatic dislocation loops as probable centers of martensite nucleation is a promising idea.

1. INTRODUCTION

After the formation of a martensitic crystal the resulting macrostrain has a shear character [1]. The shear is mainly effected along the habit plane (HP). In the majority of the cases the HP does not coincide with easy-slip planes neither of the initial nor of the final phases: the martensite lattice is rotated relative to the austenite one. Similar morphological attributes are observed in Ref. [2] and at the formation of macroshear-bands (MSB). In [2] it is shown that MSBs in the fcc single crystals arise at the stage of developed plastic deformation with the participation of two slip systems. Similarly, as noted in [3], at the intersection of two slip systems the formation of strain-induced martensite begins. It is natural to assume, that in both mentioned cases there are analogous physical carriers of macroshear. Plastic shear in a crystal, generally speaking, is connected with a carry of any discrete vectorial displacement from a spectrum of crystal lattice vectors. For the generalized carrier of such a shear the term "cryston" was introduced in [4]. That superdislocation-type carrier only in specific cases is reduced to the slip along a single plane. That is, a cryston is the carrier of displacements distributed in the volume connected to the co-operative movement on several planes of the same or different slip systems.

Let us be limited here for definiteness by consideration of orientations (*hhl*) of habits and plane borders of MSBs (designation of planes and directions are everywhere given in the basis of the fcc-lattice). We shall remind, that in systems containing up to 0.6w%C cooling-induced α-martensite exhibits typically habit planes close to (557) and for Fe-C with a C content in the interval (0.6 $\div$ 1.4)w% habits close to (225) occur. For the strain-induced martensite in iron-based alloys the displacement of poles of HP to [110] was observed, also. MSB borders of this type were observed in Ref. [2]. It is easy to show [4] that the resulting slip on (*hhl*) planes takes place at a quite determined relationship between dislocation numbers *n* and *m* with $[1\bar{1}0]$

dislocation lines and identical sizes of edge components of Burgers vectors and slipping on conjugate planes (111) and $(11\bar{1})$. Namely:

$$\frac{h}{l}=\frac{n\mp m}{n\pm m},\quad n, m = 0, 1, 2, 3, \ldots \tag{1}$$

Here the top signs concern to the case $n > m$, and bottom signs to $n < m$. For example, the pair $n = 6$, $m = 1$ (or multiples these) is adequate for the habit (557). For the habits (225) we have $n = 7$, $m = 3$, and for (110) and (001), $n = m$, see Eq. (1). The distance d_{hhl} between nearest (hhl) planes can be considerably less than the lattice parameter a: $d_{hhl}= a/(2h^2 + l^2)^{1/2}$ So, for $h/l = 5/7$ we obtain $d_{557} = a/3\sqrt{11} \approx 0.1a$.

2. CRYSTON MODELS OF SIMPLE SHEAR

We shall consider a number of models for a cryston carrying a simple shear which realizes the basic rotation of the α-martensite lattice. The direction of rotation axis coincides with $[\bar{1}10]$. If the main axis of the Bain compression is [001], this rotation leads to the Nishiyama orientation relationships. Such rotation is realized, in particular, by shear along the plane (111) in the direction $[11\bar{2}]$. In Fig.1 the triangle shaped region containing arrows corresponds to the intermediate position of a cryston which moves as whole from left to right; in this case the amount of shear is $\tan\psi_1 = \sqrt{2}/4$, and the rotation angle $\omega_1 = \tan^{-1}[(\tan\psi_1)/2] \approx 10°$. The arrows correspond to displacements which are a multiple of some minimum vector. For example, at the minimum vector $a[11\bar{2}]/4$ coinciding with the edge component of a Burgers vector of a 60°-dislocation the distance between two neighboring arrows is equal to $3d_{111} = a\sqrt{3}$. The number of arrows coincides with the number of dislocations (dislocation pairs) included in the cryston.

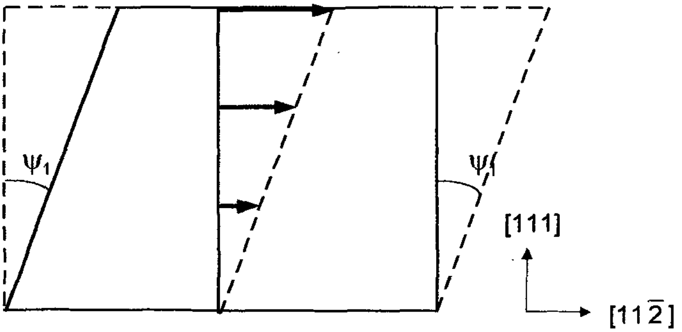

Figure 1: Cryston model for simple shear along the plane (111).

It is clear, that the position of a displacement vector on each of (111) planes results in the same shear with a minimum displacement of $a[11\bar{2}]/12$. It is possible to treat the last distribution of displacements as a collective movement of partial edge dislocations with Burgers vectors $a[11\bar{2}]/12$. However it is more natural to consider this as a nonlinear wave of located strain, as the dislocation nuclei are overlapped. Fast proceeding of the γ–α martensitic transformation is most likely connected to the participation of a cryston of such type.

According to Ref. [4] there is a tendency for 60°-dislocations with antiparallel screw components of Burgers vectors to be coupled, then the shear variant at which the minimal arrow on Fig.1 corresponds to the vector $a[11\bar{2}]/2$ is of interest. In this case the distance between the next displacement vector is equal to $6d_{111}$. The assumption that the cryston structure contains, mainly, pairs of 60°-dislocations results in interesting consequences which we shall consider with reference to the martensite with habits (557). As was marked above, the resulting shear on the plane (557) is connected with a cryston characterized by numbers $n = 6$, $m = 1$. It is obvious, that if 60°-dislocations are chosen, their total number is odd. For such a cryston the screw component of Burgers vector cannot be compensated such that it results in the Nishiyama orientation relationships. This is overcome if the numbers n and m are double using seven pairs of dislocations. Fig.2 illustrates the cryston model of shear along the (557) plane. The arrows are parallel to the $[7\ 7\ \overline{10}]$ direction; the minimal length of the arrows is equal to $a\sqrt{22}/4$; the distance between the nearest arrows is equal to $33d_{557} = a\sqrt{11}$.Once such a cryston has run, there will be the plate with thickness $d_{min}=6a\sqrt{11} \approx 20a$ in the direction [557]. Thus, the minimal value of the thickness of α-martensite crystal which has a habit (557) and which is associated with the propagation of a cryston containing coupled dislocations and which also satisfies the Nishiyama orientation relationships, is about $10a$.

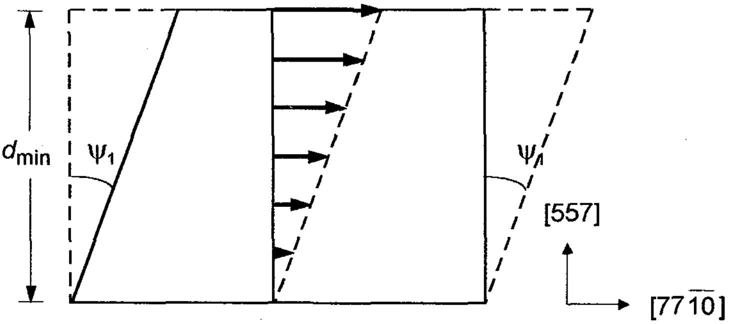

Figure 2: Cryston model of simple shear along the plane (557).

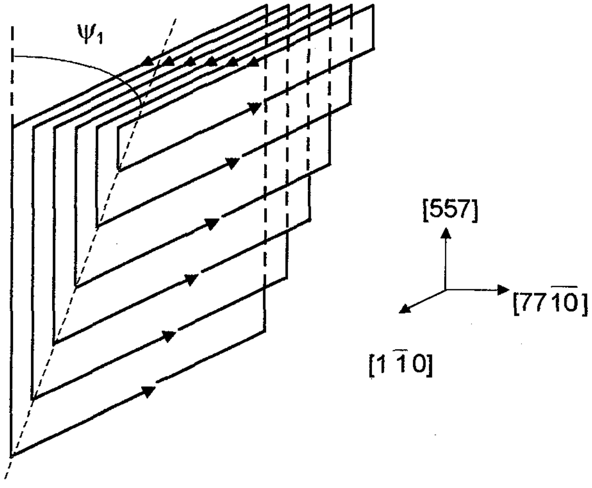

Figure 3: Cryston model of simple shear along the plane (557): distribution of prismatic dislocation loops.

The crystal size limits in [557] and in $[1\bar{1}0]$ directions corresponding with a cryston model based on dislocation loops (Fig.3), carrying out a joint prismatic movement. Certainly, the best model of cryston with reference to formation of cooling-induced martensite crystal is a nonlinear shear wave with displacements along all (557) planes in the localization area of the wave. The transition to such a wave in a dislocation model corresponds with overlapping of nuclei of strongly interacting dislocations in a connected state. Formally this transition in the model is indicated in Fig.3 by increasing the density of loops.

As was discussed in [5], the nonlinear transformation wave develops in the area, losing stability during propagation of controlling waves, carries the threshold strain $\varepsilon_{th} \sim (10^{-3} - 10^{-4})$. Cryston shear carriers detail the structure of displacement fields in the transformation wave carrying the strain on the orders exceeding ε_{th}. This indicates that three stages can be distinguished during formation of the cooling-induced martensite crystal: 1) heterogeneous origin in the elastic field of defect accompanied by excitation of controlling waves; 2) propagation of controlling waves; 3) relaxation of the lattice which lost stability by propagation of crystons. Although such division has little conditional character, it is useful because it reflects a circuit of cause-and-effect relationships.

It is obvious, that in the case of cooling-induced martensite the existence of crystons as carriers of shear is supported only at the expense of the difference between free energies of austenite and martensite lattices. When MSB is formed the energy comes from an external source. The formation of strain-induced martensite represents an intermediate variant.

3. TREATMENT OF A NUMBER OF MORPHOLOGICAL PECULIARITIES OF LATH MARTENSITE

Cryston models of shear allow to interpret peculiarities of morphology both of separate crystals and of their ensembles. For example, for lath martensite in [6] different type of boundary (557) surfaces of separate crystals (one is smooth, and second has a relief because of shear traces) was observed. This may be understood by taking into account that the break-down into i shear bands with thickness $d_i \ll d$ is favorable for martensite crystals having thickness $d \approx (0.1 - 1)\mu m$ and which are inside the sample. The presence of one smooth border means then, that the relaxation of lattice which lost stability began most likely with the propagation of a cryston carrying the shear along the (557) plane. While the shear steps on the opposite boundary are caused by a cryston carrying the shear along the (111) plane. The above mentioned is illustrated with Fig.4 where two bottom strips correspond to shear along the (557) plane, and the others correspond to shear along the (111) planes.

Moreover, in [6] a scatter in orientation relationships was noted. There both the Nishiyama orientation relationships and intermediate variants different from the Nishiyama orientation (within 2.5° towards the Kurdjumov-Sachs orientation relationships) were observed. Note that realization of intermediate relationships demands the additional rotation around the axis [111] through the angle $\omega_2 \le 2.5°$ This rotation can be carried out by means of a simple shear along the $(11\bar{2})$ plane in the $[1\bar{1}0]$ direction. The rough arrow scheme of appropriate crystons includes pure-screw dislocations with Burgers vectors $a[1\bar{1}0]/2$ and establishes the distance between the next arrows to about $8a$.

It is possible to admit that at the stage of relaxation of austenite area lost the stability the screw dislocations are born, mainly, in consequence of annihilation of edge components of a certain share of 60°-dislocations which enter into the composition of different carriers of the basic shear $\tan\psi_1$.This assumption allows to explain, on one hand, an insufficient density of screw dislocations in crystons-carriers of shear $\tan\psi_2$ to fulfill the Kurdjumov-Sachs orientation relationships, and on the other hand, a presence of significant residual density of screw dislocations $\rho_f \sim (10^{10} \div 10^{11})\mathrm{cm}^{-2}$ in the lath martensite. If it is considered that the formation of each pair of adjacent shear bands (arising at contrary run of crystons) with size $d_i \cong 10a$ was accompanied by generation of a screw dislocation pair, then the density of screw dislocations ρ is equal to $\rho = (2d_i d)^{-1} \sim (10^{10}\text{-}10^{11})\mathrm{cm}^{-2}$. Notice, that the occurrence of dislocations by pairs provides preservation of parity of the dislocation number within crystons. This condition is necessary to compensate the screw component in the cryston i.e. the carrier of the basic shear $\tan\psi_1$. The screw dislocation density correlates with the observed residual density of dislocations.

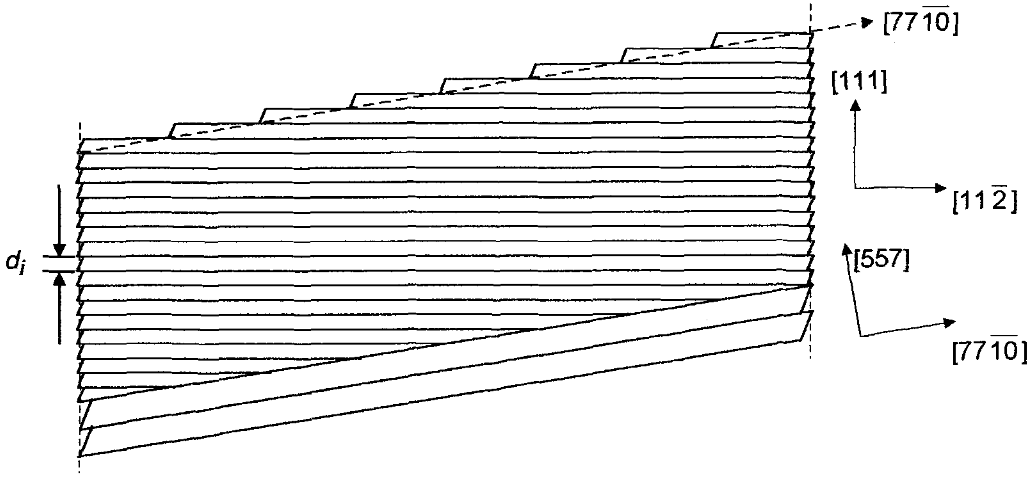

Figure 4: Cryston model for lath crystal with the habits (557). It can be seen that the lower surface is smooth whereas the upper one exhibits a relief.

The sweep of a cryston carrying the shear $\tan\psi_2$ in the band (with sizes $d_i \sim 10a$ and $d \sim (0{,}1\text{-}1)\mu\mathrm{m}$), where one screw dislocation is localized, results in rotation of the lattice through the angle $\omega_2 \cong 2°$.

Pairs of crystons with an odd number of dislocations in each of them can also participate in generation of carriers of the second shear $\tan\psi_2$. The interaction in such pair of carriers of shear $\tan\psi_1$ is accompanied by formation of one screw dislocation and a pair of crystons with an even number of 60°-dislocations whose screw components are compensated.

Note, that for laths in the near-surface area of the sample the resulting shear can be created by the sequential sweep of an ensemble of crystons, each of which has a smaller degree of localization of deformation in comparison with size d_i.

Summarizing the results by relating the cryston models to formation of a single lath martensite crystal, it is possible to describe the relaxation of an unstable austenite region in the form of a lath by ensembles of crystons which carry a shear deformation along one slip system, or along two slip systems. It is clear, that similarly crystons are equivalent as carriers of edge component of displacements and in an equal measure can participate in generation of screw dislocations.

Note, that the carriers of the basic shear $\tan\psi_1$ can include dislocation pairs containing all three 60°-dislocation lines laying in the close-packed plane, with which the given package of crystals is associated. Therefore four crystal connection types, observable inside the package [7], are explained within the framework of the unified concept of dislocation nucleation. Namely, the nucleation center of conjugated crystal is one of 60°-dislocations included in the constitution of cryston, the carrier of the basic shear in the initial crystal. It should be specified, that here a package is considered to be a set of crystals (with up to 6 different orientation) with habits close to {557}, making the least angle with one of four planes {111}.

The small fraction of dislocations from the additional slip system predetermines the observable tendency of separation of crystals which belong to the same package. However, it is important that the presence of dislocations from the additional slip systems in crystons permits at once to indicate all regular connections of crystals belonging to different packages. Thus, it is possible that an austenite with few 60°-dislocations (in the limiting case, with only one) is transformed in a self-catalytic manner to an ensemble of packed martensite crystals with the complete set of possible orientations.

In the case of strain-induced martensite which is formed in the plastic flow stage the cryston model permits to explain the tendency to form the {110} habits because the most efficient way of relaxation of external stresses is realized by the generation of small crystals of α-phase [4].

4. CONCLUSION

The model of simple shear is represented perspective for the description of a final phase of martensitic transformation, at the treatment of morphological peculiarities of both separate martensitic crystals and their ensembles. For example, the possibility to calculate elastic fields of prismatic loops capable to play the role of more realistic centers (in comparison with infinite dislocations) of martensite nucleation is obvious. The first results obtained in this direction show, in particular, that the most probable centers of nucleation for crystals with (225) habit planes are prismatic loops.

The use of the cryston model is constructive because it reveals that the physical carriers of located plastic deformation, the crystons, can describe the shear processes in a wide range of spatial scales.

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