Reconstruction of Martensitic Nucleation Process from Morphological Attributes

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Abstract

Within the framework of the concepts of heterogeneous nucleation and wave growth of martensite the refinement of a technique of account of wave normals N_w to expected habits planes are carried out. The technique allows to connect orientations of N_w with definite areas of nucleation of crystals in an elastic field of defects. The specific results are presented for system Cu-Zn. As separate rectilinear dislocations with lines [1 1 $\bar{1}$] and dislocation loops basic elements of which are pieces of these lines are considered here as probable centers of nucleation. It is shown, that the spectrum of N_w can be coordinated with experimentally observable space distribution of normals N_e in a vicinity of a pole [2 11 12]. The similar coordination opens additional opportunities to reconstruct a stage of martensite nucleation from morphological attributes and to transform a distribution of habits in the informative parameter.

1. INTRODUCTION

At the present time, there are serious objections to consider that in many cases the formation of martensitic crystal on a mesoscale is controlled by the atom displacement waves [1]. The excitation of waves occurs at the initial stage through the heterogeneous nucleation of martensite in the elastic fields of some defects. The good results take place already for the individual dislocations [2,3]. The initial excited state takes the form of elongated rectangular parallelepiped which is constructed on the eigenvectors $\vec{\xi}_i$ (i = 1,2,3) of the elastic deformation tensor of dislocation. The respective eigenvalues ε_i satisfy the conditions:

$$\varepsilon_1 > 0, \quad \varepsilon_2 < 0, \quad |\varepsilon_3| << \varepsilon_1, \varepsilon_2 \tag{1}$$

It will be recalled that the fulfillment of (1) ensures an existence of weakly distorted (or invariant if $\varepsilon_3 = 0$) planes with normals N. Both ε_i and $\vec{\xi}_i$ are the functions of the polar angle θ which lies in the plane perpendicular to the dislocation line and is measured from the slip plane. Again, ε_i are directly proportional to the ratio b/r where b is the magnitude of Burgers vector of the parent phase dislocation and r is the distance between the dislocation line and the point where the elastic field is calculated. The parameter b/r~a/r (a is the lattice constant) is considered to be small in comparison with unity. It is suggested that there is the excitation of quasilongitudinal waves vibrating in antiphase and having the normals n_1, n_2 being close to $\vec{\xi}_1$, $\vec{\xi}_2$ therewith the line of intersection of two wave fronts is parallel to $\vec{\xi}_3$. Then the prototype of the habit plane is identified with the plane which is drawn due to the movement of the front intersection line. Such a plane have the normal

$$N_w \| n_2 \pm x\, n_1, \quad |n_{1,2}| = 1, \quad x = c_2/c_1. \tag{2}$$

where c_1, c_2 are the velocities of quasilongitudinal waves. Because one of the waves transfers the compression deformation and the second - the tension one [1], the deformation of the kind (1) will be transferred in the wave regime.

Previously the concrete calculations of N used the approach:

$$N \parallel \vec{\xi}_2 \pm k\vec{\xi}_1 , \qquad k \approx (\varepsilon_1 / |\varepsilon_2|)^{1/2} , \qquad (3)$$

which is formally quite reasonable for $|\varepsilon_i| \ll 1$. However in this approach the orientation of N is found to be independent on r and, consequently, any possibility to estimate a space localization of initial state gets lost. As a result the analysis was restricted only to the establishment of the martensite nucleus localization on the polar angle θ.

By this means, for each dislocation it is possible to receive a spectrum of N and N_w, depending on the interval of corners θ and procedure of a choice of normals n_1 and n_2. The good consent between N_w and the averaged orientations of normals to the observable habits

N_e is resulted already in approximation of simple equality $n_1 = \vec{\xi}_1$, $n_2 = \vec{\xi}_2$. Nevertheless, if to put by the purpose the description of all observable distribution of N_e, it is desirable to specify a procedure of selection n_1, n_2 and to consider the dependence of orientations N_w, N on the complete set of coordinates of area of localization of initial exited state in the case of more realistic configuration of dislocation nucleation center. Taking into account a good conformity of results of account for separate rectilinear dislocation, it is natural to consider the dislocation loops, basic elements of which are pieces of lines of appropriate dislocations as dislocation nucleation centers (DNC). The similar approach allows to treat the observable distribution of N_e as the consequence of varying of coordinates of martensite nucleation areas in the elastic fields of defects.

2. UPDATING A TECHNIQUE OF ACCOUNT

The problem of the space localization was discussed in [4] in the context of the existence of minimum critical size of the parent phase grain. Clearly [2], that the area of nucleation is defined by the fulfillment of two conditions which are the condition of threshold deformation in an elastic field of DNC and the condition of generation of waves controlling the martensite crystal growth. We shall remind [1], that the fulfillment of the generation condition is only possible for waves with frequencies smaller then Debay's ones by the order of magnitude. Therefore the critical (minimum) cross size d of initial exited state area , capable to result to growth of a crystal (with the thickness d) in a wave mode makes up tens of lattice parameters. On the other hand, by consideration DNC as of power center in a field of which there is the nucleation of martensite crystal, the size d should be though on the order less than distance r up to DNC [2]. It follows that the minimum values of coordinate r of nucleation area which is physically interesting for realization of the wave growth mechanism make up hundreds of lattice parameters. Means, the indirect data about coordinates of nucleation area at $r \geq 10^2 a$ may be received by investigating the change of orientations of N and N_w depending on coordinates of area of nucleation and comparing their orientations with orientations of N_e.

It is interesting to estimate in this connection how strongly does the space dependence of N and N_w influence the selection of probable DNC of martensite? For infinite dislocations in the field of applicability of the theory of elasticity such influence should be weak. To calculate that, it is necessary, at first, to write the expression for k in (3) in the general form:

$$k = \frac{1 - |\varepsilon_2|}{1 + |\varepsilon_1|} \cdot \left[\frac{\varepsilon_1}{|\varepsilon_2|} \cdot \frac{2 + \varepsilon_1}{2 - |\varepsilon_2|} \right]^{1/2} . \qquad (4)$$

Secondly, it is necessary to take into account, that the eigenvectors of the deformation tensor $\vec{\xi}_i$ undergo the rotation, caused as a consequence of the antisymmetric part ω_{ij} of the distortion tensor χ. That is, in (3) it is necessary to replace $\vec{\xi}_i$ by $\vec{\xi}_i'$ where

$$\vec{\xi}_i' = Q\vec{\xi}_i, \qquad | \vec{\xi}_i' | = 1. \qquad (5)$$

In (5) Q is an orthogonal matrix correlated with ω_{ij}. Then, in the framework of the simplest model of the crystal growth control (the wave normals n_1, n_2 coincide with the orientations of the vectors $\vec{\xi}_1'$, $\vec{\xi}_2'$) the expression for N_w' is:

$$N_w' \parallel \vec{\xi}_2' \pm x'\vec{\xi}_1', \tag{6}$$

where x' is the ratio between the wave velocities in the new directions.

It must be stressed that both the components of the tensor ω_{ij} and the values ε_i are proportional to the ratio b/r, where b is the module of Burgers vector. It is obvious that the essential change of the orientations N and N_w compared with the orientations (3) at $r \sim 10^2 a$ can be obtained only with superdislocations with Burgers vectors $b \sim 10a$, when ε_i, $\omega_{ij} \sim 0.1$. Certainly, this estimation falls outside the limits of applicability of the theory of elasticity and its use is justified only at a qualitative level in order to reveal the tendency of change of N and N_w.

In order to describe the procedure of selection of normals n_1, n_2, behind the approximation $n_1 = \vec{\xi}_1'$, $n_2 = \vec{\xi}_2'$, it is possible to use a less rigid condition

$$\vec{\xi}_1' \parallel n_1 + e_1 , \quad \vec{\xi}_2' \parallel n_2 + e_2 , \tag{7}$$

where e_1, e_2 are the vectors of polarization of quasilongitudinal waves. The vector $(n + e)$ sets one of the main directions of deformation tensor of a plane wave. Therefore the condition (7) is carried out for a cone of directions of wave normals n_i (close $\vec{\xi}_i'$) of quasilongitudinal waves having the main axis corresponding to a tension (or compression) whose orientation coincides with one of the appropriate axis of the elastic field of DNC. The n_i satisfying (7) have been obtained with an angular accuracy of 1 minute (at known elastic modules) by the method of consecutive approximations on the basis of the Christoffel equation. It is obvious, that using the N_w from the formula (2), the condition (7) and with x' in place of x, results in directions of N_w close to the direction of N_w' calculated with the help of (6). Thus, condition (7) reflecting roughly the inheriting by wave controlling process of orientations of main axes of tension and compression in the field of nucleation allow a little to expand the range of deviations N_w from N.

We shall notice, that the comparison with observable orientation of N_e has to be conducted just for the normal N_w. Really, in the non-uniform elastic field of DNC, strictly speaking, in different areas the different local orientations of N are realized. So the extensive surfaces of interface contact are formed during propagation of wave controlling process. Nevertheless, it is natural to assume that N and N_w are close in the nucleation area and to use this condition to specify the criterion of selection. We shall remind the distortion at deformation with one invariant plane, favorable for the interface contact, is described by the diad

$$\chi = S \cdot N, \tag{8}$$

where N is the normal to the invariant plane, and S is the vector of shear. The distortion tensor can always be spread out on the sum of three diads. It is obvious, that if the module of the vector S for one of the diads is greater than two other modules of shear vectors in some area of the elastic field of DNC, then χ takes a form close to (8). Therefore, the condition $S \approx S_{max}$ can be used as one of a selection criteria of N (and, hence and $\vec{\xi}_1'$, $\vec{\xi}_2'$). The condition of local maximum of relative change of volume δ could be used as the second criterion of nucleation area selection effective for phase transition of the first order in the rigid lattice of initial phase. It is convenient to consider the results of such approach at the beginning for rectilinear infinite dislocations and then to apply it to the dislocation loops.

3. RESULTS AND DISCUSSION

For infinite rectilinear dislocations in the range of values of the parameter $a/r < 0,01$, the most interesting from the point of view of transformation physics, it is necessary to expect the weak dependence of orientations of N, N_w and N'_w on a/r. Therefore, for such dislocations it is possible to limit the comparison of N_e and N_w, as functions of parameter θ calculated by the specified technique.

Let us present here the results for an Cu - 42%Zn alloy which exhibits the shape memory effect and undergoes a cooling-induced bcc-fct martensitic transformation. As was discussed in [5], the dislocations with lines $[11\bar{1}]$, planes of sliding (011) and Burgers vectors $\mathbf{b}_1 \parallel [11\bar{1}]$, $\mathbf{b}_2 \parallel [01\bar{1}]$, $\mathbf{b}_3 \parallel [100]$, $\mathbf{b}_4 \parallel [1\bar{1}1]$ are the most probable DNC in this alloy. The elastic field of DNC was calculated by the technique [6] for the elastic moduli: $C_L = 208,15$ GPa, $C_{44} = 85,50$ GPa and $C' = 6,35$ GPa [7]. The condition $\mathbf{S} = \mathbf{S}_{max}$ [6] is carried out, for example, for $\theta = 0°$, but then $\delta = 0$, whereas the nearest local maximum of δ corresponds to $\theta \approx 13°$. The analysis of the dislocation elastic field have shown that the agreement between $N_e^0 \parallel [2\,11\,12]$ and N_w takes place at $\theta \sim 5,4°$ for $\delta > 0$. Note, that the orientation of the normal of the weakly distorted plane N nearest to N_e is obtained at $\theta = 7°$. However N remains orthogonal to the dislocation line and basically cannot coincide with the $[2\,11\,12]$ direction. Though the distinction between N_w and N is insignificant, it testifies still for the benefit of selection N_w. Fig.1 shows the fragment of the stereographic projection for described case. Numbers $i = 1,2,3,4$ mark lines, representing the orientations N'_w when changing θ in an interval $0°$-$11°$ for the infinite dislocations and the intersection determines the pole $N_e^0 \parallel [2\,11\,12]$. The narrow areas 1 and 2 in Fig.1a gives an idea of the weak dependence on parameter a/r; their left borders correspond to $a/r = 10^{-4}$ and their right ones to $a/r = 10^{-2}$. In Fig.1b the lines 3, 4 correspond to $a/r = 10^{-2}$. The normals N_w deviate $1,5°$ from N'_w and are not distinguished in figures. Consequently, the calculated set of N_w for infinite dislocations is concentrated in a rather narrow area including N_e^0 and located, mainly, to the left of the line connecting the poles N_e^0 and the $[011]$ direction. The dotted lines in Fig.1a,b determine the orientations of N'_w for superdislocations $(b_i \sim 10a)$ at $r = 10^2 a$. It is clear that for dislocations with vectors $\mathbf{b}_1$, $\mathbf{b}_2$ gravitating to screw orientation, the transition to superdislocations (as well as the reduction of r) reveals the tendency to the displacement of N_w in the area to the right of the line $[2\,11\,12]$ - $[011]$. On the contrary, for $\mathbf{b}_3$, $\mathbf{b}_4$ gravitating to the edge orientation, the increase of the displacement of N_w to the left from the pole $[2\,11\,12]$ is observed. It should be noted that the realization of orientations, indicated by a dotted line is obtained most likely from the slow growth of crystals with dislocations lines $[11\bar{1}]$.

Like the orientation of $N_e^0 \parallel [2\,11\,12]$ is averaged among the set of N_e, there are orientations located at the left, and to the right of the line N_e^0 - $[011]$ (see [8]) and the area of the observable N_e to the left of a line N_e^0 - $[011]$ appears wider than the area of orientations of N_w calculated for infinite dislocations. To interpret this result without using the superdislocations, it is necessary to search the explanation from a specification of the DNC configuration.
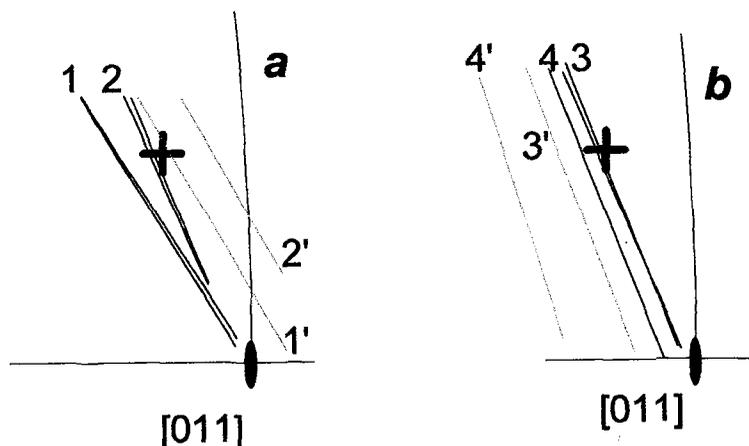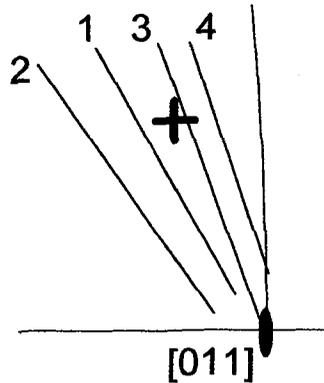
Figure 1: Position of poles N'_w relative to the pole [2 11 12] for DNC based on infinite dislocations with *Burgers* vectors: a) $b = b_1$, b_2; b) $b = b_3$, b_4.

As physically acceptable simple configurations, rhomboid and rectangular dislocation loops were considered. The basic elements of loops were pairs of pieces of lines L_1 along the $[11\overline{1}]$ directions. In the case of loops sliding in the plane (011), additional pairs of pieces of lines of length L_2 are included: $L_2 \parallel [1\overline{1}1]$ and $L_2 \parallel [100]$ (rhomboid loops) or $L_2 \parallel [2\overline{1}1]$ (rectangular loops). Prismatic loops got out of the rectangular form with $L_2 \parallel [011]$. The origin of the cylindrical coordinate system was located at the center of the loop or in the middle of the line $[11\overline{1}]$; the polar corner θ was measured from the loop plane; the axis OZ was directed along the $[11\overline{1}]$ direction. For the prismatic loops the cases of surplus ("plate") and missing ("hole") material inside a contour of a loop were considered. The sizes of loops are comparable with the critical size of a grain (about 1µm). For example, for the results presented below, the lengths of the loop sides were: $L_1 = 7000a$, $L_2 = 1000a$.

Calculations of elastic fields of slipping loops with $r = (200 - 1000)a$ and small angles θ, lead to a multitude of orientations of N_w which covers on the stereographic projection the areas 1 and 2 (Fig.1a). Note that poles to the right of line [011]-[2 11 12] are not included.

A different situation corresponds to the prismatic loops. The normals N_w for the case $b = b_4$, $z = 0$ (basis is in the center of the line $[11\overline{1}]$) are shown in Fig.2: the curves 1 ($r = 200a$) and 2 ($r = 400a$) relate to the "plate"-type loop for angles θ ranging from 80° to 90° and the curves 3 ($r = 200a$) and 4 ($r = 400a$) - to the "hole"-type loop for angles θ ranging from 90° to 100°. At $b = b_3$ and $r = 200a$ the spectrum of N_w is displaced accordingly to the left ("plate") and to the right ("hole") in an appreciable way in comparison with curves 1 and 3 in Fig.2. Thus at $b = b_{3,4}$ for prismatic loops the essential expansion of area of orientations of N'_w in the vicinity of the pole [2 11 12] is reached in a narrow range of values of r without using superdislocations. In this case the area to the left of the line [011] - [2 11 12] is related with a "plate"-type DNC and to the right - with a "hole"-type DNC.

It should be noted also that for prismatic and sliding loops the orientations of N_w in the vicinity of the pole [2 11 12] at $z = 0$ found above, are not practically changed for values of z up to ±2500a. This means that the condition for the formation of the initial exited state in the form of elongated parallelepiped are kept in certain areas of the elastic field created by the loop.

Figure 2: Position of poles N'_W relative to the pole [2 11 12] for DNC based on prismatic "plate"-type (curves 1 and 2) and "hole"-type (curves 3 and 4) dislocation loops with Burgers vectors $b = b_4$.

4. CONCLUSION

The specification of a technique to account for normals N_W and the use of dislocation loops as centers for martensite nucleation, expand the opportunities for the interpretation of the observable spectrum of orientations N_e. In particular, the results obtained for the Cu-Zn system show that martensite crystals with habit plane orientations in the vicinity of the pole [2 11 12] can be formed by nucleation in the fast wave mode on distances $r = (200-400)a$ from prismatic dislocation loops (with unit Burgers vectors) whose basic element are lines of the close-packed [11 $\bar{1}$] direction; in so doing the area to the left of the pole is connected with the nucleation near the "plate"-type loops and the area to the right, with nucleation near the "hole"-type loops. Thus, the comparison of complete sets of experimentally observed orientations of N_e and calculated wave normals N_W becomes the tool for reconstruction of a physical picture of the martensite nucleation regime.

Acknowledgments

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