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CRYSTAL DYNAMICS OF FORMING ε-MARTENSITE WITH $\{334\}_\alpha$ HABITUS PLANES IN TITANIUM

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Formation of crystals with $\{334\}_\alpha$ habitus planes often observed in titanium during the BCC-HCP (α–ε) reorganization is considered in the context of the dynamic theory of martensitic transformations. It is demonstrated that the fast wave growth of the crystals is started in elastic fields of edge dislocations with lines $<1\bar{1}0>_\alpha$ and Burgers vectors $<001>_\alpha$.

Keywords: dynamic theory, martensite, titanium, $\{334\}_\alpha$ habitus plane.

INTRODUCTION

During martensitic transformations (MT), it is convenient to identify crystals via their morphological parameters related with each other due to the action of the common control process. In the dynamic approach first applied to the γ–α MT in iron alloys [1, 2], the most convenient and evident is a description of the habitus planes (HPs). In this case, it is suffice to consider the threshold regime without transition to finishing strains.

In the theory [1, 2], the HP has purely dynamic interpretation. It is enclosed by the moving line of crossing of superimposed fronts of wave beams propagating in orthogonal directions and bearing flat tension ($\varepsilon_1 > 0$)-compression ($\varepsilon_2 < 0$) strain possessing invariant planes (with strain $\varepsilon_3 \approx 0$). It is important that at small strain values (threshold strain values ε_{1th} and $|\varepsilon_{2th}|$ are smaller than the elastic limit $\varepsilon_{e\ell} \sim (10^{-4}–10^{-3}) << 1$), their ratio is close to that of the squared velocities of the wave beams:

$$æ = \approx v_2/v_1 \ \sqrt{\varepsilon_1/|\varepsilon_2|}\,, \tag{1}$$

where the velocities v_2 and v_1 can be calculated from the Christoffel equation [3]. Investigations of the BCC-HCP (α–ε) transformations [4, 5], like the FCC-BCC transformations [6, 7], demonstrated that the ratio of strains established in the threshold regime is preserved in the case of development of final strains in the lattice that has lost stability. It is essential that during the α–ε transformation, the flat strain provides the fastest transformation of the $\{110\}_\alpha$ plane into the basic $\{0001\}_\varepsilon$ plane of the HCP lattice. The symmetry of the arrangement of atoms leads to the coupling equation between the tension and compression strains that allow final values of two transformation strains to be determined in combination with Eq. (1). As a result, all observable macroscopic morphological parameters can be described as functions of the ratio of the control wave velocities. The short-wavelength reorganization of the transformed planes that does not affect the macroscopic morphological parameters finishes the transformation.

Recall that in [4, 5], the most symmetric variant was analyzed in which the unit vectors $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$ of the control waves were chosen strictly along the symmetry axes of the second and fourth orders, that is, $\boldsymbol{n}_1 \| [110]_\alpha$ and $\boldsymbol{n}_2 \| [001]_\alpha$. Then the application of the elastic moduli C_{11} = 134 hPa, C_{12} = 110 hPa, and C_{44} = 36 hPa for the BCC titanium single crystal at a temperature of 1238 K taken from [8] allows us to find the unit vector $\boldsymbol{N}_w$ to the HP close to $[22\bar{3}]_\alpha$ (the component with $[22\bar{3}]_\alpha$ has an angle of ≈0.7°) from the formula (see [1, 2])

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$$\boldsymbol{N}_{\mathrm{w}} \parallel (\boldsymbol{n}_2 - æ\, \boldsymbol{n}_1) \quad (2)$$

for $\boldsymbol{n}_2 = [00\bar{1}]_\alpha$ and $\boldsymbol{n}_1\sqrt{2} = [110]_\alpha$.

Though orientations <223>$_\alpha$ are also observed, orientations $\boldsymbol{N}_{\mathrm{w}}$ close to <334>$_\alpha$ are more often in the literature. It should be noted that attention in [4, 5] was focused on principle questions, and investigation of extremums of elastic fields of dislocation nucleation centers (DNC), important for choosing directions of unit wave vectors $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$ of the control waves were not carried out. Therefore, the present work considers this choice and demonstrates what DNC can be juxtaposed with crystals having the most often observed habitus planes.

ANALYSIS OF THE ELASTIC DNC FIELD WITH THE <1 $\bar{1}$ 0>$_\alpha$ LINE AND EDGE ORIENTATION OF THE BURGERS VECTOR

Let us accept by analogy with [4, 5] that the role of the DNC is played by rectilinear segments of dislocation lines. Since in the BCC crystals there are three systems of planes with approximately equal occupation densities, two of them, namely, $\{110\}_\alpha$ and $\{112\}_\alpha$ comprise <110>$_\alpha$ as crossing lines, DNC with <110>$_\alpha$ lines naturally arise as a result of contact interaction of dislocations with different sliding systems when intersecting the sliding planes of sliding loops. Such DNC are characterized by the superposition of the Burgers vector and hence can create more intensive elastic fields. Obviously, this circumstance together with the requirement for the fastest crystal growth predetermines the choice of the DNC with lines $\boldsymbol{\Lambda} \parallel$ <1 $\bar{1}$ 0>$_\alpha$, though the dislocation lines typical of the BCC lattice are collinear with the most dense directions <111>$_\alpha$.

Let us consider the edge orientation of the Burgers vector $\boldsymbol{b}$ at which the formation of crystals with HP of the form $\{hh\ell\}_\alpha$ is expected. Naturally, preference should be given to such $\boldsymbol{b}$ at which extremums of elastic field tension and compression correspond to orientations of the eigenvectors $\xi_{1,2}$ of the strain tensor $\hat{\varepsilon}$ having directions close to $[110]_\alpha$ and $[001]_\alpha$. Recall [1, 2] that the synthesis of concepts of heterogenic nucleation and wave growth of the martensite crystal assumes, along with Eq. (1), fulfillment of the following conditions:

$$\boldsymbol{n}_1 = \xi_1,\ \boldsymbol{n}_2 = \xi_2. \quad (3)$$

First of all, the elastic fields were analyzed for several standard orientations $\boldsymbol{b}$. Thus, $\boldsymbol{b} \parallel [110]_\alpha$, $[111]_\alpha$, $[112]_\alpha$, and $[001]_\alpha$ were considered for $\boldsymbol{\Lambda} \parallel [1\bar{1}0]_\alpha$. The limiting case from the four cases considered above corresponds to the simplest variant of the interaction of two dislocation loops with crossed sliding planes. Indeed, two loops lying, for example, in the $(112)_\alpha$ and $(11\bar{2})_\alpha$ planes with orientations of the Burgers vectors typical of the BCC lattice (along $[11\bar{1}]_\alpha$ and $[111]_\alpha$, respectively) are intersected along $\boldsymbol{\Lambda} \parallel [1\bar{1}0]_\alpha$, and the formed DNC are characterized either by the sum ($\boldsymbol{b}_1 \parallel [110]_\alpha$) or by the difference ($\boldsymbol{b}_2 \parallel [001]_\alpha$) of the Burgers vectors. It is pertinent to emphasize that, according to the Franck criterion, the case $\boldsymbol{b}_2 \parallel [001]_\alpha$ corresponds to a decrease in the elastic energy of interacting dislocations. Therefore, the case in point is most probable, especially when the material undergoes transformation at sufficiently high temperatures and hence dislocations in the initial α-phase are sufficiently mobile for implementation of the reactions with decreasing energy.

Nevertheless, it is useful to compare the angular dependences of the eigenvalues ε_i (i = 1, 2, 3) of the strain tensor $\hat{\varepsilon}$ for $\boldsymbol{b}_1 \parallel [110]_\alpha$ and $\boldsymbol{b}_2 \parallel [001]_\alpha$. It is convenient to illustrate the discussion by the results of calculations of the elastic field of the rectangular loop with side orientations $\boldsymbol{\Lambda}_1 \parallel [1\bar{1}0]_\alpha$ and $\boldsymbol{\Lambda}_2 \parallel [110]_\alpha$ and the corresponding lengths (in units of the lattice parameter) $L_1 = 7 \cdot 10^3$ and $L_2 = 10^4$ at the distance $R = 10^3$ from the center of the side $\boldsymbol{\Lambda}_1$. The angle θ is counted from the plane of the $(001)_\alpha$ loop. It is clear that the prismatic loop corresponds to the case $\boldsymbol{b}_2$, and the loop capable of sliding corresponds to the case $\boldsymbol{b}_1$.

A comparison demonstrates that in both cases, it is possible to juxtapose definite regions of angular elastic field localization with the habitus planes $(33\bar{4})_\alpha$ and $(334)_\alpha$. However, this region has an extremum point for the compression strain at $\boldsymbol{b} \parallel \boldsymbol{b}_2$. In addition, it is important that at $\boldsymbol{b} \parallel \boldsymbol{b}_2$, the conditions of negative change of the specific volume (which is natural during reorganization upon cooling into a more densely packed lattice) together with the

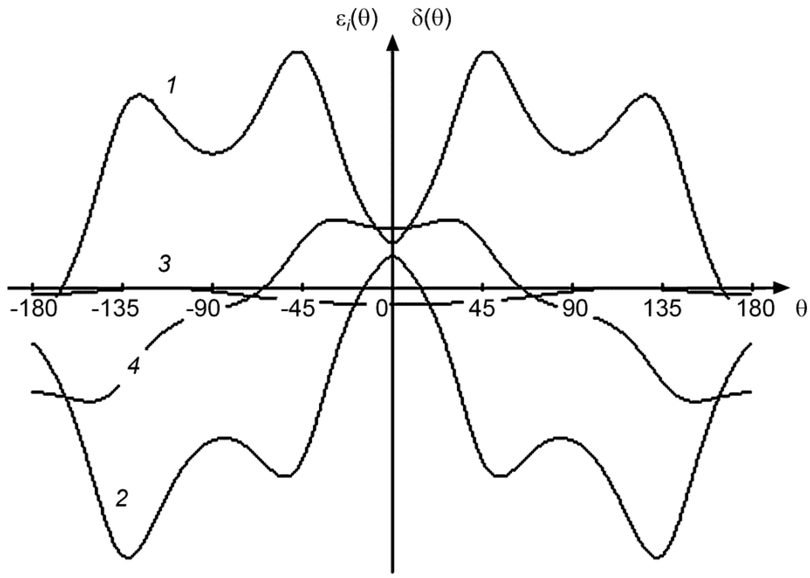

Fig. 1. Dependences $\varepsilon_i(\theta)$ (curves *1*, *2*, and *3*) and $\delta(\theta)$ (curve *4*).

proximity of the tension axis to $[110]_\alpha$ and of the compression axes to $[001]_\alpha$ are satisfied. The above-indicated selection conditions are not satisfied simultaneously at $\boldsymbol{b} \parallel \boldsymbol{b}_1$. Therefore, Fig. 1 shows the data only for $\boldsymbol{b} \parallel \boldsymbol{b}_2$.

For $\boldsymbol{b} \parallel \boldsymbol{b}_2$, $\boldsymbol{N}_w$ coincides with $[33\bar{4}]_\alpha$ (to within the one hundredth degree) at $\theta_1^* \approx -139°$ and $\theta_1^{**} \approx 133.5°$. In turn, $\boldsymbol{N}_w$ coincides with $[334]_\alpha$ at $\theta_2^* \approx -133.5°$ and $\theta_2^{**} = 139°$. Here θ_2^* and θ_1^{**} correspond to maximum values of compression $|\varepsilon_2|_{max}$ (see curve *2* in Fig. 1), and θ_1^* and θ_2^{**} are shifted toward the *plateau* of the minimum relative change of the volume δ (curve *4* in Fig. 1) with the points $\theta_\delta \approx \pm 147°$ nearest to θ_1^* and θ_2^{**}. The presence of pairs of angles (for example, θ_1^* and θ_2^*) for which $\boldsymbol{N}_w$ coincides either with $[33\bar{4}]_\alpha$ or with $[334]_\alpha$ is quite natural if we consider the possibility of changing the direction of any of the unit vectors $\boldsymbol{n}_{1,2}$ into the opposite one in Eq. (2). We now write down the orientations of vectors $\xi_{1,2}$ at θ_1^* and θ_2^*:

$$\xi_1(\theta_1^*) = [-0.706578 \quad -0.706578 \quad -0.0038671],$$

$$\xi_2(\theta_1^*) = [0.00273446 \quad 0.00273446 \quad -0.9992520], \tag{4}$$

$$\xi_1(\theta_2^*) = [0.706578 \quad 0.706578 \quad -0.0038671],$$

$$\xi_2(\theta_2^*) = [-0.00273446 \quad -0.00273446 \quad -0.9992520]. \tag{5}$$

It is obvious that Eqs. (4) and (5) can be derived from the pairs of symmetry axes $[-1/\sqrt{2} \;\; -1/\sqrt{2} \;\; 0]$, $[00\bar{1}]$ and $[1/\sqrt{2} \;\; 1/\sqrt{2} \;\; 0]$, $[00\bar{1}]$ rotated about the $[1\bar{1}0]$ axis through equal small angles, but in opposite directions. From here it is clear that Eqs. (4) and (5) differ due to the opposite direction of the vector $\xi_1(\theta_2^*)$. It is also clear that the angle $\theta^* \approx (\theta_1^* + \theta_2^*)/2$ to which the exact coincidence of the tension and compression axes with the symmetry axes $[110]_\alpha$ and $[001]_\alpha$ corresponds lies between θ_1 and θ_2^*.

Recall that the fact that the wave vectors lie in the symmetry plane $(1\bar{1}0)_\alpha$ provides its fastest reorganization and incorporation into the orientation relationship with orientation orthogonal to the habitus.

CONCLUSIONS

The treatment of formation of ε-martensite crystals with often observed habitus planes $\{334\}_\alpha$ has naturally and unambiguously been explained in the context of the dynamic theory of forming martensitic crystals as a consequence of the fastest transformation of the plane $\{1\,\bar{1}\,0\}_\alpha$. The DNC with lines $\mathbf{\Lambda} \parallel \langle 1\,\bar{1}\,0\rangle_\alpha$ and the Burgers vectors with the edge orientation $\langle 001\rangle_\alpha$ are juxtaposed with them. The directions of the unit vectors that control over the wave reorganization are selected from the extremum of the compression strain of the elastic DNC field. The formation of crystals with other (more rarely observed) orientations of the habitus planes will be discussed separately in our future work.

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