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THEORY OF METALS

Elastic Fields of $(774)_\gamma[4\ 4\ \overline{14}]_\gamma$ Crystons and the Formation of a Lath Structure of Bainitic Ferrite

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Abstract—An analysis has been performed for elastic fields of crystons that simulate the carriers of shear deformation on planes close to the habit plane of the additional-to-$\{558\}_\gamma$ component of the bimodal distribution of ferrite habits in a bainite macroplate. The conclusion has been drawn that the additional component arises according to the same mechanism as the main component, but in the region of austenite with a twin orientation.

Keywords: bainitic ferrite, dynamical theory, cryston, elastic fields, lath crystals, bainitic-ferrite macroplate

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1. INTRODUCTION

As has been noted in the literature (see, e.g., [1, 2]), a macroplate of bainite can represent a packet of crystals of the α phase in the form of laths. It is interesting [2] that such a packet is characterized by the presence of crystals with habits of two types. One variant of habits is close, according to literature data, to the variants of the $\{hh\ell\}_\gamma$ type with $h < \ell$ (e.g., $\{223\}_\gamma$, $\{335\}_\gamma$, $\{557\}_\gamma$, $\{558\}_\gamma$), which is typical of lath martensite. According to [3], the second variant of habits, is close to $\{0.373\ 0.663\ 0.649\}_\gamma$. In the approximation of small integer Miller indices and the equality of two largest indices, this variant is intermediate between $\{477\}_\gamma$ and $\{599\}_\gamma$.

Just as in [4], we will assume that the lath crystals are formed in the supersonic regime via the martensitic mechanism [5, 6]. This means that, in the elastic fields of defects there exist local regions with lowered interphase barriers for the development of initial excited states (IESs) in the form of extended rectangular parallelepipeds. The pairs of wave beams propagating from the region of the excited state initiate a threshold deformation of the extension–compression type in the orthogonal directions $\mathbf{n}_{1,2}$ specified by the eigenvectors $\xi_{1,2}$ of the deformation tensor of the elastic field of the defect in the region of the development of the IESs.

It can easily be shown [4, 5] that the normal $\mathbf{N}_w$ to the habit plane, which is related to the propagation of the control wave process, is specified by the relationship

$$(\mathbf{N}_w)_{1,2} \parallel \mathbf{n}_2 \pm \mathbf{n}_1 æ, \quad \mathbf{n}_{1,2} = \xi_{1,2}, \qquad æ = v_2/v_1, \quad \mathbf{n}_1 \perp \mathbf{n}_2, \ |\mathbf{n}_i| = 1, \tag{1}$$

where v_1 and v_2 are the moduli of the velocities of propagation of the waves in the directions $\mathbf{n}_1$ and $\mathbf{n}_2$, respectively. The relationships (1) are convenient for the identification of possible dislocation nucleation centers (DNCs) via a comparison of the calculated orientations $\mathbf{N}_w$ with the observed orientations. Indeed, in the course of the primary choice of potential DNCs it is natural to find the extrema of the eigenvalues $\varepsilon_{1,2}$ of the tensor of elastic deformation of the field, to choose the corresponding orientations $\xi_{1,2}$, and to find $\mathbf{N}_w$. It can be expected that, upon the description of the habits of $\{hh\ell\}_\gamma$ type, a decisive role is played by the rectilinear segments of dislocation loops (or separate segments of dislocations pinned at defects) oriented along close-packed directions $\Lambda_1 \| \langle 1\,\bar{1}0 \rangle$, therefore, we will choose segments such as basic DNCs for the formation of a first lath. In addition, the formation of each lath is accompanied by a macroshear with the main component lying in the habit plane. This means that, like a DNC, the lath creates a defect that, in the cryston model of the simple shear [7, 8], can conveniently be simulated as a set of parallel prismatic loops. Figure 1 shows a cryston model for a carrier of shear with $\tan\psi$ on the plane $(557)_\gamma$ in the direction $[77\overline{10}]_\gamma$.

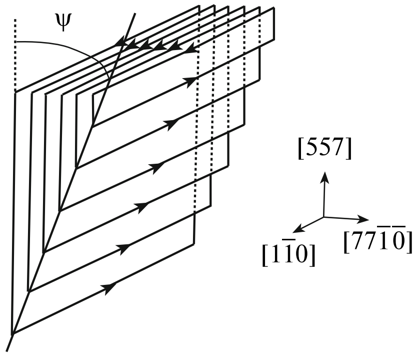

Fig. 1. Dislocation model of a cryston, i.e., carrier of simple shear of the $[77\overline{10}]_\gamma$ $(557)_\gamma$ type (schematic).

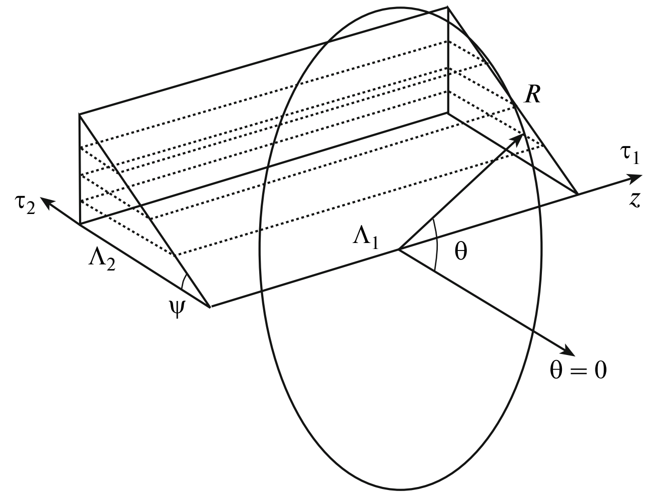

Fig. 2. Cylindrical coordinate system used to calculate elastic fields of dislocation loops.

The orientation $\mathbf{\Lambda}_2$ of the second segment of any of the loops of a cryston carrier of shear is chosen to be orthogonal to $\mathbf{\Lambda}_1$.

It has been shown in [9] that the results of calculations for the case of $\mathbf{\Lambda}_2\|[558]_\gamma$, the direction of which is close to $[557]_\gamma$ in Fig. 1, confirm the possibility of the formation of a lath composition of a bainite macroplate including crystals with habits of the $(hh\ell)_\gamma$ type at $h < \ell$ and $h > \ell$. The case of $(hh\ell)_\gamma$ with $h < \ell$, which in fact represents the reproduction of the initial DNCs, corresponds to the choice of wave vectors (of control waves) in the region of the extrema of eigenvalues of the tensor of the elastic field of DNCs. The case of $(hh\ell)_\gamma$ with $h > \ell$ corresponds to the maxima of the relative changes in volume.

The aim of this work is to study (using the same scheme) the elastic field of a DNC at $\mathbf{\Lambda}_2\|[774]_\gamma$, which corresponds to the cryston model of shear that should accompany the appearance of a lath with a habit $(774)_\gamma$ related to the second component of the bimodal composition. This problem is of large importance for determining the mechanism of the formation of an additional component of the lath composition of the bainite macroplate.

2. ELASTIC FIELD OF A CRYSTON CARRIER OF SHEAR $(774)_\gamma$ $[44\ \overline{14}]_\gamma$

Let us choose, as the basic (widest) loop of the cryston model of shear $(774)_\gamma$ $[44\ \overline{14}]_\gamma$, a dislocation loop with dimensions (in the units of the lattice parameter a) $\mathbf{L}_1 = 10^4$ along $\mathbf{\Lambda}_1\|[1\ \overline{1}\ 0]_\gamma$ and $\mathbf{L}_2 = 10^3$ along $\mathbf{\Lambda}_2\|[774]_\gamma$ with a Burgers vector $\mathbf{b}_1\|[44\ \overline{14}]_\gamma$. The spatial orientation of the cylindrical coordinate system with respect to the rectangular dislocation loop with the orientations of the sides specified by the unit vectors $\boldsymbol{\tau}_1$ and $\boldsymbol{\tau}_2$ is given in Fig. 2.

It can be seen from Fig. 2 that the origin is chosen to lie at the center of the segment $\mathbf{\Lambda}_1$ and that the angle θ is counted from the loop plane. The positive values of θ correspond to the counterclockwise rotation (when seeing from the end of the vector $\boldsymbol{\tau}_1$). The distance (in the units of the lattice parameter a) of the point of observation R is chosen so that, by increasing the number of loops in accordance with Fig. 1, we could investigate the superimposed elastic field.

Figure 3 shows the elastic fields of a cryston carrier of shear with the above-indicated parameters of the basic loop for the case of ten loops at $R = 1500$. In accordance with [10], as the model set of elastic moduli, we chose $C_L = 0.2508$, $C' = 0.0271$, and $C_{44} = 0.1034$ TPa for the Fe–31.5Ni alloy at a temperature $T = 673$ K. Compared to the case of the carrier of shear $(558)_\gamma$ $[88\overline{10}]_\gamma$, considered in [9], the transition to the shear $(774)_\gamma$ $[44\ \overline{14}]_\gamma$ (apart from the interest in the consideration of a variant $|h|/|\ell| > 1$) requires that we increased $\tan\psi$. In accordance with the results of [6], we assume that $\tan\psi = 0.22$.

Here, the main attention is given to the angular localization of the extrema in the dependences of the eigenvalues $\varepsilon_{1,2}(\theta)$ of the tensor of elastic deformation, to the relative change in the volume $\delta(\theta)$, and to the calculation of the corresponding orientations of $\xi_{1,2}(\theta)$ eigenvalues. The values of the eigenvalues ε_3 are small compared to ε_1 and $|\varepsilon_2|$, and the corresponding $\varepsilon_3(\theta)$ curve is not shown. The absolute values of $\varepsilon_{1,2}$ (on the order of 10^{-4}) are not given. The graphs are given on a suitable scale.

Since the transformation occurs with an increase in the specific volume, it is suitable to use, when analyzing the intense extrema of the $\varepsilon_{1,2}(\theta)$ and $\delta(\theta)$ dependences, the condition $\delta \geq 0$ as one of the criteria for the choice. Then, substituting the eigenvectors $\xi_{1,2}(\theta)$ and the values of æ found via Christoffel equations [11] into (1), we can easily find a correlation between the extremal values of θ and habits of the expected lath

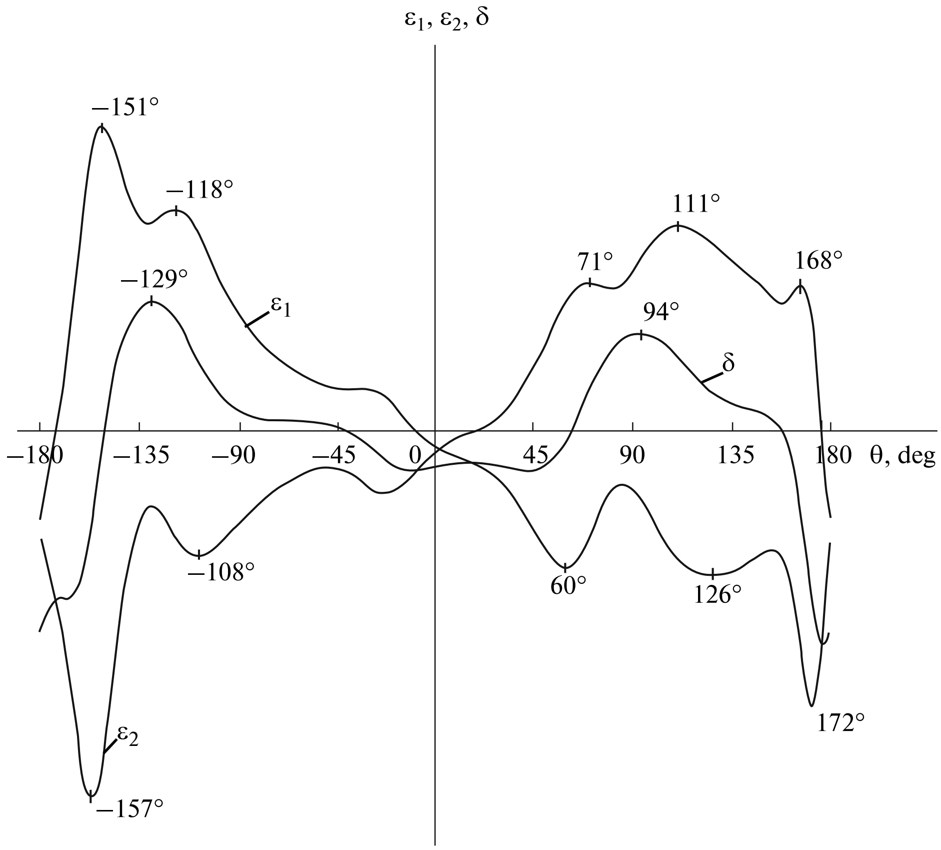

Fig. 3. Angular dependences of eigenvalues $\varepsilon_{1,2}$ of deformation tensor and relative change in volume δ of the elastic field of a cryston consisting of ten loops for the shear $(774)_\gamma$ $[44\ \overline{14}]_\gamma$ at $\tan\psi = 0.22$ and $R = 1500$. Elastic moduli are taken to be $C_L = 0.2508$, $C' = 0.0271$, and $C_{44} = 0.1034$ TPa.

crystals. Let us present the results of this comparison using approximate designations in the form of small integer Miller indices for the habits as follows:

$$\begin{aligned}&\theta = -151° \to (11\ 11\ 15)_\gamma,\\ &\theta = -129° \to (-14-14\ 3)_\gamma,\\ &\theta = 94° \to (-5-5\ 3)_\gamma,\quad \theta = 111° \to (-3-34)_\gamma,\\ &\theta = 126° \to (2\ 2\ 3)_\gamma.\end{aligned} \qquad (2)$$

Note that the orientations of the eigenvectors $\xi_{1,2}$ that correspond to the extrema of $\varepsilon_{1,2}(\theta)$ are close to the symmetry axes $[110]_\gamma$ and $[001]_\gamma$. However, if we take into account that, in the absence of transformation twins, for the initiation of the transformation it is necessary for the tensile axis to be close to the $[110]_\gamma$ axis and the compression axis be close to the $[001]_\gamma$ axis, the two last variants, $\theta = 111° \to (\bar{3}\bar{3}4)_\gamma$ and $\theta = 126° \to (223)_\gamma$, can be excluded from the consideration.

Thus, there remains an $(11\ 11\ 15)_\gamma$ habit that makes a small angle $\approx 4.6°$ with the habit $(558)_\gamma$, the main component of the lath structure of the macroplate. Then, it can be assumed that, in the case of the $(774)_\gamma$ $[44\ \overline{14}]_\gamma$ shear, the conditions necessary for the initiation of the growth of the main component of the bimodal composition are also reproduced.

On the contrary, the elastic fields of crystons that correspond to the extrema of $\delta(\theta)$ do not reproduce conditions necessary for the initiation of the growth of crystals with habits of the $(hh\ell)_\gamma$ type at $h > \ell$ that make small angles with the initial habit $(774)_\gamma$. Indeed, as can be seen from (2), the signs of two Miller indices differ from the sign of the third index.

Strictly speaking, as was shown in [9], for the carrier of shear of the $(558)_\gamma$ $[88\ \overline{10}]_\gamma$ type with $\tan\psi = 0.15$ one of the maxima of $\delta(\theta)$ at $\theta = 126°$ corresponds to the habit $(\bar{3}\ \bar{3}\ 2)_\gamma$ of the bainitic ferrite. Therefore, to check the completeness of the set of orientations of the expected habits in this work, it is possible to start from the calculation of the field of the $(\bar{7}\ \bar{7}\ 4)_\gamma$ $[4\ 4\ 14]_\gamma$ cryston. It can easily be shown that the images in the left- and right-hand sides of the graphs in Fig. 3 replace sites and the condition for the choice at $h < \ell$ for $\theta = 151°$ is satisfied at the habit $\left(11\ 11\ \overline{15}\right)_\gamma$. This means that the field of the $(\bar{7}\ \bar{7}\ 4)_\gamma$ $[44\ 14]_\gamma$ cryston does not create DNCs that correspond to the crystals of the main lath component with the equal signs of all three indices. Correspondingly, at $h > \ell$, the rules of selection for a crystal with a habit $(553)_\gamma$ that forms a significant angle (≈±135°) with $(\bar{7}\ \bar{7}\ 4)_\gamma$, are obeyed.

3. DISCUSSION

The results considered in [9] and in this work show that the cryston carriers of shear of the $(hh\ell)_\gamma$ $[\ell\ell\overline{2h}]_\gamma$ type at $h < \ell$ and $h > \ell$ are not equivalent from the viewpoint of creating conditions for the reproduction of self-similar carriers that play the role of DNCs. If both variants of the cryston DNCs were equal in the process of the formation of a bainitic macroplate, then the set of orientations of the lath habits in the macroplate would include at least the habits of the $(hh \pm \ell)_\gamma$ type at $h < \ell$ and $h > \ell$. Note that this expansion of the set of habits were sharply different from the well-known [12] feature observed for packet martensite. Indeed, a feature characteristic of packet martensite is the spatial insulation of lath crystals with orientations (up to six orientations) that make the least angles with the same close-packed plane of the initial austenite that enters into the orientation relationships for the crystals of the packet. Note also that the orientations of the eigenvectors $\xi_{1,2}(\theta)$ in the region of the maxima of $\delta(\theta)$ deviate substantially (by more than 20°) from the symmetry axes $[110]_\gamma$ and $[001]_\gamma$; this should noticeably decrease the efficiency of the control wave process [13].

These difficulties are removed if we assume that the process of the formation of crystals with the $(774)_\gamma$ habits occurs via the same scenario as for crystals with $(558)_\gamma$ habits, but with respect to the crystallographic basis of the austenite twin with a twinning plane $(111)_\gamma$. This variant has been discussed in [14]. In particular, it was shown that, with the transition to the crystallographic basis of the austenite twin, the $(774)_\gamma$ habit becomes analogous to the $(558)_\gamma$ habit. However, it seemed premature to draw any certain conclusions before calculations of the DNCs would be performed. At present, this scenario can only be considered to be the most likely. In connection with this, it is worthy of noting that, in [6], the formation of austenite twins was noted to accompany the formation of lath crystals of bainitic ferrite.

4. CONCLUSIONS

The results of the analysis given in this work and in [9, 14] show that the formation of a bimodal lath composition of the macroplate of bainitic ferrite is related not only to the relay mechanism of the formation of the main component, but also to the accompanying process of the formation of twinned plates of austenite, in which additional components of the bimodal composition are formed. In connection with this, detailed experimental information on the accompanying twinning of austenite is of undoubted interest.

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