CRYSTALLOGRAPHY

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COMPARISON OF MARTENSITE CRYSTAL PROFILES, CALCULATED IN A GROWTH WAVE MODEL AND OBSERVED BY EXPERIMENT

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A number of typical martensite crystal profiles observed by experiment are compared with the results of profile calculations obtained within the framework of a model of a controlling wave process in an inhomogeneous material. The satisfactory conformity obtained makes it possible, in principle, to reconstruct the nature of an inhomogeneous material according to profile shape.

Key words: controlling wave process, inhomogeneous material, forms of crystal profiles.

INTRODUCTION

In transition metals and alloys based on them a version of limiting (supersonic with respect to a longitudinal elastic wave) growth rate if fine lamellar martensitic crystals is possible. A classical example is the growth of α-martensite in disordered alloys based on iron with $\gamma \to \alpha$-martensitic transformation (MT) during quenching. A supersonic crystal growth rate is naturally explained within the framework of a wave model [1]. Since transformation develops with significant supercooling below the T_0 point of phase equilibrium, and the temperature for absolute loss of austenite stability is absent, the M_s temperature for the start of MT should necessarily comprise some differences from the zero of the threshold value for strain ε_{th}, transferred by a controlling wave process (CWP). It is well known hat external elastic stresses shift the M_s point. This indicates that the value of ε_{th} is placed in the elastic region, and consequently in describing a wave entering into the composition of the CWP, it is permissible to use superimposition of elastic waves, for which in turn, it is correct to use harmonic description. The MT in question exhibits clearly expressed signs of phase transition of the first order, and as analysis shows [1, 2] it has a specific nature of heterogeneous generation. In fact, transformation commences with appearance of an initially excited (oscillatory) condition in the form of an extended rectangular parallelepiped, whose sides coincide with the orientation of the eigenvectors of the elastic strain field tensor for an individual dislocation, playing role of a force center, disrupting the original austenite symmetry. As a rule, a pair of strains ε_1, ε_2 in orthogonal directions ξ_1, ξ_2, perpendicular to the long axis of a parallelepiped ξ_3, have opposite signs, and strain in direction ξ_3 is close to zero. Excitation of the conditions is a source of wave beams whose superimposition causes propagation of a plane threshold strain of the "tension – compression" type with supersonic velocity $v = v_1 + v_2$, where v_1, v_2 are longitudinal (or quasilongitudinal) wave velocities in direction ξ_2, ξ_2 respectively.

A steady-state scheme is presented for control of lamellar crystal growth with a constant thickness in an inorganic uniform material. Without limiting the generality of directions ξ_1, ξ_2 they are selected coinciding with axes x and y. Transverse dimensions d_1, d_2 satisfy the inequality $d_{1,2} < \lambda_{1,2}/2$, prescribing the CWP limit. In fact, with harmonic description of points standing at distance $\lambda/2$, strain reverts to zero, so that the final threshold strains are achieved in the inner region of a cell with dimensions less that $\lambda_{1,2}/2$. It is apparent that extreme values of strain are achieved in the center of a cell.

A CWP propagates through a metastable steady-state material. As a result of this in the field of a lattice, losing stability, energy is released making it possible to maintain the level of strain exceeding threshold values with respect to modulus. It is clear that when a CWP falls in a region of inhomogeneous material leading to effective energy dissipation, the value of strains in a moving boundary of the controlling process (prescribing in a dynamic regime the habit plane) will be reduced. As a result of this dimensions d_1, d_2

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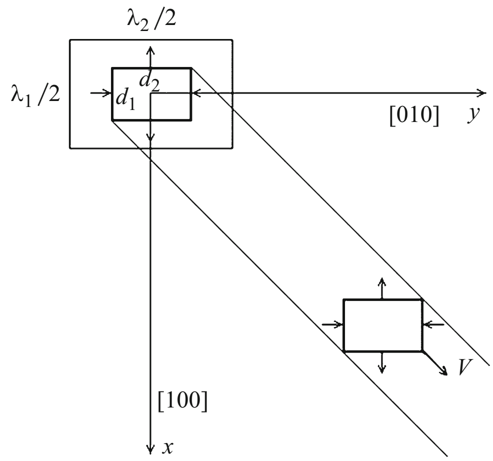

Fig. 1. Formation of a lamellar region, losing stability with propagation of threshold strain.

will decrease, leading to a reduction in crystal profile. In contrast, at the start of crystal growth in a region with high energy dissipation in the area with the least level of it, should be accompanied by an increase in plate thickness. Grain boundaries, martensitic crystals, forming in the preceding stage, and inclusions of different nature within the volume of a grain, may serve as typical sources of inhomogeneity.

METHODS FOR CALCULATIONS

Description of superimposition of wave beams running in x- and y-directions is carried out using two simple wave equations in special first order derivatives, obtained with factorizing the d'Alambertian operator from the required reversion to zero of one of the multiples [3]. Expressions for effective coefficients of wave beam damping $b_{1,2}(\varepsilon_1, \varepsilon_2)$ reflect the dissipation mechanism in electron and lattice sub-systems, and within the region of a lattice, losing stability, consideration is given to the contribution of wave generation by non-equilibrium electrons. As a result of this the signs of $b_{1,2}$ within and outside the region, losing stability, are opposite. Additional dissipation in the inhomogeneity region is reflected by introducing into $b_{1,2}$ additive components depending correspondingly on coordinates x and y.

For the purpose of illustration in analytical description of the change in values of $d_{1,2}$ it is assumed that $d_1 = d_2$, $|v_1| = |v_2|$, and the center of inhomogeneity localization agrees with planes $x = \bar{x}$, $y = \bar{y}$, $|v| = \sqrt{2}|v_{1,2}|$. The dependences of $b_{1,2}$ on coordinates are similar:

$$b_1(\varepsilon_1, \varepsilon_2, x) = \kappa\left[1 - \frac{\sigma_0}{\sigma_{th}}\theta(\varepsilon_1 - \varepsilon_{th1})\theta(\varepsilon_{th2} - \varepsilon_2) + \delta_0\varphi\left(\frac{x-\bar{x}}{\lambda}\right)\right],$$

$$b_2(\varepsilon_1, \varepsilon_2, y) = \kappa\left[1 - \frac{\sigma_0}{\sigma_{th}}\theta(\varepsilon_1 - \varepsilon_{th1})\theta(\varepsilon_{th2} - \varepsilon_2) + \delta_0\varphi\left(\frac{y-\bar{y}}{\lambda}\right)\right]. \quad (1)$$

In Eq. (1) the "intensity" of inhomogeneity is specified by parameter δ_0, introduction of wavelength λ corresponds to a change in distance in units of λ, $\sigma_{th} - \sigma_0 \leq 0$. within the region, losing stability (the region is separated by derivation of units Heavyside function θ). We recall (for example [1]) that in Eq. (1) parameter $\kappa > 0$ specifies damping of elastic waves (phonons) in the absence of a mechanism for wave generation, σ_0 prescribes the value of the difference of inverted population of pairs of electrons of conditions (IPPEC), σ_{th} is the threshold value of IPPEC, and the dependence of φ on coordinates x and y concretizes the form of spatial inhomogeneity.

In order to determine the thickness of a crystal one of the pairs of symmetrical wave equations is considered of the form (indices 1, 2 for strain in orthogonal directions are discarded):

$$\dot{\varepsilon} + v\varepsilon' + b(x)\varepsilon = 0,$$
$$b(x) = \kappa\left[1 - \frac{\sigma_0}{\sigma_{th}} + \delta_0\varphi\left(\frac{x-\bar{x}}{\lambda}\right)\right]. \quad (2)$$

The value of $d_{1,2}$ obtained by means of Eq. (2) is $\sqrt{2}$ times less than the thickness of d of the crystal prototype. Everywhere subsequently in diagrams be the dependence $d_1(x)$ will be provided, corresponding to steady-solution of Eq. (2).

Four versions are considered of relationship $\varphi\left(\frac{x-\bar{x}}{\lambda}\right)$, three of which (3$b$, 3$c$, 3$d$) are briefly elucidated in [4]:

$$\varphi\left(\frac{x-\bar{x}}{\lambda}\right) = 0, \quad (3a)$$

$$\varphi = \exp\left(\frac{-|x-\bar{x}|}{\lambda}\right), \quad (3b)$$

$$\varphi = \left(\frac{(x-\bar{x})^2}{\lambda}\right), \quad (3c)$$

$$\varphi = \left(\frac{(x-\bar{x})^{-2}}{\lambda}\right). \quad (3d)$$

A solution of Eq. (2) is found in the form $\varepsilon(x,t) = \tilde{\varepsilon}(x,t)\cos(\omega t \pm kx)$, for sufficiently slowly changing amplitude $\tilde{\varepsilon}(x,t)$, so that to a first approximation it is possible to ignore the change in frequency ω, and signs $\pm$ in describing the phase of wave reflect the possibility of propagation in directions $\pm k$. Then from expression (2) taking account of the condition $v = \omega k$, we obtain an equation for amplitude $\tilde{\varepsilon}(x,t)$:

$$\dot{\tilde{\varepsilon}} + v\tilde{\varepsilon}' + b(x)\tilde{\varepsilon} = 0, \quad (4)$$

that with substitution in the dependence $b(x)$ of function (3) makes it possible to obtain an analytical solution for $d_1(x)$.

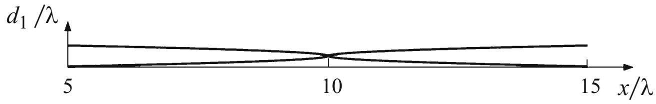

Fig. 2. Dependence $\tilde{d}_1(\tilde{x})$ for form of function φ = 0 with parameters $\tilde{\tilde{x}} = 10$; $\frac{\kappa}{v}\left(\frac{\sigma_0}{\sigma_{th}} - 1\right) = 10^{-3}$.

The relative width $\tilde{d}_1(x) = d_2(x)/\lambda$ with harmonic description of strain in a threshold regime gives a relationship

$$\tilde{d}_1(x) = \frac{1}{n}\arccos\left(\varepsilon_{th}/\tilde{\varepsilon}(x)\right). \qquad (5)$$

In the next section, mainly in graphical form, a representative collection of profiles of martensite crystal prototypes obtained from Eqs. (2), (3) and (5) are provided.

RESULTS

For the simple case of a material not containing significant inhomogeneity, we assume that $\varphi\left(\frac{x - \bar{x}}{\lambda}\right) = 0$. Then with fulfilment of the generation condition $1 - \sigma_0/\sigma_{th} < 0$ and realistic values of parameters we select $\frac{\kappa}{v}\left(\frac{\sigma_0}{\sigma_{th}} - 1\right) = 10^{-3}$. Then assuming that the initial fluctuation with a threshold of strain ε_{th} corresponds to coordinate $\tilde{x}$, after integrating the steady-state version of Eq. (2) and introducing $\tilde{x} = x/\lambda$ we find

$$\tilde{\varepsilon}/\varepsilon_{th} = \exp\left(10^{-3}\,|\tilde{x} - \tilde{\tilde{x}}|\right). \qquad (6)$$

From Eqs. (5) and (6) we obtain a relationship $\tilde{d}_1(x) = \frac{1}{\pi}\arccos\left(\exp\left(10^{-3}\,|\tilde{x} - \tilde{\tilde{x}}|\right)\right)$, shown in Fig. 2. This trivial case corresponds to the possibility of forming pairs of crystals with a generation center at point $\tilde{\tilde{x}}$, uniformly expanding with distance from it. In accordance with the inequality $d_{1,2} < \lambda_{1,2}/2$ provided above, it is clear that the width $\tilde{d}_1(x)$ cannot exceed the value $\tilde{d}_{1\max}(x) = 1/2$.

In fact [1], for phase transition of the first order generation has a heterogeneous character, and the choice of coordinates $\tilde{\tilde{x}}$ cannot be arbitrary, and due to the action of elastic field of defects, as a rule, individual dislocations, reducing the interphase energy barrier in the generation field.

Without writing out analytical expressions for the cases (3*b*), (3*c*), and (3*d*) we provide in graphical form the most typical results with the same values of parameters κ, σ_0, σ_{th} as above, permitting variation of parameter δ_0.

For the exponential version of function φ [case (3*b*)] in Fig. 3, an example is presented for the existence of a change

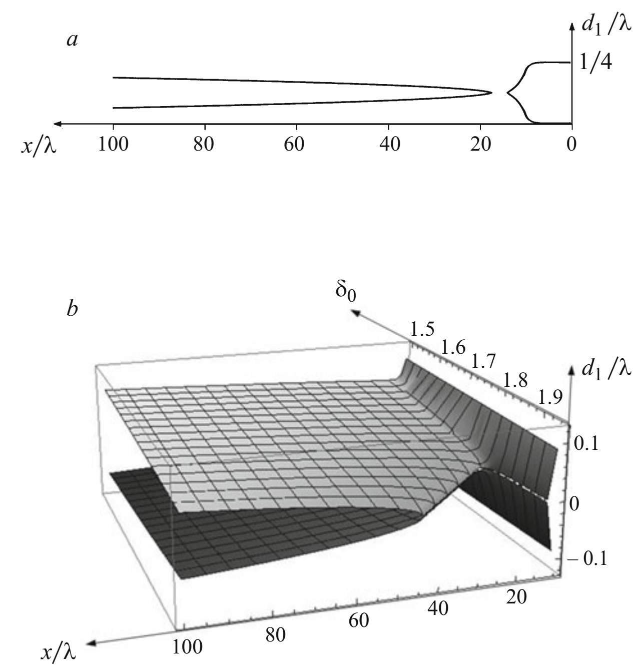

Fig. 3. Dependence $\tilde{d}_1(\tilde{x})$ for the exponential form of function φ [see Eq. (3*b*)] with parameters $\tilde{\tilde{x}} = 10$; $\frac{\kappa}{v}\left(\frac{\sigma_0}{\sigma_{th}} - 1\right) = 10^{-3}$; $\delta_0 = 1.82 \times 10^2$ (*a*); $1.5 \times 10^2 \le \delta_0 \le 1.95 \times 10^2$ (*b*).

in $\tilde{d}_1(\tilde{x})$. It is shown (Fig. 3*a*) that in a region of quite strong inhomogeneity, adjacent to $\tilde{\tilde{x}}$, due to high damping controlling crystal growth a formation wave for a martensite crystal appears to be impossible. The left-hand part of Fig. 3*a* corresponds either to the initially excited state, whose center *x* may be localized at any point of region $x^* \le x < \infty$ (with $x \to \infty$, $d \to \lambda/2$), if a crystal grows in direction of a reduction in *x*, or to the initially excited condition, whose center *x* is localized at point x^*, if a crystal grows in a direction of an increase in *x*. The right-hand part of Fig. 3*a* corresponds to typical behavior of $\tilde{d}_1(x)$ in immediate vicinity of the center of inhomogeneity.

It may be seen from Fig. 3*b* that a reduction in parameter δ_0 maintains the possibility of forming a martensite crystal within the whole region of a change in *x*, and here the width of the crystal profile $\tilde{d}_1(x)$ changes uniformly, reaching for each value of δ_0 a minimum at some point *x*, placed between x^* and $\tilde{\tilde{x}}$. This contraction in a crystal is due to traverse of region $\tilde{\tilde{x}} = 10$, within which damping is at a maximum.

We note that in Figs. 2 and 3 the scales in orthogonal directions differ markedly for the demonstration of change in crystal form within a large spatial interval along the growth direction, prescribing the crystal long axis. The dependence $\tilde{d}_1(\tilde{x})$ is presented in Fig. 4, obtained after substitution in Eq. (2) of quadratic and inverse quadratic forms of function φ in Eqs. (3).

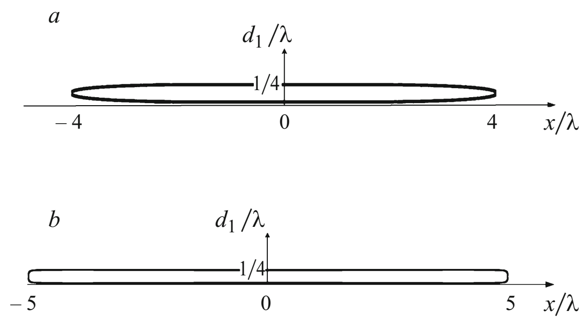

Fig. 4. Examples of dependences $\tilde{d}_1(\tilde{x})$: *a*) $\varphi\left(\frac{x-\bar{x}}{\lambda}\right)=\left(\frac{(x-\bar{x})^2}{\lambda}\right)$, $\delta_0 = 10^2$, $\tilde{\bar{x}} = 0$; *b*) $\varphi\left(\frac{x-\bar{x}}{\lambda}\right)=\left(\frac{(x-\bar{x})^{-2}}{\lambda}\right)$, $\delta_0 = 10$, $\tilde{\bar{x}} = 5$.

For both versions in Fig. 4 point $x = 0$ is the central point of a region for the initially excited condition. Symmetry of the diagrams with respect to a change in x by $-x$ signifies that the solutions in question, relating to wave beam propagation in directions $\pm k$ from the generation region. We note that with a change of k to $-k$ there should be a change in $\bar{x}$ to $-\bar{x}$ in function $\varphi\left(\frac{x-\bar{x}}{\lambda}\right)$. Since with $\varphi\left(\frac{x-\bar{x}}{\lambda}\right)=\left(\frac{(x-\bar{x})^{-2}}{\lambda}\right)$ planes $x=-\bar{x}$, $x=\bar{x}$ correspond to an undetermined hindrance, there is a difference in the forms of curves in the region of crystal growth cessation (close to point $x/\lambda = \pm 4$ in Fig. 4*a* and $x/\lambda = \pm 5$ in Fig. 4*b*).

DISCUSSION

The forms of profiles provided above have been obtained in the vicinity of threshold strains and correspond to prototypes of real crystal profiles. Development of strain in the region of lattice, losing stability, is accompanied by development of macroshear and lattice turning, as a shown in [5, 6]. The amount of shear with $\gamma \to \alpha$-transformation in iron alloys is close to 0.2. Transition from threshold to finished strain (by means of shear) makes it possible to move to comparison of calculated forms of crystal profiles with the versions observed.

Two versions of this comparison are provided in Fig. 5. For clarity in an expanded fragment (Fig. 5*a*) taken from [7, Fig. 2.16a), a section of twinned crystal martensite is presented, for one of the components of a twinned structure for the calculated profile applied. The profile is separated by dark lines and marked by the number *1*. We note that comparison in fact with a component twin is entirely correct within the framework of the simplification $d_1 = d_2$ adopted above, since the component of a twin forms mainly, with a pair of wave beams, running along the orthogonal axes of fourth order symmetry, so that the section of an active cell has a quadratic form [8]. The form of the profile applied corresponds to the profile provided in Fig. 4*b*, after modification by shear. Now we comment on versions *2* and *3* shown in Fig. 5*b*.

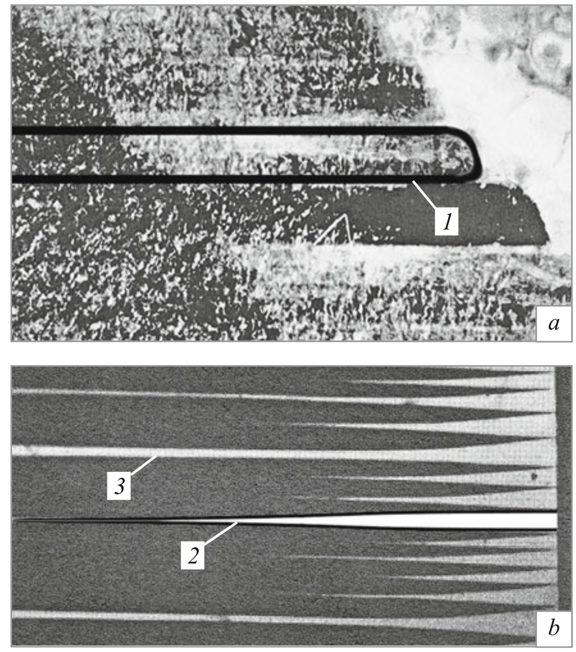

Fig. 5. Comparison of calculated and experimentally observed profiles of twinned structure components: *a*) steel 55Kh2N23; *b*) alloy Cu – 14 wt.% Al – 3.9 wt.% Ni.

Version *2* illustrates conformity of the calculated profile with that of martensite in the form "white needles" (these are precisely the same "needles" observed in [9], Fig. 1). The calculated profile *2* corresponds to a profile provided in the right-hand part of Fig. 3*a*, and with selection of identical spatial scales in the horizontal and vertical directions.

Version *3* in Fig. 5*b* illustrates the case observed in [9, Fig. 1] of a nonuniform change in twinned component profile thickness. This behavior, as noted above, corresponds in Fig. 3*b* to the region of parameters $\delta_0 < 1.815 \times 10^2$ for a model of inhomogeneity, described by Eq. (3*b*). We also not that the nonuniform behavior of the thickness of the profile is also observed with intersection of martensite crystals.

CONCLUSIONS

Results of this work indicate that there is, at least, qualitative conformity between the forms of profiles, calculated in a wave model for martensite crystal grain growth and those observed. This makes it possible in principle to pose the reverse problem of reconstructing the nature of spatial inhomogeneity of a specimen with respect to the features observed for crystal section form. The results obtained make it possible to add a restoration scheme to the dynamic picture of martensite reactions according to the choice of experimental morphological data.

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