DYNAMIC MECHANISM OF LATERAL GROWTH OF THIN-LAMELLAR MARTENSITE CRYSTALS IN IRON-NICKEL ALLOYS UNDER EXTERNAL TENSILE STRESS

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Abstract. Within the framework of the dynamic theory of martensitic transformations, the possibility of cooperative growth of the faces of the resulting crystal is discussed using the example of the formation of a layer parallel to the habit plane. This growth is comparable to the lateral crystal growth typical of shape memory alloys, but not typical of α-martensite in iron alloys upon simple cooling. However, under conditions of external tensile stress, rapid lateral growth of thin-lamellar α-martensite crystals was observed. It is shown that the formation of a layer parallel to the habit plane is similar to the formation of the original crystal. The functions of the dislocation nucleation center (DNC*) for this layer are performed by a dislocation loop framing the habit plane with the Burgers vector **b***, and **b*** is specified by the macroshift in the initial crystal. An example of a crystal with a habit close to (3 14 9) is considered. The results of calculation of the elastic field of the DNC* loop are presented using data on the elastic moduli of the Fe–31.5%Ni alloy at a temperature $M_s = 239$ K. In the approximation of longitudinal waves for a pair of relatively long-wave components in the control wave process, the practical coincidence of the layer habit with the initial habit is demonstrated. The value of b^* has been estimated.

Keywords: *martensitic transformations, dynamic theory, habit planes, dislocation nucleation centers, initial excited state, controlling wave process, lateral growth*

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INTRODUCTION

It is well known (see, e.g., [1, 2]) that iron-based alloys undergo γ–α martensitic transformation (MT) by cooperative rearrangement of the initial structure (austenite, γ-phase) with face-centred cubic (HCC) lattice into the final structure (martensite, α-phase) with volume-centred cubic (OCC) or tetragonal (TCT) lattice.

The transformation has pronounced signs of phase transition of the I kind (specific volume change δ~1%, temperature hysteresis up to hundreds of degrees). Moreover, despite significant supercooling below the phase equilibrium temperature T0, austenite is metastably stable at the temperature Ms of the beginning of the transformation during cooling of austenite.

Martensite crystals are characterized by a set of interrelated macroscopic morphological features (orientations of habit planes, interphase orientation relationships, magnitude and direction of macroshear). It is appropriate to note that in iron-nickel alloys, when the nickel concentration changes, martensite of several morphotypes is formed, and M_s decreases with increasing nickel content. At Ni content up to 29% (here and below Ni content is given in at.%), packet martensite with habits close to the {557} family is observed. At 30–31% nickel, lenticular martensite is observed, the central part of which (midrib) has the shape of a plate, defining habit planes close to {3 10 15}. And, finally, at 32–35% Ni shows thin-plate martensite, which, like the midrib of lenticular crystals, is completely twinned (less often "single-crystal", i.e. instead of the second component of the twin structure it contains transformation dislocations [3]).

It should be emphasized that subsequent growth of the crystals that have arisen is not typical for α-martensite in iron alloys. The increment of the martensite phase during cooling occurs due to newly arising crystals. In particular, spontaneous lateral growth is not observed for such crystals.

In contrast, for titanium nickelide-based alloys, martensitic transformations with shape memory effect (SME) occur, which are characterized not only by the formation of new crystals during cooling but also by lateral growth [4]. MTs in alloys with SME have less pronounced features of first-order transitions; naturally, it can be assumed that such alloys have lower stability of the initial phase than the γ-phase. Apparently, this circumstance is the main reason for the absence of lateral growth of α-martensite crystals. This is supported by experiments [5], in which lateral growth of thin-plate α-martensite crystals was observed, but not during cooling, rather under external tensile stresses. Schematically, this effect is shown in Fig. 1, which is part of Fig. 7 in [5].

Fig. 1. Diagram of lateral growth of thin-plate martensite in Fe - 31Ni - 10Co - 3Ti alloy, induced by tensile stress at temperature $M_s = 83$ K (part of Fig. 7 in [5]).

Importantly, the formation rate of midribs in α-martensite crystals is supersonic. This unambiguously indicates the existence of a dynamic controlling wave process (CWP), the propagation of which carries threshold deformation and ensures the cooperativity of MT (see, e.g., [6, 7]).

Regarding the completeness of description of both morphological and kinetic features of individual martensite crystals growth, the dynamic approach remains relevant for describing spontaneous (during cooling) MTs in samples with relatively large grains (as well as in single crystals). Therefore, modern works in the field of MT focus on the occurrence of MT under extreme conditions (for example, under intense external deformations and high external pressures (see [8])), with manifestation of pronounced combined effects (as in the case of Heusler alloys [9]), in ultrafine-grained samples. Of course, research continues on structural features with almost atomic resolution (see, e.g., [10]), phase compositions, and discussion of potential possibilities for MT in multicomponent alloys (in particular, in so-called high-entropy alloys [11]).

In the present work, attention is focused on the development of a dynamic approach applied to the classical variant of γ-α-MP in iron alloys.

Note that within the framework of the dynamic theory of MP, macroscopic morphological features are successfully described both for α-martensite and for martensite in alloys with SME [12]. Therefore, the aim of the work is to clarify the possibility of a dynamic description and lateral growth of martensite crystals.

SCHEME OF WAVE CONTROL OF MARTENSITE CRYSTAL GROWTH

For the convenience of readers, let us briefly recall the main conclusions of the dynamic theory of MP.

1. Crystal growth starts with the emergence of an initial excited state (IES). The IES has the form of an elongated rectangular parallelepiped, the edges of which are collinear to the eigenvectors ξ_i (i = 1, 2, 3) of the strain tensor $\hat{\varepsilon}$ of the elastic field of the dislocation nucleation center (DNC). Moreover, the elongated axis of the parallelepiped is chosen along the axis ξ_3, corresponding to the eigenvalue $\varepsilon_3 \approx 0$ of the tensor $\hat{\varepsilon}$ close to zero. The transverse orientations of the IES along ξ_1 and ξ_2 correspond to different signs of the eigenvalues $\varepsilon_1 > 0$, $\varepsilon_2 < 0$ of the tensor $\hat{\varepsilon}$. The regions of IES localization correspond to extreme values of deformations.

2. The IES appears when supercooled below the point T_0 as a result of rapid synchronous displacements of atoms to new equilibrium positions in the IES region. Such a cooperative jump of atoms is accompanied by the excitation of oscillations that generate a CWP. The CWP inherits information about the nature of the elastic field of the DNC in the IES region. The CWP violates the symmetry of the initial phase and forms a "transformation channel." The relaxation of the atomic lattice inside the transformation channel leads to final deformations and the observed set of morphological features.

3. The description of the fine structure of transformation twins is achieved by including in the CWP composition, along with relatively long-wavelength pairs of waves (l -waves), relatively short-wavelength displacements (s -waves).

4. A fundamental simplification of crystal morphology analysis is achieved due to the fact that to describe the orientation of the habit plane (HP), it is sufficient to know only *l-waves.* In the simplest case, the normal **N** to the HP is defined by the kinematic formula:

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

$$\mathbf{n}_1 = \xi_1, \quad \mathbf{n}_2 = \xi_2, \qquad (2)$$

where the index W explicitly indicates the wave description, $\mathbf{n}_1$, $\mathbf{n}_2$ – unit wave normals of a pair of l -waves, having velocities $\mathbf{v}_1$, $\mathbf{v}_2$, and the choice (2) corresponds to the longitudinal wave approximation, convenient for qualitative assessments. The HP is "swept" by the intersection line of wave fronts, moving at supersonic speed $\mathbf{v}$, equal to the vector sum of velocities $\mathbf{v}_1$ and $\mathbf{v}_2$:

$$\mathbf{v} = \mathbf{v}_1 + \mathbf{v}_2. \qquad (3)$$

As a result, the NWS also propagates at velocity $\mathbf{v}$, sweeping out a plate-shaped region, as schematically shown in Fig. 2.

Fig. 2. Wave scheme for the formation of a prototype of a martensite plate.

5. The orientation of the habit can also be expressed through tensile and compressive strains:

$$\mathbf{N}_D \parallel \xi_2 \pm k\, \xi_1, \quad |\xi_{1,2}| = 1, \qquad (4)$$

$$k = \frac{1 - |\varepsilon_2|}{1 + \varepsilon_1} \left(\frac{\varepsilon_1}{|\varepsilon_2|} \frac{(2 + \varepsilon_1)}{(2 - |\varepsilon_2|)} \right)^{\frac{1}{2}}, \qquad (5)$$

in (4) the index D indicates the specification of the orientation of the normal to the habit as an invariant plane during plane deformation of the "tension – compression" type.

6. Since the waves carry threshold deformation, it is natural to identify $\mathbf{N}_W$ and $\mathbf{N}_D$, assuming $\mathbf{N}_W = \mathbf{N}_D = \mathbf{N}$. Then, comparing (1) and (2) with (4) and (5) and taking into account that for threshold deformations $\varepsilon_{1,2} << 1$, we obtain the relationship between the ratios of wave velocities and deformations:

$$æ = k \approx \sqrt{\varepsilon_1 |\varepsilon_2|^{-1}}. \qquad (6)$$

Fig. 3. Fragments demonstrating: a – cross-section of a flat transformation channel forming during UWP propagation. The values of relatively small threshold deformations are not shown; b – rotation of the material by angle φ and the appearance of pure shear deformation ($\Delta \mathbf{S}_1 = -\Delta \mathbf{S}_2$) during finishing deformations in the case of a positive volume effect.

7. The transition of the material in the area of the transformation channel (Fig. 3a) to the final state (Fig. 3b), under the condition of preserving the HP orientation and macroscopic continuity, is accompanied by lattice rotation and macroshear. The lattice inside the channel loses stability at the contact points of the diagonal (with direction **d**) of the parallelepiped cross-section in relation to the plane deformation of compression-tension. As a result, the lattice inside the channel experiences a constrained rotation by angle φ, reflected in Fig. 3b by the change in orientation from **d** to **d′**.

DYNAMIC MECHANISM OF LAYER-BY-LAYER GROWTH OF CRYSTAL FACES, INCLUDING LATERAL GROWTH

The main idea that allows extending the described dynamic mechanism of crystal formation to the description of the growth of the faces of the formed crystal is to associate each crystal face with a dislocation loop framing that face. Such loops can be considered as new DCNs*, assuming that the Burgers vector $\mathbf{b}^*$ is collinear with the direction of macroshear of the formed crystal.

Let us illustrate this with an example of the formation of a layer with the calculated (in the longitudinal wave approximation) normal:

$$\mathbf{N} \parallel [0.171867\ 0.832798\ 0.526221]. \qquad (7)$$

Normal (7) in the approximation of integer indices is close to [3 14 9]. Note that the HP (3 14 9) of a thin-plate crystal makes an angle of ≈ 1.2º with (3 15 10), and HP (3 15 10) approximately corresponds to the experimental data of Greninger - Troiano [13]. When calculating **N** the elastic moduli (in GPa) $C_L = 218$, $C' = 27$, $C_{44} = 112$, found in [14] for the Fe - 31.5%Ni alloy at temperature $M_s = 239$ K were used. A DCD with Burgers vector $\mathbf{b} \parallel [01\text{-}1]$ and segments $\mathbf{\Lambda}_1 \parallel [11\text{-}2]$, $\mathbf{\Lambda}_2 \parallel [111]$, having lengths (in lattice parameters a) $L_1 = 7000$, $L_2 = 10000$ was considered. Normal (7) in the cylindrical coordinate system (with the origin at the center of $\mathbf{\Lambda}_1$) corresponds to the angle $\theta \approx 116^{\circ}$ and R =1200.0020

From the perspective of the dynamic theory of MT, it is natural to choose a rectangular loop with segments $\mathbf{\Lambda}_1^* \parallel \xi_3$ and $\mathbf{\Lambda}_2^* \parallel \mathbf{v}$, where ξ_3 and **v** are determined from the analysis of the elastic field of the initial DCD as the DCD* framing the HP. Then crystals with HP (7) can be matched with

$$\mathbf{\Lambda}_1^* \parallel [0.949954\quad 0.001357\ -0.312385], \qquad \mathbf{\Lambda}_2^* \parallel [-0.260868\quad 0.553574\quad -0.790887],$$

$$\mathbf{b}^* \parallel [0.214711\quad -0.708892\quad 0.671841].$$

A number of characteristics of the elastic field of DCD* while maintaining the values of $L_{1,2}$ in the cylindrical coordinate system (see Fig. 4) are presented in Fig. 5 in a scale convenient for perception. To avoid overloading the notations, the symbol (*) is implied but not used.

Fig. 4. Parameters of the cylindrical coordinate system linked to the dislocation loop: $\mathbf{\Lambda}_1$, $\mathbf{\Lambda}_2$ **-** directions of the loop segments, axis Z is collinear to segment $\mathbf{\Lambda}_1$, angle θ is measured from the loop plane.

Fig. 5. Dependence on the angle θ of the shift value S, strains $\varepsilon_{1,2}$, relative volume change δ, at $Z = 0$, $R = 200\,a$ (a – austenite lattice parameter; reference point – center of segment $\mathbf{\Lambda}_1$, vertical lines separate areas of dominance of shifts S_1 or S_2, all characteristics refer to CWB in the form of a loop framing the habit plane, but the symbol (*) is omitted).

Preference is given to the localization of IPS in areas of angles θ close to ± 180º, for which, along with large values of S_2, δ also has the largest positive values. The selected orientation of the normal to the layer surface **N** * ‖ [0.151942 0.833740 0.530841] is close to [2 11 7]. Since the angle between **N** * and normal (7) is small (≈ 1.23º), the agreement with the expected result can be considered quite satisfactory. The resulting direction of macroshift **S*** ‖ [0.210347 –0.693324 0.689243] is close to **b** *, and the orientation ξ_3* ‖[0.959100 0.005396 –0.283016] is close to $\mathbf{\Lambda}_1$*, so that the increment of the next layer maintains an orientation practically coinciding with the HP.

DISCUSSION OF RESULTS

According to the dynamic theory of MT, the formation of rectangular dislocation loops framing the habit, which play the role of DCN*, seems completely natural. Due to the increase in specific volume (during γ–α-MT), the austenite region adjacent to the formed martensite crystal experiences compression deformation, which prevents the formation of NWS*, which generates lateral growth, since the area of NWS* formation should be characterized by a positive value of specific volume. Therefore, excitation in the NWS* region and the NWS*-associated controlling wave process CWP* can occur if the elastic field of the dislocation loop is capable of leading to a resulting positive change in the specific volume δ in austenite. Considering that the Burgers vector **b** * is associated with macroshear, it can be expected that the magnitude of b * will significantly exceed the lattice parameter. Since, according to [5], a tensile strain of 1% is sufficient to initiate lateral growth, it is natural to assume that the strain value $\varepsilon^* \approx b^*/2\pi R$ will be of the same order. Then with $R = 200\,a$ and $\varepsilon^* = 10^{-2}$, we get $b^* = 2\pi R \cdot \varepsilon^* = 6.3 \cdot 200\,a \cdot 10^{-2} = 12.6\,a = b_1^*$.

Apparently, this estimate looks acceptable for the case of a crystal that does not reach the surface of the sample. It should be kept in mind that the crystal is in a compressed state. As a result, the deformation of shape is characterized by a relatively small magnitude of macroshear tg ψ. The vector $\mathbf{b}_1$* refers to the core of a superdislocation-type dislocation, but distributed in volume. Such carriers of crystallographic shear are briefly called crystons (see, e.g., [15]). The emergence of crystals on the sample surface is accompanied by the formation of a surface relief, clearly reflecting the presence of macroshear. Therefore, the estimation of b * can be carried out based on the parameters of such relief. For example, with a shear value of tgψ ~ 0.1 and a thickness of thin-plate crystals $d \sim 0.1$ µm ~ 300 a, the estimate gives $b^* \sim \mathrm{tg}\psi \cdot d \sim 30\,a = b_2^*$. The excess b_2* over b_1* is quite expected, since, as already noted, b_1* refers to the case when the state of the formed martensite crystal and the surrounding austenite is elastically stressed, and the shear is inhibited. The dislocation model of macroshear is presented in sufficient detail in [16].

The formation of individual martensite layers, parallel to the habit plane, can lead to the formation of stacks of parallel crystals separated by layers of distorted austenite. Such stacks, for example, are well known for packet martensite with habits close to {557}. However, the process of spatial scaling [17] of the initial excited state in the elastic field of DWC* can ensure the closure of the emerging layers, providing rapid lateral growth of the crystal.

Of course, the scenario of rapid lateral crystal growth is potentially possible and does not exclude other options. As noted in [2], during isothermal holding, thin-plate α-martensite crystals, initiated by the action of a strong magnetic field, can thicken due to the growth of thin transformation twins.

Lateral growth of a martensite crystal in shape memory alloys with lower values of final deformations does not require the application of external stresses and can proceed in both rapid and thermoelastic variants. The case of extremely thin (on the order of a) layers of lateral crystal increment corresponds to short-wave displacements with strong damping. Therefore, the growth of crystal thickness, visually perceived as a continuous process, occurs through discrete jumps with relatively long pauses. Such a dynamic picture essentially corresponds to the concept of "transformation dislocation" long introduced into phenomenological theory, which naturally correlates with an extremely narrow transformation front.

Note that obtaining an exact match of the calculated habit layer with the original habit is easily achieved when considering the quasi-longitudinal *nature of waves*. However, this is not necessary, given that the differences between habits (3 14 9) and (2 11 7) fit within the measurement error of plane orientations. Thus, the approximation of longitudinal waves used above is sufficient to demonstrate the capabilities of the dynamic theory of MT in describing the lateral growth of a martensite crystal.

CONCLUSION

The lateral growth of a martensitic crystal (like any other face) can proceed via a rapid cooperative pathway, similar to the dynamic scenario of the original crystal formation. In this case, the role of the dislocation nucleation center is played by a rectangular dislocation loop framing the habit plane, characterized by a Burgers vector that is determined by the macroshear.

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CONFLICT OF INTERESTS

The authors of this paper declare that they have no conflict of interest.

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