PHYSICAL NATURE OF fcc-bcc MARTENSITIC TRANSFORMATION IN IRON BASED ALLOYS

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Abstract

The summary of the models offered by the author revealing features of the physical mechanisms controlling processes of martensite crystal formation is resulted. The rapid growth of a cooling martensite crystal is considered as a self-organized process controlled by the quasi-longitudinal lattice displacement waves (DW). It is shown, that processes of the heterogeneous nucleation and wave growth have the genetic connection in case of spontaneous \( \gamma \rightarrow \alpha \) martensitic transformation. The exposition of strain martensite formation is considered in the context of a cryston model.

1. Introduction

One of the most characteristic features of \( \gamma \rightarrow \alpha \) martensitic transformations (MT) is their diffusionless transformation mechanism, by means of cooperative rearrangement of the face-centered cubic (fcc) high-temperature \( \gamma \)-phase (austenite) into the body-centered cubic (bcc) or body-centered tetragonal (bct) low temperature \( \alpha \)-phase (martensite). The disclosure of the dynamical mechanisms and principles underlying the process of martensitic transformations would enlighten their intrinsic characteristics and physical nature, and can thus be regarded as one of the fundamental problems of metal physics. The reconstructive phase transitions, to which the MT is related, demonstrate pronounced features of the first-order transitions, namely, considerable temperature hysteresis (between the direct and reverse transformations) and thermal and volume effects. As is known [1] the spontaneous (cooling-induced), stress-induced and strain-induced \( \alpha \)-martensites are distinguished. Processes of martensite nucleation in all cases are heterogeneous.

Theoretical research on the \( \gamma \rightarrow \alpha \) MT is mainly characterized by the parallel development of the lattice-geometrical, thermodynamic and wave approaches. Now it is obvious that only the wave approach would have the full potential for a comprehensive description of the dynamical aspects of the transformation process in the cases of spontaneous and stress-induced martensites. In the stage of rapid martensite crystal growth there exists a boundary area between the phases being characterized by intensive electron currents within coexisting strongly pronounced temperature and - even more important - chemical potential gradients.
An electronic drift current leads to an inverted occupation of those pairs of electronic states being localized in the proximity of the s-surfaces in quasi-momentum space. This surfaces are defined by the condition that the projection of electronic group velocity towards the orientations of $\nabla T$ or $\nabla \mu$ must vanish at all points of the s-surfaces. The number of pairs of inversely occupied electronic states of the 3d-bands of iron is a macroscopic quantity. The process of generation of atomic displacement waves is energized by stimulated emission of phonons during transitions of the non-equilibrium 3d-electrons between the inversely occupied states. The microscopic theory of generation of waves is in detail stated in [2] (see also [3,4]).

The constructive description of strain-induced martensite is achieved in frameworks of cryston model (definition of cryston it has been entered in [5]). In this case the crystons (the shear carriers of superdislocation type) are direct carriers of threshold strain. Thus there is clear enough fathoming of physical mechanisms for all alternatives of the $\gamma - \alpha$ martensitic transformation in iron-based alloys. The purpose of the report to have given the evident representation being accessible not only for narrow experts about the simplest models that will allow, in author opinion, to optimize the further researches of martensitic transformations.

2. Waves controlling the growth of martensite crystal

The displacement waves controlling the process of martensitic crystal growth are of the longitudinal type (or quasi-longitudinal) with frequencies of $\nu \sim 10^{10} \text{ s}^{-1}$ (region of hypersound) and amplitudes ensuring the required level of lattice deformation of $\varepsilon \sim 10^{-3}$ needed for initiation of the $\gamma - \alpha$ martensitic transformation. The mode of initial excitation of waves during the nucleation stage of the $\alpha$ phase is a hard mode [6,7]. The certain combinations of displacement waves are important but not separate waves. Thus for instance, the stage of rapid growth of a spontaneous (and stress-induced) martensitic lamellae is correlated with the propagation of a pair of perpendicularly oriented waves, stimulating the process of flat lattice deformation of a combined tensile-compressive type.

It is easy to conceive from Fig.1 that the hatched area of wave-superposition, as well as the intersecting area of the wave-fronts, are simultaneously propagating at the velocity equivalent to the vector-sum (i.e. geometrical sum) of their individual velocities $c_1 \perp c_2$, i.e.

$$c = c_1 + c_2, \quad c = |c| = \sqrt{c_1^2 + c_2^2}. \quad (1)$$

As the value of $|c|$, on the one hand, characterizes the frontal speed of growth
Figure 1. Fundamental growth pattern of a martensite lamella in the notion of two flat longitudinal waves propagating perpendicular to each other: $c_1, c_2$ - wave-velocities, $\lambda_1, \lambda_2$ - wavelengths.

of a martensite lamella, and on the other hand can exceed the longitudinal velocity of sound in direction of $c$ in Fig.1 it is possible in principle to explain this way the aligned supersonic growth of martensite crystals (being controlled by a pair of ordinary longitudinal waves), thus inherently representing an important kinetic particularity of the growth stage. From Fig.1 it is also obvious that the normal line to a habit plane of a growing crystal is set to the vector $\vec{N}$, being collinear with the normal vector of the plane defined by the vectors $[c_1, c_2]$ and $c$, by the following vector-product

$$N = [c, [c_1, c_2]] = c_1 \cdot c_2^2 - c_2 \cdot c_1^2.$$  \hspace{1cm} (2)

If the concerning short waves are included into control waves system the fine twinning may be described too [8,9].

3. **Heterogeneous nucleation in elastic fields of dislocations**

The elastic field of dislocations disarranges the original lattice symmetry by selecting regions being most favorable for martensitic nucleation. Such a region features the shape of a perpendicular parallelepiped, its edges being oriented along the
eigenvectors $\vec{\xi}_i$ of the distortion tensor $\hat{\varepsilon}$, its eigenvalues $\varepsilon_i$ satisfying the following conditions:

$$\varepsilon_1 > 0, \quad \varepsilon_2 < 0, \quad |\varepsilon_3| \ll |\varepsilon_{1,2}|,$$  \hspace{1cm} (3)

thus ensuring the existence of slightly distorted surfaces (SDS) with normals

$$(\mathbf{N}_{SDS})_{1,2} \parallel \vec{\xi}_2 \mp \vec{\xi}_1 \sqrt{\frac{\varepsilon_1}{|\varepsilon_2|}}, \quad |\vec{\xi}_{1,2}| = 1.$$ \hspace{1cm} (4)

Obviously, from a point of view of minimization of elastic distortion energy, phase-coupling is supported by weakly distorted (with $\varepsilon_3 = 0$ invariants) planes. Thus it would be reasonable to expect that the normal of the habit-plane of the martensite crystal should match with one $\mathbf{N}_{DS}$. In fact, among the $\mathbf{N}_{DS}$, there exist $60^\circ$-dislocations with lines $\langle 110 \rangle$ situated near $\langle 557 \rangle$, $\langle 225 \rangle$ and $30^\circ$-dislocations with lines $\langle 121 \rangle$ situated near $\langle 259 \rangle$, $\langle 31015 \rangle$, being evidence of certain differences among the NC of packet vs. explosive-martensite. Moreover, in the orientational relationship of the phase-lattice, there are included the slip-plane and the dislocation line, the latter one acting as a nucleation center, which suggests us to give preference to the Kurdjumov-Sachs- or Nishiyama-relationships, for various NC.

The question related to the orientation of macroscopic shear $\mathbf{S}$ will be resolved in conjunction with the choice of one of the two orientations of the normal $\mathbf{N}_{SDS}$. For this aim, let us consider the notation of the distortional tensor in the elastic field, being represented as the sum of two diad products, and discriminate the part containing two addends:

$$\mathbf{S}_1 \cdot \mathbf{N}_1 + \mathbf{S}_2 \cdot \mathbf{N}_2, \quad |\mathbf{N}_{1,2}| = 1.$$ \hspace{1cm} (5)

We recall that the diad product $\mathbf{S} \cdot \mathbf{N}$ defines a deformation with an invariant plane, where $\mathbf{N}$ - normal of a plane and $\mathbf{S}$ - vector characterizing the deformation. Further considering that austenite is metastable at the beginning of the martensitic transformation at $M_S$ temperature, it is justified in the case of $|\mathbf{S}_1| > |\mathbf{S}_2|$, to surmise that the plane with the normal $\mathbf{N}_1$ is distinguished, and that the anticipated orientation of macroscopic shear is close to $\mathbf{S}_1$. And vice-versa, for $|\mathbf{S}_2| > |\mathbf{S}_1|$, the components $\mathbf{N}_2$ and $\mathbf{S}_2$ will be discriminated, respectively. The results of this approach are in good accordance with experimental results [10,11].
4. Synthesis of concepts of the heterogeneous nucleation and of the wave growth of martensite crystals

With this approach, all macroscopic morphological characteristics of martensite attain a reasonable interpretation within the conceptual notion of nucleation at dislocations, where dislocations act as centers of forces disturbing the original lattice symmetry, their effect not being confined to the nuclear volume. These findings match in detail with the ideas of the wave theory of growth, presupposing that the transformation starts with the emergence of an excited state with the shape of a parallelepiped, built up of vectors $\vec{\xi}_i$, its pairs of edges oscillating in opposed phase, thereby exciting controlling displacement waves orientated in the wave-normal $\vec{n}_{1,2}$ close to $\vec{\xi}_{1,2}$. In the most simple approximation of the equations

$$\mathbf{n}_1 = \vec{\xi}_1, \quad \mathbf{n}_2 = \vec{\xi}_2,$$  \hspace{1cm} (6)

the requirement of correspondence of $\mathbf{N}_{SDS}$ with the wave-habit (2) delivers the following condition:

$$\kappa = \frac{c_2}{c_1} = \left( \frac{\varepsilon_1}{|\varepsilon_2|} \right)^{1/2},$$  \hspace{1cm} (7)

which, if satisfied, ensures the possibility of a kinematic agreement of the wave description with the deformation description of the habit. Fig.2 diagrammatically reflexes the process of nucleation in an elastic field of an edge dislocation and the growth controlling by the waves. As against Fig.1 the image three-dimensionally. The displacement waves exist in the shape of the wave bundles propagating in co-ordination with the spatially limited front of a wave of relative volume deformation and making the function of a ”pilot-waves”, paving the way for the martensitic reaction in their wake.

Obviously, given the case that the ratio of tensile and compressive deformation in the wave-mode corresponds with $\kappa^2$, then dynamic agreement will also be achieved. We further note that for the $\gamma - \alpha$ -transformation, which proceeds with increase of specific volume: $\varepsilon_1 > |\varepsilon_2|$. Consequently, $c_2 > c_1$, so that the tensile strain can be prescribed by the wave propagating with the smaller velocity $c_1$, whereas compressive strain can be prescribed by the wave propagating with the larger velocity $c_2$. (In the case of the $\alpha - \gamma$ -transformation, the situation will just be inverted.)
5. Crystons controlling the growth of $\alpha$ strain induced martensite crystal

The strain-induced martensite formation is considered as a consequence of carry of a threshold plastic deformation by crystons. The sources of crystons (carriers of shear of a superdislocation type) are caused by interaction of dislocations belonging to systems with intersected slip planes. Thus, the role of a pinned segment of an individual dislocation in the classic Frank-Read source is now played by a dislocation braid (Fig. 3, region AC restricted by dashed lines), and the result of generation is a cryston (superdislocation) loop, which can be considered as a set of closed loops localized in the region bounded by a surface that is topologically similar to a torus.

As is shown in [12,13] the basic features of the strain-induced martensite is described if to consider the cryston as the carrier of the threshold deformation having character of simple shear.
Figure 3. Typical for $\gamma$-phase generalized Frank-Read source of crystons with the total (superpositional) Burgers vector $\vec{b} \parallel n\vec{b}_1 + m\vec{b}_2$.

6. Conclusion

It is significant that concepts of the heterogeneous nucleation and the strain controlling the crystal growth (the last is localized in the frontal region of the growing crystal) are the universal for the exposition of martensite crystal formation. However the dynamic nature of controlling processes, as well as mechanisms of their energy support, essentially discriminate. For case of the cooling martensite this is the controlling wave process that is supported in the maser regime by nonequilibrium electrons due to the generation of energy in transforming phase. For case of the strain martensite this is the process of the cryston propagations that are supported in basic by energy of exterior stresses.

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