DOI 10.1007/s11041-016-9998-3
Metal Science and Heat Treatment, Vol. 58, Nos. 5 – 6, September, 2016 (Russian Original Nos. 5 – 6, May – June, 2016)

UDC 669.1'24:539/371

PROMISING VERSIONS OF α-MARTENSITE ROD-LIKE CRYSTAL INITIATION IN IRON ALLOYS BY THREE ELASTIC WAVE SOURCES

M. P. Kashchenko[1, 2] and V. G. Chashchina[1, 2]

Translated from *Metallovedenie i Termicheskaya Obrabotka Metallov*, No. 5, pp. 9 – 13, May, 2016.

Versions are provided for α-martensite rod-shaped crystal initiation by three orthogonal longitudinal elastic waves propagating in orthogonal directions of the types $\langle 001\rangle_\gamma$ and $\langle 110\rangle_\gamma$ in Fe – 31% Ni single crystals. The probability is considered of direct initiation by Bain-type deformation waves. It is demonstrated within the scope of dynamic theory that the anticipated orientation of rod-like crystals is close to $\langle 111\rangle_\gamma$ or to $\langle 905\rangle_\gamma$. Possible features of martensite crystal tetragonality are discussed. Ultrasound source power required for initiating martensitic transformation is determined.

Key words: dynamic theory, martensitic transformation, rod-shaped crystals, tetragonality, ultrasound power source.

INTRODUCTION

The entirety of describing features of martensitic transformation (MT) in iron alloys achieved currently [1] points to the adequacy of the theory. Nonetheless, it is interesting to set up experiments making it possible either to introduce clarification in the value of parameters, or to demonstrate the direct consequences of the theory. We recall that the simplest but entirely adequate scheme for martensite crystal growth is based on the concept of a controlled wave process (CWP).

The essence of the new paradigm, supplementary to the traditional equilibrium thermodynamic scheme, comes down to interpretation of the dynamic structure of the excited state of a metal lattice in the equilibrium region of a non-linear transformation wave front. Spontaneous (during cooling) MT commences with development of an initial excited state (IES) in an elastic field of a dislocation generation center. The oscillatory nature of IES generates a controlled wave process, supporting threshold strain, and disturbing original phase stability.

The typical lamellar shape of martensite crystals (or their central regions-midribs), and also their crystallographic orientation, is naturally described in the CWP model including a pair of quasilongitudinal (or longitudinal) wave beams, generating IES in the form of an elongated rectangular parallelepiped [1 – 4]. In the case of γ – α MT waves supporting the threshold strain of a compression-tension type facilitate the start of Bain type deformation.

We recall (see for example [5]) that Bain deformation includes compression along one of the axes $\langle 001\rangle_\gamma$ and synchronous tension along a pair of orthogonal axes $\langle 100\rangle_\gamma$, $\langle 010\rangle_\gamma$ (or $\langle 110\rangle_\gamma$, $\langle 1\bar{1}0\rangle_\gamma$). Versions of a CWP, including participation of short-wave movements, for describing almost all features of spontaneous γ – α MT (for cooling martensite) have been described in sufficient detail in [6].

In this work the task is set and discussed of physical modeling of the initial excited state of metal in the form of a vibrating cube (with ribs along the $\langle 100\rangle_\gamma$ axis) or a rectilinear parallelepiped with a pair of equal ribs a along axis $\langle 110\rangle_\gamma$ and a third rub c along $\langle 001\rangle_\gamma$ with a c/a ratio close to $\sqrt{2}$.

As first noted in [7], with occurrence of IES in the form of an oscillating cubic cell with vibration directions along rib $\langle 100\rangle_\gamma$ it is possible to expect formation of rod-shaped martensite crystals along $\langle 111\rangle_\gamma$. In fact, the moving line (line of intersection of two wave fronts) "marks" the plane of lamellar crystal habit. Similarly the moving point (point of intersection of three fronts) "marks" the line prescribing orientation of a rod-shaped crystal.

The aim of this work is to consider the most promising versions of forming a rod-shaped morphotype for α-martensite crystals by direct stimulation of Bain type deformation.

[1] Ural Federal University, Ekaterinburg, Russia (e-mail: mpk46@mail.ru).
[2] Ural State Wood Technology University, Ekaterinburg, Russia.

METHODS OF STUDY

A suitable material for preparing single-crystal specimens may be alloy Fe – 31% Ni. The M_s temperature for the start of spontaneous $\gamma - \alpha$ MT for this alloy is below room temperature ($M_s \approx 230$ K). as a result of this it is comparatively simple to prepare a required specimen shape with three orthogonal edges having a normal along axis $\langle 100 \rangle_\gamma$. In order to simulate conditions for occurrence of an IES in the form of an oscillating cube it is natural to place three identical sources of longitudinal elastic waves at orthogonal boundaries close to one rib of a specimen. Normally as typical elastic wave sources films of substance are used with a piezoelectric or magnetostriction effect. The position of sources (in the form of deposited films) shown in Fig. 1 schematically corresponds to three gray areas in orthogonal areas of a cube, adjacent to one tip. Presence of parallel specimen boundaries in Fig. 1 creates the potential possibility of forming a regular structure of standing waves due to application of incident and reflected waves in the case of weakly attenuated waves (for example for ultrasound of the megahertz frequency range). However, it cannot be considered with a pulsed wave source regime (as also for waves of gigahertz range, exhibiting marked attenuation).

Indeed, simulation of conditions independent of the dislocation center for generation of an IES occurrence will be more probable, the lower the dislocation density appears (ideally their zero density). In the opposite case stress-induced martensite will be realized, not entirely typical, when crystals arise with a habit similar for cooling martensite, but with a markedly smaller number of versions compared with the complete collection of 24 versions.

As discussed in detail in [2 – 4, 6, 8] a transverse IES diameter typical for spontaneous MT is $d \approx 10^{-2} L$, where L is size of a region free from defects, with a distantly acting elastic wave. At the same time $d \sim \lambda/2$. This means that with values of $d \sim 1$ μm typical for the first finely lamellar crystals we are talking about waves with a frequency of $\nu \sim 1$ GHz and scales $L \sim 10^2$ μm; the latter corresponds to a dislocation density $L^{-2} \sim 10^4$ cm^{-2}.

It is pertinent to remember that in the arrangement of the problem under discussion wave length λ markedly exceeds the lattice parameter, and therefore it is entirely adequate in describing controlling wave process propagation to use approximation of a solid (but anisotropic) medium.

In the case when the role of the generation center produces an individual dislocation, independent of the type of dislocation, Burger's vector b has a value of the order of the lattice spacing.

Then at distances r from a linear defect of the order of $0.1L$ as an estimate of the value of threshold strain it is possible to take a value comparable with dislocation elastic deformation field, and in fact $\varepsilon_t \sim b/2\pi r$. This means that for perfect single crystals with $L \sim (10^2 - 10^3)$ μm roughly $\varepsilon_t = (10^{-5} - 10^{-6})$. Considering an estimate of strains based on conversion of the thermal effect during martensitic transformation into vibration energy of two longitudinal modes with orthogonal polarization vectors [1, 2], the values provided may be considered as limiting the value of ε_t from below.

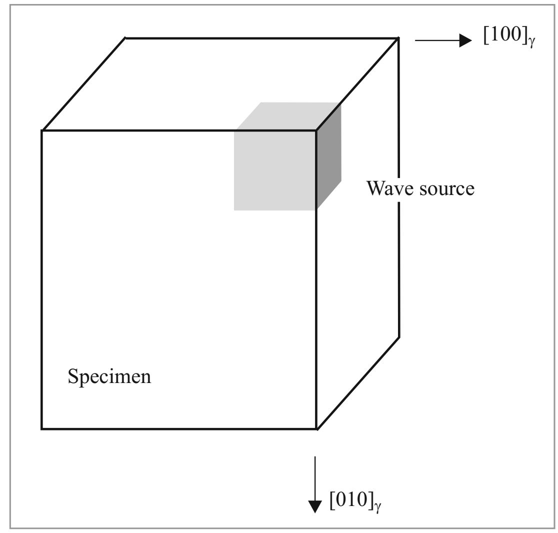

Fig. 1. Diagram of the arrangement of longitudinal elastic wave sources for initiating rod-like crystal grain growth along $\langle 111 \rangle_\gamma$. Deposited material coating films are colored gray, exhibiting piezoelectric or magnetostriction effects providing elastic wave excitation.

By carrying out specimen cooling with three active wave sources, providing fulfilment of the condition $\varepsilon > \varepsilon_t$, it is possible to calculate the start of rod-shaped crystal growth along $\langle 111 \rangle_\gamma$ in the region of wave source application (region to the right in the upper part of Fig. 1). Since below room temperature in Fe – Ni alloys component diffusion is almost entirely suppressed, cooling may be carried out slowly and make it possible to establish reliably the temperature for the start of transformation with a prescribed wave source power.

It should be noted that the fact of appearance of rod-shaped crystals would indicate realization of IES physical modeling of a new (equiaxed) configuration. We recall that physical modelling of an IES in the form of an extended parallelepiped by action of laser pulses with a track shape close to linear, has been realized previously at the surface of a single crystal (for example [9 – 12]). In addition, the possibility also arises of refining the estimate of threshold strains.

CALCULATION PROCEDURE AND DISCUSSION OF RESULTS

Connection of threshold strains with maximum strains in waves

In evaluating threshold strains it is convenient to consider elastic description of a material since as is well known application of elastic deformation shifts the temperature for the start of deformation.

It easy to be sure that by analogy with a two-wave scheme [6] that in a region of compressive and tensile strain application

$$\varepsilon_1(\zeta_1, \zeta, \zeta_3) = \varepsilon_{1\max}\cos(k_1\zeta_1)\,\varphi(\zeta_1, \zeta_2, \zeta_3);$$

$$\varepsilon_2(\zeta_1, \zeta_2, \zeta_3) = -\,|\varepsilon_2|_{\max}\cos(k_2\zeta_2)\,\varphi(\zeta_1, \zeta_2, \zeta_3); \quad (1)$$

$$\varepsilon_3(\zeta_1, \zeta_2, \zeta_3) = \varepsilon_{3\max}\cos(k_3\zeta_3)\,\varphi(\zeta_1, \zeta_2, \zeta_3),$$

where $\zeta_1 = y - v_1 t$, $\zeta_2 = y - v_2 t$, $\zeta_3 = z - v_3 t$, Θ is Heaviside singularity function. The function

$$\begin{aligned}\varphi(\zeta_1, \zeta_2, \zeta_3) = [\Theta(\zeta_1 - d_1/2) - \Theta(\zeta_1 + d_1/2)] \times \\ [\Theta(\zeta_2 - d_2/2) - \Theta(\zeta_2 + d_2/2)] \times \\ [\Theta(\zeta_3 - d_3/2) - \Theta(\zeta_3 + d_3/2)]\end{aligned} \quad (2)$$

describes movement of an excited region with a rate equal to the vector sum of velocities v_1, v_2, v_3 of longitudinal wave beam propagation with wave numbers $k_{1,2,3}$ along mutually perpendicular directions *x*, *y*, and *z* respectively; $d_{1,2,3}$ are IES dimensions.

In describing strains in an IES it is natural to consider that the threshold strain is realized at the boundaries of an effective cell, within which an inequality is fulfilled: $\varepsilon_1 > \varepsilon_{1t}$, $|\varepsilon_2| > |\varepsilon_{2t}|$, $\varepsilon_3 > \varepsilon_{3t}$.

It is clear that with a totally identical nature of wave sources an equality will be fulfilled $k_1 = k_2 = k_3$, $d_1 = d_2 = d_3$, $v_1 = v_2 = v_3 = v$, $(\varepsilon_1)_{\max} = |\varepsilon_2|_{\max} = (\varepsilon_3)_{\max}$. For a linear connection $\omega = vk$ between cyclic frequency ω of radiation and quasipulse *k* it is easier to find the connection of useful power P_{use} of a wave source with $\varepsilon_{\max}$. In fact, vibration energy density

$$\begin{aligned}W = 1/2\rho\omega^2 u_{\max}^2 = 1/2\rho(vku_{\max})^2 = \\ 1/2\rho v^2(2\pi u_{\max}/\lambda)^2 = 1/2\rho v^2\varepsilon_{\max}^2,\end{aligned} \quad (3)$$

where ρ is substance density; $u_{\max}$ is vibration amplitude. The product *wv* is the value of energy flow (analog of the Umov–Poynting vector). Consequently,

$$P_{\text{use}} = wvS = 1/2\rho v^3\varepsilon_{\max}^2 s, \quad (4)$$

where *s* is specimen surface contact area with a wave source. With a known frequency (and this means wavelength λ), taking $\tilde{d}$ for thickness of a rod-shaped martensite crystal diagonal length $d\sqrt{3}$ of a cubic IES cell, in a harmonic approximation (1) we find:

$$\begin{aligned}\varepsilon_t = \varepsilon_{\max}\cos(kd/2) = \varepsilon_{\max}\cos(k\tilde{d}/2\sqrt{3}) = \\ \varepsilon_{\max}\cos(\pi\tilde{d}/\lambda\sqrt{3}).\end{aligned} \quad (5)$$

This means that by establishing the value of $\varepsilon_{\max}$ from data for the wave source power and measuring thickness $\tilde{d}$ from (5) we can easily find ε_t.

Possibility of using ultrasonic wave sources

As the analysis carried out above showed, with quite low dislocation densities (about 10^4 cm^{-2}) the frequency of external sources is of the order of 10^9 Hz, i.e., it pertains to the hypersonic range ($10^9 - 10^{13}$) Hz. Normally a frequency of 10^9 Hz is taken conditionally as an upper boundary of the ultrasonic range. However, if due to thorough annealing of single crystals it is possible to prepare specimens with a lower order of dislocation density, then it is possible to calculate for appearance of an IES also with use of ultrasonic waves close to the upper frequency limit.

We show that fulfilment of condition $\varepsilon \geq \varepsilon_t$ is entirely real, at least with $\varepsilon_t \approx 10^{-6}$. For this we evaluate the useful power of an electronic wave source. Assuming that $\varepsilon_{\max} \approx \varepsilon_t \approx 10^{-6}$, $S = 1$ cm$^2 = 10^{-4}$ m^2, $v = 5 \times 10^3$ m/sec, $\rho = 8 \times 10^3$ kg/m^3, from Eq. (4) we find: $P_{\text{use}} = 5 \times 10^{-2}$ W. With a condition that P_{use} is of the order of 0.1 of the total power, we are talking about an ultrasonic wave generator with power of 0.5 W, which is suitable for existing generators.

It might be expected that with a sufficient approximation to M_s, strains in waves propagating from an IES essentially (by an order of magnitude) exceed the threshold level. As evaluation in [1] shows, on the basis of the value observed for a thermal effect, this is very probable.

Transition from threshold strains to final

The term “final” (or “finishing”) strains has been introduced in order to avoid ambiguity in using the term “finite” applied to strains. In fact, for martensitic transformation with clear signs of first order phase transition, threshold strains are also finite. Final strains ε_f markedly exceed threshold strains and are realized after transition of austenite lattice losing stability into a metastable steady state, corresponding to α-phase. We recall [1 – 4] that in a threshold regime for pure longitudinal waves the ratio of k^2 of tensile strains ($\varepsilon_1 > 0$) to compressive strain modulus ($|\varepsilon_2|$) almost equals the ratio of the squares of wave velocities $\kappa_2 = (v_2/v_1)^2$. Previous analysis of spontaneous martensitic transformation shows that the ratio of strains prescribed in a threshold regime remains unchanged up to achievement of final values. In view of this it is interesting to follow the conclusion to which this requirement leads as applied to a version of initiating MT by elastic wave sources.

1. We assume that all ultrasound sources are identical and excite wave beams along axis $\langle 100\rangle_\gamma$. Then the expected form of IES will be a vibrating cube. Application of three running wave beams, stimulating triaxial Bain type deformation will initiate formation of rod-shaped crystals, extended along the $\langle 111\rangle_\gamma$ direction growing with a supersonic velocity

equal to $\sqrt{3}v_\Delta$ is, where v_Δ is longitudinal wave velocity along fourth order axis of symmetry $\langle 100\rangle_\gamma$. It should be noted that the rate of rod-shaped crystal growth exceeds the growth rate not only of lamellar crystal with a $(1\bar{1}0)_\gamma$ habit, equal to $\sqrt{2}v_\Delta$, but also the growth rate for crystals with $(259)_\gamma - (3\ 10\ 15)_\gamma$. habits typical for these compositions. As a result of this if it is possible to realize threshold conditions for the start of rod-shaped crystal growth with approach towards the M_s temperature, their formation may have be entirely competitive in depletion of the energy resource, releasing energy of a metastable persistent phase. It is typical that for rod-shaped crystals orientated along the $\langle 111\rangle_\gamma$ direction, the emerging BCT lattice will have tetragonality

$$t = \sqrt{2}\,(1 - \varepsilon_{1f})/(1 + \varepsilon_{1f}). \qquad (6)$$

In case of its realization this tetragonality will be a natural consequence of equality in a threshold regime of values of all strains and assumption about retention of the ratio of strains with a change-over from a threshold regime to a final stage. These conditions are entirely fulfilled [1 – 4, 6, 13, 14] for spontaneous $\gamma - \alpha$ and $\alpha - \varepsilon$ (BCC – HCP) martensitic transformations. If a typical value of $\varepsilon_{1f} = \varepsilon_{1B} \approx 0.13$ is adopted for Bain deformation, then $t \approx 1.09$, which is an anomalously high value for Fe – Ni-alloys in the absence of carbon. If it is assumed that $t = 1$, then the value of final strain is $|\varepsilon_{2f}| = \varepsilon_{1f} = 0.1716$. We note that with this strain the BCC lattice parameter $a_\alpha = a_\gamma$ will markedly exceed a_α for standard (Bain value) of compressive strains $|\varepsilon_{2B}| = 0.2$.

2. Let a pair of sources stimulate expansion strains along axes $[110]_\gamma$ and $[1\bar{1}0]_\gamma$, and a third source provides compressive strains along axis $[001]_\gamma$. Then growth of a rod-shaped crystal will occur with velocity $v_\Delta\sqrt{1+2/\kappa^2} > \sqrt{3}v_\Delta$ since $\kappa < 1$. Rods have an orientation along direction $\langle\sqrt{2}\ 0\ \kappa\rangle_\gamma$. We select for illustration evaluation of elastic moduli [15] for alloy Fe – 31.5Ni, TPa: $C_L = 0.218$; $C' = 0.027$; $C_{44} = 0.112$; $C_{11} = C_L + C' - C_{44} = 0.133$. Then $\kappa = \sqrt{C_{11}/C_L} \approx 0.78108$. This means orientation of rod-shaped crystals will be close to $\langle 905\rangle_\gamma$.

By changing the power of sources it is easy to fulfil a condition for equality of the ratio of squares of wave and strain velocities [1 – 4, 6]. In this case assuming as previously retention of the ratio of strains with transition from a threshold regime to the final stage we obtain

$$t = \sqrt{2}(1 + \varepsilon_{2B})/(1 + \varepsilon_{1B}). \qquad (7)$$

If the final vale of tensile strain $\varepsilon_{1B} \approx 0.13$, then for compressive strain we obtain $\varepsilon_{2B} \approx -\varepsilon_{1B}/\kappa^2 \approx 0.13/0.61 \approx 0.213$, and according to (7) $t \approx 0.985 < 1$, i.e., in this case parameter c of a BCT lattice is less than parameter a.

It is clear that with presence of two final characteristics ε_{1B} and t, only connected by one Eq. (6) or (7), it is impossible to determine both values clearly. However, by selecting one of the characteristics of some reasonable range of values it is easy to find the value of the other. A search for an additional defining relationship (for example from any extreme principle) in this case leads to incorrect complication of the problem not guaranteeing calculation of all significant factors. As a result of this an entirely constructive way of carrying an experiment is with fulfilment of morphological analysis making it possible to establish a specific pair of quantities of final values.

CONCLUSIONS

In single-crystal alloys with compositions close to Fe – 31% Ni and Fe – 31.5% Ni using three longitudinal wave beam sources (with wave vectors strictly along the axis of fourth order symmetry or fourth and second orders) it is possible to expect initiation of α-martensite rod-shaped crystal growth along direction $\langle 111\rangle_\gamma$ or $\langle 905\rangle_\gamma$. It should be noted that these orientations do not depend on values of final characteristics.

With retention of the ratio of threshold strains up to the final stage it is also possible to expect additional morphological differences between rod-shaped crystals and crystals of cooling martensite, depending however on the amount of final strain.

Confirmation of clear differences with respect to orientation (and possibly degree of tetragonality) for rod-shaped crystals initiated by three ultrasound sources is important since it opens up additional research possibilities. Finally, the main difficulties in realizing atypical morphotypes is connected with the use of relatively high-frequency elastic wave sources and fulfilment of threshold conditions. In view of this the situation may appear to be more favorable in stimulating martensitic transformation in an alloy with small strains, both threshold and final, for example with martensitic transformation $B2 - B19$ in alloys based on titanium nickelide.

Work was carried out with financial support of the RFFI (project number 14-08-00734).

REFERENCES

1. M. P. Kashchenko, *Wave Model for Growth of Martensite with γ – α Transition in Alloys Based on Iron* [in Russian], NITs “Regular and random dynamics,” Izhevsk Inst. Of Computer Research, Moscow – Izhevsk (2010).
2. M. P. Kashchenko and V. G. Chashchina, “Dynamic model of supersonic martensite crystal growth,” *Usp. Fiz. Nauk*, **101**(4), 345 – 364 (2011).
3. M. P. Kashchenko and V. G. Chashchina, “Formation of martensite crystals in the limiting case of supersonic growth rate,” *Pis’ma Mater.*, **1**, 7 – 15 (2011).
4. M. P. Kashchenko and V. G. Chashchina, “Fundamental achievements of the dynamic theory of reconstructive martensitic transformation,” *Mater. Sci. Forum*, **738 – 739**, 3 – 9 (2013).

5. G. V. Kurdyumov, L. M. Utevskii, and R. I. Éntin, *Transformations in Steel and Iron* [in Russian], Nauka, Moscow (1977).
6. M. P. Kashchenko and V. G. Chashchina, *Dynamic Model of Twinned Martensite Crystal Formation with* $\gamma - \alpha$ *Transformation in Iron Alloys* [in Russian], UGLTU, Ekaterinburg (2009).
7. M. P. Kashchenko and V. P. Vereshchagin, "Generation centers and wave schemes for martensite growth in iron alloys," *Izv. Vyssh. Uchebn. Zaved., Fizika*, No. 8, 16 – 20 (1989).
8. M. P. Kashchenko, V. G. Chashchina, and S. V. Konovalov, "Evaluation of the stored elastic energy resource with assembly of similar martensite crystals in a symmetrical model," *Metalloved. Term. Obrab. Met.*, No. 7, 33 – 37 (2012).
9. M. P. Kashchenko, V. V. Letuchev, S. V. Konovalov, and S. V. Neskoromnyi, "Laser sounding of the initial stage of $\gamma - \alpha$ martensitic transformation," *Izv. Ross. Akad. Nauk, Ser. Metally*, No. 2, 105 – 108 (1992).
10. M. P. Kashchenko, V. V. Letuchev, S. V. Konovalov, and S. V. Neskoromnyi, "Physical modeling of α-martensite generation," *Fiz. Met. Metalloved.*, **67**(1), 146 – 147 (1992).
11. V. V. Letuchev, S. V. Konovalov, S. V. Neskoromnyi, and M. P. Kaschenko, "Initiation of the $\gamma - \alpha$ martensitic transformation in iron-based alloys by picosecond pulses," *J. Mater. Sci. Lett.*, No. 11, 1683–1684 (1992).
12. V. V. Letuchev, S. V. Konovalov, and M. P. Kashchenko, "Dynamical lattice state at the initial stage of martensitic transformation and possibilities of its physical realization," *J. de Physique IV, Colloque C2*, **5**, 53 – 58 (1995).
13. M. P. Kashchenko and V. G. Chashchina, "Mechanism of HCP – BCC martensitic transformation with the most rapid rebuilding of densely packed planes. 2. Orientation relationships," *Izv. Vyssh. Uchebn. Zaved., Fizika*, No. 11, 42 – 47 (2008).
14. M. P. Kashchenko and V. G. Chashchina, ""Crystal dynamics of BCC – HCP martensitic transformation. 2. Martensite morphology," *Fiz. Met. Metalloved.*, **196**(1), 16 – 25 (2008).
15. G. Haush and H. Warlimont, "Single crystalline elastic constants of ferromagnetic centered cubic Fe – Ni invar alloys," *Acta Metall.*, **21**(4), 400 – 414 (1973).