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Correlation of velocities of the waves controlling the thin-plate α-martensite formation and the modulation of the transformation twin structure

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For the case of γ-α martensitic transformation (MT) in iron alloys, the concept of transformation twins is developed. As a rule, crystals of α-martensite having the form of thin plates are characterized by a fine twin structure (TS) with interchanging orthogonal directions of main compression axes. An example of the real structures of transformation twins that are not strictly regular is given. It is shown that in dynamic theory of MT the regular TS initiation is associated with coherent propagation of long (ℓ) and short (s) displacement waves belonging to controlling wave process (CWP). An analytical approximation of the dispersion law of s-waves is obtained. The threshold conditions of deformation and the qualitative picture of modulated TS formation are discussed. The correlation of velocities of the waves controlling thin-plate α-martensite crystals formation is established by the example of Fe-30Ni alloy. It is shown that at the real correlation of wave velocities a modulated structure of transformation twins is induced. Such structure contains fragments each of which is connected with the short-wave excited cell. The fragment size is associated with N_{bas} — the number of layers of the main component inside the TS fragment generated by a single spontaneously activated s-cell. Fragments' sizes depend on the site of localization of spontaneously appearing s-cell generating the fragment in the area of the CWP front. It is shown that the N_{bas} value can vary within rather wide limits. Therefore, in contrast to regular TS forming, we should expect repeated s-cells spontaneous excitements for long enough twinned thin-plated crystals. Along with difference of s- and ℓ-waves velocities, consideration of waves (especially s-waves) decay is one more quite determined factor making its contribution into TS modulation. Estimation of this contribution seems to be very actual.

Keywords: martensitic transformations, transformation twins, dynamic theory, controlling wave process, fragment of twin structure.

Соотношение скоростей волн, контролирующих формирование тонкопластинчатого α-мартенсита, и модуляция структуры двойников превращения

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Для случая γ-α мартенситного превращения в сплавах железа разъясняется понятие двойники превращения. Как правило, кристаллы α-мартенсита в форме тонких пластин характеризуются тонкой двойниковой структурой (ДС) с чередующимися ортогональными направлениями главных осей сжатия. Приводится пример реальных структур двойников превращения, не являющихся строго регулярными. Показывается, что в динамической теории мартенситных превращений инициация регулярной ДС связывается с согласованным распространением относительно длинноволновых (ℓ) и коротковолновых (s) смещений в составе управляющего волнового процесса (УВП). Проводится аналитическая аппроксимация закона дисперсии s-волн. Обсуждаются пороговые условия деформации и качественная картина формирования модулированной ДС. На примере сплава Fe-30Ni установлено соотношение скоростей волн, управляющих формированием тонкопластинчатых кристаллов α-мартенсита. Показано, что при реальном соотношении скоростей волн индуцируется модулированная структура двойников превращения. Подобная структура содержит фрагменты, каждый из которых связан со своей коротковолновой возбужденной ячейкой. Размер фрагмента связывается с числом слоев N_{bas} основной компоненты внутри фрагмента ДС, порождаемого единственной спонтанно активированной s-ячейкой. Размеры фрагментов зависят от места локализации возникающей спонтанно s-ячейки, порождающей данный фрагмент, в области фронта УВП. Показано, что величина N_{bas} может изменяться в достаточно широких пределах. Значит, в отличие от формирования регулярной ДС, для достаточно длинных двойникованных тонкопластинчатых кристаллов следует ожидать неоднократных спонтанных возбуждений s-ячеек. Наряду с различием скоростей s- и ℓ- волн, учет затухания волн (в первую очередь s-волн), является еще одним вполне детерминированным фактором, оценка вклада которого в модуляцию ДС представляется весьма актуальной.

Ключевые слова: мартенситные превращения, двойники превращения, динамическая теория, управляющий волновой процесс, фрагмент двойниковой структуры.

1. Introduction

Crystals of α-martensite in the form of thin plates generated during martensitic transformation (MT) in iron-based alloys are characterized by habit planes (habits) close to $\{31015\}_\gamma-\{259\}_\gamma$ [1]. In most cases, such crystals have a fine twin structure (TS) with interchanging orthogonal directions of main compression axes. However, as experiments on initiating MT by strong magnet fields have shown [2], thin-plate crystals having no transformation twins can be formed as well. In crystal geometry approach [3] the occurrence of a regular TS (or regular shift system) is a necessary condition for initiation of crystals with habits $\{31015\}_\gamma-\{259\}_\gamma$. To provide a macroscopic invariance of habits during MT, each habit plane should correspond to a strictly determined ratio β of TS components. However, as seen from Fig. 1, TS specifies only a tendency for regularity, and β magnitude can vary inside one martensite crystal (intervals of such variations are given in [4]).

Such data are incompatible with conclusions of [3] and especially with the above-mentioned fact of TS absence in some cases.

The general ideology and main applications of the dynamic theory of MT in the case of γ-α MT in iron-based alloys have been reported in [5–11]. In particular, the problem related to the formation of a regular structure of transformation twins in supersonic mode has been fairly completely elucidated in [6, 9, 10]. TS initiation is associated with a coherent propagation of long (ℓ) and short (s) displacement waves belonging to the controlling wave process (CWP). Although in [6, 9, 10] variants of a dynamic formation of regular TS were analyzed, there is no grounds for the above-mentioned collision between calculated and experimental data because only ℓ-waves are responsible for the generation of a habit surface. The key role of TS description (along with supersonic rate of crystal growth) in understanding of the nature of MT was underlined in [11], where the reasons leading to variations in the volumes of TS components have been also enumerated.

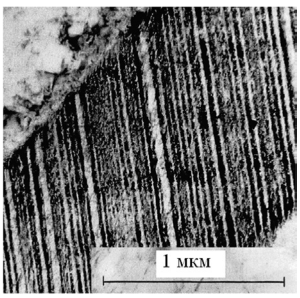

Fig. 1. Typical structure of martensite crystals in 52KhN23 steel (twinned thin-plate crystal) [2]. Pulsed magnetic field 100 kOe, temperature 77 K.

The purpose of the present work is to analyze the effect of a very important factor upon modulation of TS structure, namely, the deviation of the ratio of s- and ℓ-waves velocities from the value characteristic for a regular TS structure realization.

2. The dynamic model of regular TS formation

Let us remind, for the readers' ease, the model of TS formation. According to [5, 6, 9, 10], the condition of ideal synchronizing of s- and ℓ-waves looks as:

$$v_s = v'_\ell \cos\psi, \qquad (1)$$

where v'_ℓ is the projection of velocity v_ℓ onto the surface $(001)_\gamma$, and ψ is the sharp angle between v'_ℓ and $v_s \parallel <001>_\gamma$ (see Fig. 2).

The condition (1) itself can easily be obtained from the requirement that the times of propagation of s-waves superposition along the legs of the triangle marked out at Fig. 2 with velocity $\sqrt{2}v_s$ and along the hypotenuse of this triangle — with velocity v'_ℓ are equal. In the model presented at Fig. 2, the exciting of neighbor s-cell in vicinity to previously activated cell takes place with a lag $T_s/2$, where T_s is the period

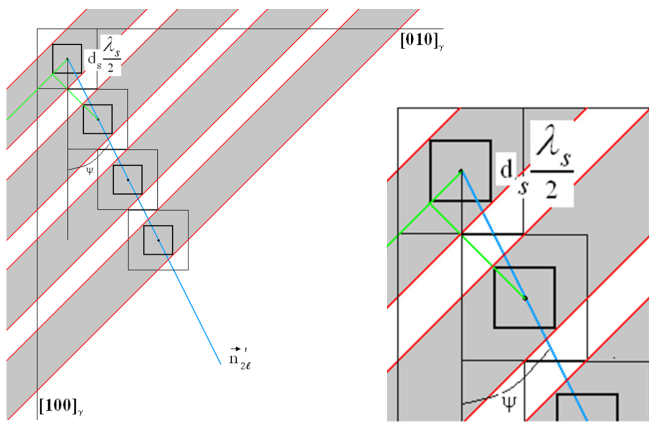

Fig. 2. The dynamic model of formation of regular laminated structure with the ratio of components' volumes 2:1.

of s-oscillation (in our previous works this obstacle has been considered though without accentuation). Such a condition seems to be natural. The oscillations in adjacent quadratic cells with side $\lambda_s/2$ really occur in antiphase. Therefore, after $T_s/2$ the phase of oscillations that occurred in previously activated s-cell will be reproduced in neighbor area. Besides, short lag restricts the possibility of substantial decay of s-waves, which fact is important for fulfillment of the threshold condition of lattice stability loss in the site of a new s-cell activation. It is also useful to remind that superposition of the pair of s-wave beams running in orthogonal directions «sweeps up» a plate-formed area $\lambda_s/\sqrt{2}$ thick. However, as deformations vanish at the bounds of this area, lattice stability is lost only in the area $d_s/\sqrt{2}$ thick provided that $d_s < \lambda_s/2$. By the way, forming of a new crystal of main TS component also occurs inside the area $\lambda_s/\sqrt{2}$ thick adjacent to the area $d_s/\sqrt{2}$ thick that has just appeared.

Let us state additionally that formation of regular TS structure presupposes fulfillment of the following conditions. At the initial moment of time s-cell is so localized that its center is congruent with ℓ-cell center, the oscillation phases match up the maximum deformations in cell centers, the wave velocities satisfy condition (1), and wave decay may be neglected. It must be underlined that, if all these conditions be kept, a single s-cell is enough for regular TS initiation.

3. The approximation of *s*-waves dispersion law and the estimation of difference between the wave velocities by the example of alloy Fe-30%Ni

Condition (1) of regular TS formation requires knowledge of the laws of phonon ε_k dispersion along $<001>_\gamma$-directions for any wave vectors $\mathbf{k}$, as matching of ℓ- and s-waves velocities for k_ℓ and k_s, at $k_s >> k_\ell$ is necessary. The law of ε_k dispersion along $<001>_\gamma$ for $0 \le k \le k_{max} = 2\pi/a$ (a — lattice parameter) is approximated in dimensionless variables y and x by the function

$$1 - y = (1 - x)^p, \quad y = \varepsilon_k/(\varepsilon_k)_{max}, \quad x = k/k_{max}. \qquad (2)$$

For example, for alloy Fe30Ni with fcc lattice, a satisfactory concordance with experimental data (both in long-wave and short-wave areas) is achieved at $p \approx 1.733$. Excluding short-wave range, the values of group $v_g(x) = dy/dx$ and phase velocities $v_p(x) = y/x$ for s-waves are not significantly different ($v_p(x) \ge v_g(x)$). Therefore, assuming that k_s values are at least one order of magnitude lower than k_{max}, we conserve nomination v_s without such detailing, paying attention to difference between the velocities v_s and v'_ℓ in (1).

For crystals with habits close to $\{31015\}_\gamma - \{259\}_\gamma$, the angle ψ is changed from ≈16.7° to ≈21.8° and $0.9578 \ge \cos\psi \ge 0.9285$. At values of elastic modules [12] for alloys Fe-Ni even without taking into account the dispersion along $<001>_\gamma$, the values v_s/v'_ℓ do not belong to the interval of $\cos\psi$ values, although close to it. Thus, for habits $\{31015\}_\gamma$ $v_\ell/v_s \approx 1.17$, and $v'_\ell/v_s \approx 1.155$, i.e. $v_s/v'_\ell \approx 0.8655$. Estimation shows that, considering the concrete alloy Fe-30Ni, we get an inequality

$$v_s < v'_\ell \cos\psi, \qquad (3)$$

and $\Delta v = v'_\ell \cos\psi - v_s \approx 0.11 v_s$, can be accepted as a real value of the difference in velocities leading to TS modulation.

4. The threshold conditions of deformation and the qualitative picture of modulated TS formation

The information on Δv value principally allows to comprehend the zones with decreasing or increasing thickness of TS components observed (see Fig. 1) in twinning areas.

Let us remind that in dynamic theory [6] it is accepted that local loss of stability by initial phase lattice takes place in s-cells that satisfy the threshold condition for compressive strain ε_2

$$|\varepsilon_2| = |\varepsilon_{[100]}| = |\varepsilon_{2\ell}(d_s/2)| + |\varepsilon_{2s}(d_s/2)| \ge |\varepsilon_{2\mathrm{th}}| \qquad (4)$$

along the main axis of Bain's deformation [100] where $\varepsilon_{2\ell,s}(d_s/2)$ are the contributions of ℓ- and s-waves at the border of s-cell with cross size $d_s < \lambda_s/2$, and $\varepsilon_{2\mathrm{th}}$ is the threshold value. Certainly, the tensile strain in ℓ-wave running in the direction practically orthogonal to Fig. 2 surface is also important for three-dimensional deformation start, but for the purpose of our article it's enough to examine the compressive strain.

As the formation of thin-plate crystals (as well as crystals of packet martensite) may occur without transformation twins [2, 11], it is obvious that ℓ-waves (responsible for habits description) are able to disturb lattice stability in the area of localization of the initial excited state (IES) with cross size $d_\ell < \lambda_\ell/2$ regardless of s-waves existence. Therefore, the contribution of $\varepsilon_{2\ell}(d_s/2)|_{\mathrm{th}}$ is significant, and fast growth of main TS component takes place in the lattice losing its resistance against ℓ-waves. Thus it is quite natural that the growth of twin components is terminated on the boundary (habit) surfaces of martensite crystal (it's well seen at Fig. 1).

Concerning the fact that threshold deformations at temperatures close to M_s are minimal (M_s is a temperature of MT start), it will be acceptable to use harmonic approximation in our analysis to describe the wave deformations. Then, if we place the coordinate origin in the center of quadratic s-cell, the deformation at cell border will have such standard look in moment t:

$$|\varepsilon_{2\ell}(t, d_s/2)| = |\varepsilon_{2s}|_{max} \cos(\omega_s t - k_s d_s/2), \quad \omega_s = v_s k_s, \quad k_s d_s/2 = \pi d_s/\lambda_s. \qquad (5)$$

The initial phase in (5) is chosen so that the cell center corresponds to maximum deformation $|\varepsilon_{2s}|_{max}$ at $t = 0$ (as seen at Fig. 1). Similarly, for the compressive strain in ℓ-wave

$$|\varepsilon_{2\ell}(t, d_s/2)| = |\varepsilon_{2s}|_{max} \cos(\omega_\ell t - k_\ell d_s/2), \quad \omega_\ell = v_\ell k_\ell, \quad k_\ell d_s/2 = \pi d_s/\lambda_\ell. \qquad (6)$$

It is obvious from (5) that the decrease of size d_s is accompanied by the increase of $|\varepsilon_{2s}(d_s/2)|$, therefore fulfillment of the request (4) at some interval of deviations from regular TS formation conditions appears to be possible due to the decrease of d_s value.

5. The estimation of the number of laminas of the main TS component generated by a single spontaneously activated cell

Let us accept that the centers of s- and ℓ-cell coincide in a moment $t = 0$ in the area of IES localization, wave decay is not considered (as it's accepted by conclusion (1)), but the inequality (3) is fulfilled. Thus it is obvious that initiation of the next s-cell at the front will lag behind in respect to ℓ-cell center transfer. Let us evaluate by what magnitude $|\varepsilon_{2\ell}(d_s/2)|$, level will decrease at that. If difference between the velocities after $T_s/2$ makes Δv, in the area of activation of the nearest new s-cell a path-length difference $\Delta v\, T_s/2$ will arise between s- and ℓ-waves deformation maximums. As a result, levels of deformations $|\varepsilon_{2\ell}(\pm d_s/2)|$ will change and be different.

Taking for example $\Delta v \approx 0.11 v_s$, we find $\Delta v\, T_s/2 \approx 0.11\, \lambda_s/2$. According to the data from Table 2 in [6], for our case of interest the values $\text{tg}\psi = 1/3$, $d_s/\lambda_s = 1/5$ are acceptable at the ratio of regular TS components $\beta = 3/2$. It means that path-length difference $0.11\, \lambda_s/2$ makes near 27% of d_s. Therefore, the level of $|\varepsilon_{2\ell}(t, +d_s/2)|$ at one of the borders of the lattice (*here and further the coordinate is measured from the center of new excited cell*) will first increase (at successive activation of four new cells) and then decrease. And the level of $|\varepsilon_{2\ell}(t, -d_s/2)|$ at other border of the cell will be only decreased. However, if the inequality $\lambda_s << \lambda_\ell$ is fulfilled, changes of $|\varepsilon_{2\ell}(t, d_s/2)|$ may be relatively small. Assuming, for certainty, $|\varepsilon_{2\ell}(t, -d_s/2)|$, we'll illustrate the above words, regarding that $|\varepsilon_{2\ell}(t, -d_s/2)|$ will drop from the value $|\varepsilon_{2\ell}(0, -d_{s0}/2)| = |\varepsilon_{2\ell}|_{\max}\cos(k_\ell d_{s0}/2)$ in the initial moment of time to the value

$$|\varepsilon_{2\ell}(nT_s/2, -d_{s0}/2)| = |\varepsilon_{2\ell}|_{\max}\cos[k_\ell(n\Delta v T_s/2 + d_{s0}/2)] \qquad (7)$$

in the moment $t_n = nT_s/2$. In (7) n corresponds to the number of s-cell in the succession of cells that are activated in discrete moments of time $t_n = nT_s/2$ by the superposition of s-waves after spontaneous activation of zero cell, but the change of cell width is not considered. Thus at $\lambda_\ell = 50\lambda_s$ and $\Delta v T_s \approx 0.11\,\lambda_s/2$ and initial size $d_{s0}/\lambda_s = 0.2$, from (7) for normalized deformations Δ_n

$$\Delta_n = |\varepsilon_{2\ell}(nT_s/2, -d_{s0}/2)| \,/\, |\varepsilon_{2\ell}|_{\max} \qquad (8)$$

we find:

$$\Delta_n = \cos[\pi(n\,0.11 + 0.2)\,\lambda_s/\lambda_\ell] = \cos[\pi(n\,0.11 + 0.2)/50] \qquad (9)$$

Estimations obtained using (9) and differences of normalized deformations values $\Delta_n - \Delta_0$ at distances $d_{s0}/2$ from centers of the cell (the same that in zero cell) are given for comparison in Table 1.

Consequently, at the indicated conditions and parameters values, n increase is accompanied by monotonic Δ_n decrease, and its compensation has to lead to reduction of thickness of the crystals of main TS component and, correspondingly, to monotonic growth of twin component thickness. As value $\beta \geq 1$ by definition, it's possible to estimate the number of s-cell, for which inferior limit $\beta = 1$ should be achieved. According to «reference» data from Table 2 in [6], at the same $\text{tg}\psi = 1/3$, $d_s/\lambda_s = 1/6$ corresponds to value $\beta = 1$. Then, at additional condition of proximity of s- and ℓ-waves contributions into the threshold deformation, we may consider that the transition from $d_s/\lambda_s = 1/5$ to $d_s/\lambda_s = 1/6$ accompanied by growth of the level of normalized deformations from start value $\Delta_s \approx 0.81$ to finish value $\Delta_f = \sqrt{3}/2 \approx 0.866$, i.e. by ≈ 0.056, just compensates diminution of contribution $|\varepsilon_{2\ell}(t, -d_s/2)|$. From the estimates given in Table 1 it's obvious that such compensation will exist for cells with numbers $40 < n < 50$.

Let us note that value $n = 50$ listed as the last in Table 1 corresponds to maximum value $n_{\max}$ at chosen ratio $\lambda_\ell = 50\lambda_s$, because only s-cells located not more than $d_\ell/2$ far from the central one can be activated.

Let us label the number of main TS component laminas initiated by one spontaneously activated s-cell by symbol N_{bas}. As follows from the data of analysis, the maximum size $(N_{bas})_{\max}$ is achieved when the generated s-cell is localized at one of the borders of $d_\ell/2$ (signified as $+d_\ell/2$). It is the border for which the activation of successive s-cells is first accompanied by monotonic growth of $|\varepsilon_{2\ell}(t, -d_s/2)|$ and, correspondingly, monotonic growth of d_s. Then, after achievement of maxima $|\varepsilon_{2\ell}(t, -d_s/2)|_{\max}$ and $(d_s)_{\max}$, according the above scenario monotonic d_s decrease follows. The value $N_{bas} = 1$ corresponds to spontaneous s-cell localization near the second border $-d_\ell/2$. Such variant can be revealed as single basis components sharply different in width from adjacent ones. It's obvious that the probability of spontaneous activation of a cell in $d_\ell/2$ wide band substantially exceeds the probability of activation only along the central line of the band between borders $\pm d_\ell/2$. Therefore, in general number of transformation twins TS fragments with numbers N_{bas} satisfying the inequalities $2n_{\max} > N_{bas} > n_{\max}$ have to prevail. Evidently, $(N_{bas})_{\max} = 2n_{\max}$ and at $n_{\max} = 50$ we have $(N_{bas})_{\max} = 100$. By the way, TS fragments' appearance at $n_{\max} > N_{bas} > 1$ is also quite expectable.

Let us mark at last that not only the consideration of additional factors blocking the formation of regular TS structure, but also the increase of λ_s/λ_ℓ ratio, as well as the growth of Δv, lead to reduction of N_{bas} numbers correlated with different TS fragments.

6. Conclusion

Taking into account the real ratio of s- and ℓ-waves velocities on the example of Fe-30Ni alloy leads to deviation from ideal condition for regular TS formation. As a result, a modulated TS structure containing of fragments is formed. Fragments' sizes depend on the site of localization of spontaneously appearing s-cell generating the fragment in the area of CWP front. Therefore, in contrast to regular TS forming, we should expect repeated s-cells spontaneous excitements for long enough twinned thin-plated crystals.

The consideration of additional factors breaking the conditions of regular TS realizing can only reduce the length

Table 1. The dependence of normalized deformation on the number of s-cell.

n	0	1	10	30	40	50
Δ_n	0.99992	0.99981	0.99667	0.97592	0.95852	0.93655
$\Delta_0 - \Delta_n$	0	$\approx 1.1\cdot 10^{-4}$	$\approx 3.25\cdot 10^{-3}$	$\approx 2.4\cdot 10^{-2}$	$\approx 4.14\cdot 10^{-2}$	$\approx 6.34\cdot 10^{-2}$

of TS fragments (as compared with the cited values).

Along with the difference between s- and ℓ-waves velocities, the consideration of waves (especially s-waves) decay is one more quite determined factor making its contribution into TS modulation. Estimation of this contribution seems to be very actual and will be examined in another work.

The analysis provided indicates the way of reconstruction of local dynamics of the wave TS formation basing on the observed fragments of modulated TS structure, going beyond the limits of simple averaged description.

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