Shape Memory Alloys: Properties, Technologies, Opportunities

Edited by Natalia Resnina Vasili Rubanik

Shape Memory Alloys: Properties, Technologies, Opportunities

Special topic volume with invited peer reviewed papers only

Edited by

Natalia Resnina and Vasili Rubanik



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Preface

The collective monograph "Shape memory alloys: properties, technologies, opportunities" presents the scientific results obtained by leading scientific teams studying shape memory alloys in former Soviet Republics during the last decade. The scientists from Russia (Moscow, Saint Petersburg, Ekaterinburg, Chelyabinsk, Tomsk), Ukraine (Kiev) and Belarus (Vitebsk) together with their colleagues from other countries made contributions to prepare this monograph.

The collective monograph consists of five parts covering of all aspects of shape memory alloys from theory and modelling to applications. The first part is devoted to the theory of martensitic transformations and the modelling of functional properties of shape memory alloys. New methods for the simulation and prediction of the behaviour of shape memory alloys under different stress temperature regimes are described. The wave model for the description of martensite crystal growth at different sequences of martensitic transformations and the analysis of recent achievements in theoretical description of phase transformation in Heusler alloys are presented. The second part is devoted to the physical basis for the development of shape memory alloys, including unique properties such as high-temperature shape memory alloys, high-strength single crystals of shape memory alloys and ferromagnetic shape memory alloys. The third part is devoted to the methods for controlling functional properties of shape memory alloys by thermomechanical treatment, warm deformation, electroplastic deformation, high strain rate loading, ultrasonic vibration and neutron irradiation. The fourth part is devoted to the study of martensitic transformation and shape memory effects in special objects such as porous alloys, thin ribbons, high-strength precipitation-hardening austenitic steels and alloving TiNi-based alloys. Finally, the fifth part contains a review of shape memory alloy applications in Russia.

All chapters were peer-reviewed by expert referees. As the guest editors of the volume, we are grateful to the authors who prepared the chapters. We wish to acknowledge all those who reviewed the papers submitted to the monograph.

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I. Theory and Modeling of Martensitic Transformation and Functional Properties

Possible Wave Processes Controlling the Growth of Martensite Crystals at B2-B19, B2-B19' and B2-R Transformations

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Keywords: dynamic model, martensitic transformation, morphological parameters, titanium nickelide, intermediate mesoscopic state.

Abstract. Basic directions in the theory of martensitic transformations are briefly listed. Within the framework of the dynamic theory based on the synthesis of concepts of heterogeneous nucleation and wave growth of martensite crystals, the possibilities of description of morphological parameters during the B2 \rightarrow B19, B2 \rightarrow B19', B2 \rightarrow R transformations are analyzed. It is demonstrated that the calculated and observed habit planes and orientation relationships can be matched.

In particular it is demonstrated that an introduction of the notion of the intermediate mesoscopic state during the $B2 \rightarrow B19'$ transformation is expedient for a description of the observed morphological parameters. The {78 39 48}_{B2} habit planes of the B19' phase can be associated with standard dislocation nucleation centers.

It is noted that the exact inheriting of elastic fields of a dislocation nucleation center is possible. This is a necessary condition for explanation of the effect of transformation reversibility upon thermocycling.

The results obtained are briefly discussed.

Introduction

The phenomenon of martensitic transformation (MT) as a specific variant of the realization of a polymorphic transformation associated with a cooperative mechanism of atomic displacements attracts wide attention of researchers. On the one hand, an MT modifies the properties of a material and therefore plays an important practical role (it suffices to mention the process of quenching steels or a shape memory effect in NiTi alloys). On the other hand, it is quite interesting to construct a physical theory of MTs that would not be limited to fragmentary explanations of separate aspects of this phenomenon but rather would enjoy a high degree of completeness of description of all significant observable properties. It is obvious that such a theory should be based on a clear understanding of the physical nature of the mechanism of control of the structure rearrangement. It is evident that in the case of metals and alloys that represent electron-ion systems, we should first of all understand what features and states of the subsystems are necessary for the development of the MT. The issue is complicated by the fact that in different metallic systems, the MT can occur via different scenarios, which include the differentiation not only of the structures of the initial and final phases but also of the character of the phase transition, whose manifestations in some cases correspond to a limit version of a second-order transition, while in other cases, - to a clearly pronounced first-order transition. The understanding of both limit cases seems to be important. Until recently, the main problems are currently related precisely to the explanation of the MT mechanism in the case of distinctly pronounced first-order transitions.

This is not surprising because such a transition occurs upon a significant deviation from the point of equilibrium of the phases, and the strongly supercooled (or superheated) system is an active medium capable of liberating energy. Consequently, under nonequilibrium conditions, the MT mechanism that ensures the fastest rate of energy liberation may be unrivaled. Detecting such a mechanism requires revising familiar concepts of first-order phase transitions, in particular, revising the problem of the existence of equilibrium (quasi-equilibrium) nuclei of a new phase. It is obvious that in a metallic system, the mechanism of propagation of the fastest relaxation of energy is related to a wave process, and the appearance of waves is related to the initial excited (oscillatory) state of ions, which is maximally efficient for triggering the process of rapid growth of the new phase. In turn, this initial state is localized in those regions of space where, owing to the influence of the elastic fields of defects (e.g., ordinary dislocations), a significant decrease occurs in the interphase energy barrier. This explains the specific character of heterogeneous nucleation. And, finally, the case that is richest in physical contents is where the maintenance of a high (threshold) level of deformations at the front of the control wave process (CWP) is possible due to the participation of the electronic subsystem.

The physically transparent picture described in an above general representation corresponds to a new paradigm of MTs that allows consistently describing a large body of observed facts and removing problems that seemed to be insurmountable for theoretical constructions based on the traditional quasi-equilibrium approach.

In making the final conclusions, we can state that the current model of the formation of a martensite crystal (including the stages of heterogeneous nucleation, wave growth, and accommodation of the coexisting phases) in the case of a spontaneous (in the process of cooling) $\gamma-\alpha$ martensitic transformation in iron alloys realized in single crystals or in polycrystals with large grain sizes D is generally complete [1-4]. The high degree of the completeness of the description of the observed features of the transformation suggests a new paradigm of the dynamic theory of the spontaneous $\gamma-\alpha$ MT.

The scheme in fig. 1 reflects an important role of the concept of initial exited state (IES) within the limits of new paradigm of MT. This concept has essentially completed the ideas of physics of first-order phase transitions on the initial stage of transformation. A deduction on the existence of the controlling wave process and its supersonic speed is a direct consequence of this.

IES is a region having the shape of an elongated rectangular parallelepiped with transverse dimensions d1, 2 (d1 \sim d2 \sim d) that is constructed on orthogonal eigenvectors of the tensor of elastic deformations of the defect (as a rule, a dislocation). It is important that d makes about one hundredth of the size of defect-free volume. The relation between spatial scales together with the condition for occupation of states of the electrons generating waves allows explaining an Ms dependence on D (Ms is the temperature of MT start and D is the size of austenite grain).



Fig. 1. Key position of the concept of Initial Excited State in dynamical theory of MT [2]

This conclusion can also be related to the dynamic theory of the formation of stress-assisted martensite (upon cooling in an external elastic field), in which case we simply observe a reduction in the number of realized variants of orientations of martensite crystals (compared to that observed in the case of a spontaneous transformation).

For the completeness of the analysis, we recall that at grain sizes exceeding the critical size D_c , apart from the above-considered cooling-induced martensite, crystals of deformation-induced martensite can be formed (at the stage of plastic flow), which is related to the carriers of threshold

deformation called crystons. The crystons (shear superdislocation carriers that arise upon the contact interaction of dislocations with intersecting slip planes) specify the orientations of habit planes during their propagation [5-7]. Fig. 2 displays the formation scheme of a cryston due to the interaction of n and m dislocations with different initial slip systems.



Fig. 2. Generalized Frank-Read source (typical of the fcc phase) of crystons each of which is characterized by a total (superposition) Burgers vector $\vec{b} = n\vec{b}_1 + m\vec{b}_2$.

The cryston concept is also efficient in describing shear bands with an arbitrary crystallographic orientation of planar boundaries.

Fig. 3 schematically shows the logical structure of the dynamic approach to the description of martensitic transformations.

The conformity of the theory to the observed picture of a γ - α MT is beyond doubt. Here is a list of the main obtained achievements and solved problems. 1. The new model of martensite nucleation in elastic fields of dislocations. 2. The concept of the initial exited state. 3. The identification of the characteristic spatial scales at the nucleation. 4. The mechanism of generation of elastic waves by nonequilibrium electrons. 5. The supersonic growth speed of martensite crystals. 6. The transition from threshold to ultimate deformations. 7. The interpretation of all observed macroscopic morphological features (habitus, macroshear and orientation relationships of the initial and final phase lattices). 8. The martensite crystal twinning in the course of $\gamma - \alpha$ martensitic transformation [4, 8]. 9. Analytical formula for the critical size of austenite grains $D_c (M_s (D_c) = 0)$ has been obtained [1, 9, 10]. 10. The dependence of D_c on significant physical parameters was analyzed. 11. The existence of the special concentration C* (for $C \rightarrow C^*$, $M_s \rightarrow 0$, $D_c \rightarrow \infty$). 12. An explanation of the dependence of the size D_c on the strong magnetic field H and, as a result, the effect of destabilization of austenite preliminarily stabilized via grain refinement or severe plastic deformation. 13. An estimation of the macroscopic fraction of martensite for self-similar kinetics of ensembles of martensitic crystals in the model of symmetric orthogonal joints [11]. 14. The description of the profiles of martensite crystals formed in a medium containing planar inhomogeneities [12, 13]. 15. The calculation of critical rates of cooling of an austenite [14]. 16. The estimations of scales of incubatory times during the forming of a macroplate of bainitic ferrite [15].

This opens a wide field of activity for using the diverse tools of physical acoustics in the analysis of the morphological features of separate crystals (e.g., of plate-like or wedge-like forms), their junctions (acute and obtuse), mutual intersections, interactions with grain boundaries, etc., on the basis of the concepts of the CWP as a superposition of wave beams propagating in metastable austenite and capable of disturbing its stability. As regards other promising avenues of investigations, we note the possibility of extending the applicability of the theory to bcc-hcp and hcp-bcc transitions [16, 17], which require an additional short-wavelength "reshuffling" of planes (which does not affect the macroscopic morphological features).

The purpose of this paper is to show that the concept of the controlling wave process is efficient also in the case of MTs in titanium nickelide-based alloys.



Fig. 3. Key points of the description of a martensitic reaction in single crystals and in polycrystalline materials with the grain size exceeding the critical size D_c .

Theory Procedure

The key role in a new paradigm is played by the concept of the IES appearing in the elastic field of a dislocation nucleation center (DNC). The oscillatory character of the IES generates a control wave process resulting in the threshold deformation disruption of the stability of the initial phase. In the simplest case the synthesis of concepts of heterogeneous nucleation and wave growth is reached if we consider that the wave normals \vec{n}_1 and \vec{n}_2 of wave beams in the CWP, describing in the superposition region the tensile ($\varepsilon_1 > 0$) and compression strain ($\varepsilon_2 < 0$), are collinear to the eigenvectors $\vec{\xi}_i$ (*i* = 1, 2) of the strain tensor of the elastic defect field in the nucleation region (see Fig.4):



Fig. 4. Wave model of controlling growth of a martensite crystal (the segment bounded by the symbols \perp corresponds to a dislocation line).

$$\vec{\mathbf{n}}_1 \| \vec{\xi}_1, \, \vec{\mathbf{n}}_2 \| \vec{\xi}_2, \, \vec{\mathbf{n}}_1 \perp \, \vec{\mathbf{n}}_2, \, | \, \vec{\mathbf{n}}_1 | = | \, \vec{\xi}_i | = 1.$$
 (1)

The normal \vec{N}_w to the habit plane associated with CWP propagation is set by the relationship

$$\dot{N}_{w} \parallel \ddot{n}_{2} - \ddot{n}_{1} a, \ a = v_{2} / v_{1},$$
 (2)

where v_1 and v_2 are the moduli of the velocities of wave propagation in the \vec{n}_1 and \vec{n}_2 directions. For the small threshold strains ε_{th} , there holds true the relationship

$$\mathbf{a} = \mathbf{v}_2 / \mathbf{v}_1 = \mathbf{k} = \sqrt{\varepsilon_1 / |\varepsilon_2|} \tag{3}$$

The reconstructive γ - α MT in iron-based alloys possess clearly pronounced properties of cooperative phase transitions of the first kind, whereas in the B2 titanium–nickelide-based alloys, the characteristics of transitions of the first kind are expressed to a lesser degree. From three widespread MT variants (B2 \rightarrow B19, B2 \rightarrow R, and B2 \rightarrow B19'), we consider at first the B2 \rightarrow B19 transition with the greatest relative change of the volume.

Results and Discussion

 $B2 \rightarrow B19$ MT for simplest variant (wave vectors along the axes of symmetry). Here the attention is focused on CWP cases [16-18] providing the fastest transformation of the $\{110\}_{B2}$ planes. The present paragraph is aimed at demonstration of the possibility of a choice of the deformable plane convenient for a description of the B2 \rightarrow B19 (and B2 \rightarrow B19') MT through the intermediate mesoscopic state.

We begin by considering of expected habit planes and DNC for quenched martensitic crystals. Based on the data on the elastic moduli of Ti–Ni–Cu and Ti50–Ni38–Cu10–Fe2 systems presented in [19-22], the elastic moduli (in GPa) are assumed to be

$$C_{11} = 165, C_{12} = 139, C_{44} = 34.$$
 (4)

Setting in Eq. (2) $\vec{n}_1 \parallel [110]_{B2}$ and $\vec{n}_2 \parallel [001]_{B2}$ (the $(1 \overline{1} 0)_{B2}$ plane is deformed), we find

$$\vec{N}_{w} \parallel [-\boldsymbol{x} - \boldsymbol{x} \sqrt{2}]_{B2}, \, \boldsymbol{x} = \sqrt{\frac{2C_{11}}{C_{11} + C_{12} + 2C_{44}}} \,.$$
 (5)

Substitution of elastic moduli (4) into Eq. (5) yields

$$a \approx 0.9419 \text{ and } N_w \parallel [\overline{1} \ \overline{1} \ 1.5015]_{B2}$$
 (6)

that is, the $\{223\}_{B2}$ habit planes, as well as $\{334\}_{B2}$ ones (for small deviations of \vec{n}_1 and \vec{n}_2 from the symmetry axes), are easily realized in the wave description. It is well known (for example, see [23, 24]) that the necessary conditions for the formation of the corresponding IES exist in elastic fields of edge dislocations with a $\begin{bmatrix} 1 & 1 & 0 \end{bmatrix}_{B2}$ direction of dislocation lines. Recall that the habit planes, close to $\{223\}_{B2}$ and $\{334\}_{B2}$, are observed in Ti–Ni–Cu [25].

The B19 phase is orthorhombic; therefore, the additional requirement caused by the lattice symmetry during an α - ϵ MT (see [17]) is absent, and it is impossible to determine analytically the final strains only from the known ratio of their values. However, knowing the lattice parameters for the initial and final phases, it is possible to verify whether the observable ratio of final strains is in agreement with the ratio of threshold strains according to the requirement (3). Fig. 5 taken from [19] shows elementary cells of phases.



Fig. 5. Elementary cells of B2 (*a*), B19 (b and c), and B19' phases (d) in titanium nickelide alloys and their size-orientation relations and reorganization schemes determined by shuffle (of $\{011\}<100>$ and $\{01\overline{1}\}<011>$ types) displacements of atoms (the $\{011\}_{B2}$ shear planes are hatched). The Fig. 5 corresponds to Fig. 3.12 in [19].

It should be borne in mind that Fig. 5 displays only approximate correspondence of cell sizes of the initial B2 phase. For example, setting the cell size in the $[100]_{B2}$ direction equal to $a_{B2} = 0.3$ nm, the sizes in the $[011]_{B2}$ and $[01\overline{1}]_{B2}$ directions must be set equal to $\sqrt{2} a_{B2} \approx 0.42426$ nm rather

than 0.43 nm. Below it is expedient to take advantage of experimental data for the lattice parameters with greater number of significant digits. Thus, according to [25], we have

$$a_{\rm B2} = 0.3030 \text{ nm}, a_{\rm B19} = 0.2881 \text{ nm}, b_{\rm B19} = 0.4279 \text{ nm}, c_{B19} = 0.4514 \text{ nm}.$$
 (7)

A comparison of data (7) with data in Fig. 5 demonstrates the maximum difference between values of the parameter b_{B19} .

From Fig. 5 it is clear that the final strains of the B2 phase cell are determined by formulas

$$\varepsilon_{[100]} = (a_{B19} - a_{B2})/a_{B2}, \ \varepsilon_{[01\bar{1}]} = (b_{B19} - \sqrt{2} a_{B2}) / (\sqrt{2} a_{B2}), \ \varepsilon_{[011]} = (c_{B19} - \sqrt{2} a_{B2}) / (\sqrt{2} a_{B2}).$$
(8)

From Eq. (8) with values of the parameters given by Eq. (7) we obtain

$$\varepsilon_{[100]} \approx -0.04917, \varepsilon_{[01\bar{1}]} \approx -0.00142, \varepsilon_{[011]} \approx 0.05343.$$
 (9)

Since the strain $\varepsilon_{[01\overline{1}]} \approx -0.00142$ in Eq. (9) is 10 times less than the two others, it is obvious that the plane $(01\overline{1})_{B2}$ experiences the fastest tensile-compressive strain in the orthogonal $[100]_{B2}$ and $[011]_{B2}$ directions. Choosing $\varepsilon_{[011]} \approx 0.05343$ for ε_1 and $\varepsilon_{[100]} \approx -0.04917$ for ε_2 , we obtain the ratio of strains

$$\varepsilon_1 / |\varepsilon_2| \approx 1.0865. \tag{10}$$

From Eq. (6) we obtain $a^2 \approx 0.8872$. According to Eq. (10), $\varepsilon_1/|\varepsilon_2| > 1$ and $a^2 < 1$; therefore, the ratio of the final strains deviates from that set by condition (3) in the threshold regime.

We note that the fulfillment of condition (3) would mean smaller tensile strain value in comparison with the compressive strain for a pair of relatively long-wavelength beams (ℓ -beams), responsible for the formation of the habit plane of a martensite crystal. An analogous situation is observed during a γ - α MT in iron-based alloys. Moreover, by analogy with [16], it is clear that in the presence in the CWP structure of relatively short-wavelength displacements (*s*-beams) responsible for the formation of the main component of transformation twins (with alternating principal tension axes), condition (3) can be met for ℓ -beams up to the final strains for the B2–B19 MT as well.

However, B19 martensite, as a rule, is not twinned. In this case, in our opinion, another transformation scenario not discussed earlier can be observed.

Hypothesis about the intermediate mesoscale state. Since the strain rate of B19 martensite crystals is high and the observed habit planes are easily described by the wave model, it is possible to assume that actually, the CWP induces the first (main) stage of the fastest strain of the $(01\overline{1})_{B2}$ plane. In this stage, the final compression strain ε_2 and the intermediate value of the tensile strain ε_1 are attained. The subsequent stage is associated with additional (rather small) stretching in the [011]_{B2} direction caused, most likely, by electron correlations. Then the CWP will determine the parameters a_{B19} and c'_{B19} according to the condition $\varepsilon_1/|\varepsilon_2| \approx \alpha^2$. For example, for $|\varepsilon_2| = 0.04917$ and $ae^2 = 0.8872$, we obtain $\epsilon_1 \approx 0.04362$, i.e., the strain $\epsilon_1 \approx 0.01$ is retained for the second stage. The lattice parameter c'_{B19} is $\sqrt{2} a_{B2}(1 + \epsilon_1) \approx 0.4472$ nm. This sequence of transformations is also suitable for a description of the $B2 \rightarrow B19'$ transformation. Indeed, it is convenient to consider the fast formed (due to CWP stimulation) state as an unstable intermediate mesoscale state (IMS), which has emerged after realization of the compression strain ε_2 along [100]_{B2} and tensile strain ε_1 = $(c'_{B19}-\sqrt{2} a_{B2})/(\sqrt{2} a_{B2})$ along $[011]_{B2}$. The IMS \rightarrow B19 transition is accompanied by additional stretching in the $[011]_{B2}$ direction (and possibly by a smaller strain in the $[01\overline{1}]_{B2}$ direction). The IMS $\rightarrow B19'$ transition is associated with the coordinated tension along $[011]_{B2}$ and compression along $[01\overline{1}]_{B2}$. We note that tensile and compressive strains for the IMS \rightarrow B19' transition are approximately equal. This means that the IMS \rightarrow B19' transition can proceed in the wave mode for which the condition (3) holds true, because the velocities of waves in the equivalent directions are identical and hence $\alpha = 1$.

Orientation relationship. First of all, proceeding to orientation relationships (OR) for the IMS, we note that for the fastest transformation of a plane, for example, $(011)_{B2}$, it is possible to expect that this plane will enter into OR:

$$(011)_{B2} \| (001)_{B19}, \tag{11}$$

and the given plane will be orthogonal to the habit one. The misorientation angle $\Delta \varphi$ for the corresponding directions is equal to $\varphi(\alpha)-\varphi_0$. Value φ_0 is the misorientation angle for the corresponding directions after homogeneous deformation without turning the lattice as a whole. According to [4, 17], one of the variants of recording the analytical dependence of the $\varphi(\alpha)$ on the wave velocity ratio α has the form

$$\varphi(\boldsymbol{x}) = \arccos \frac{\Gamma + \boldsymbol{x}^2}{\sqrt{(\Gamma^2 + \boldsymbol{x}^2)(\boldsymbol{x}^2 + 1)}}, \quad \Gamma = \frac{1 + \varepsilon_1}{1 - |\varepsilon_2|}.$$
(12)

In the case of the B2–IMS transition, the replacement $\varepsilon_1 \rightarrow \varepsilon'_1$ in Eq. (12) should be borne in mind. In the examined case, the angle $\varphi(\mathfrak{x})$ describes rotation of the $<100>_{B2}$, $<01\overline{1}>_{B2}$ reference basis vector pair about the $<011>_{B2}$ axis. Substituting in Eq. (12) $\mathfrak{x}^2 \approx 0.8872$, $\varepsilon_1 \approx 0.04362$, $|\varepsilon_2| = 0.04917$, and $\Gamma \approx 1.0976$, we obtain $\varphi(\mathfrak{x}) \approx 2.6516^\circ$.

Additional strain during IMS-B2 and IMS-B19 rearrangements leads to an increase in $\varphi(a)$ within the limits of 3°. It should be noted that the Bain variant of the orientation relations equivalent to the special case of OR (11) and (12) at $\varphi = 0$ was indicated in [19] as the OR for the B2 \rightarrow B19' and B2 \rightarrow B19 transformations. Our estimate of the OR demonstrates that the OR must be determined as exact as possible to judge the mechanism of cooperative transformation. In our opinion, the exact fulfillment of the Bain OR would demonstrate that the conditions for material rotation of the lattice were not met in experiments with foils under examined conditions. In the general case, OR (11), (12) are preferable.

Dynamical model of the B2 \rightarrow B19'MT with taking into account an intermediate state. As indicated in [19], the B19' phase can be formed directly from the B2 phase after (or simultaneously with) the B2–B19 and B2–R transitions. In particular, the possibilities for initiation of the direct B2–B19(19') transformation with the formation of the habit planes close to $\{78 \ 39 \ 48\}_{B2}$ observed in [26] within the limits of the concepts of heterogeneous nucleation and wave growth were studied in [24, 27, 28]. Based on the data about the orientation relationships between the lattice of Ti₃Ni₄ particles (precipitated in the process of aging) and the lattice of the B2 phase, the dislocation with line orientation $<1\overline{2}0>_{B2}$ associated with the elastic field of particles and untypical of the homogeneous B2 phase was chosen. It was demonstrated that this dislocation can play the role of a nucleation center for the crystals with the habit planes $\{78\ 38\ 48\}_{B2}$ and for the crystals with the habit planes $\{0.868 \ 0.269 \ 0.414\}_{B2}$ observed in [29]. In [30, 31] it was shown that the $\{78 \ 38$ 48_{B2} habit planes for crystals of the B19' phase can also be associated with the standard orientations of dislocation lines $\Lambda \parallel <111>_{B2}$ and $\Lambda \parallel <110>_{B2}$. For this purpose, it must be taken into account that the initial stage of forming the B19' phase is associated with the influence of elastic fields of dislocations inherited by an intermediate mesoscopic state (IMS) after the $B2 \rightarrow IMS$ transition [30] or by the B19 phase after the B2 \rightarrow B19 transition [31]. It was shown that dislocations change the orientation of the lines $\vec{\Lambda}$ by $\vec{\Lambda}'$ due to strain of unit cells and of the lines $\vec{\Lambda}'$ by $\vec{\Lambda}''$ due to material rotation (12). As a result, the martensite crystals with the {0.78 0.39 0.48_{B2} habit planes are associated with nucleation in elastic fields of dislocations with lines whose

orientations $\vec{\Lambda}''$ virtually coincide with the habit planes after strain and material rotation as it is evident from Table 1.

This means you can describe the growth of martensitic crystals in the wave mechanism, but with the change in the orientation of the dislocation lines in inheritance. Thus, the use of orientations $\vec{\Lambda} \parallel < 1 \, \overline{2} \, 0 >_{B2}$ is not obligatory though possible [23, 27, 28].

Table 1. Transformation of Orientations of Dislocation Lines Λ	during the B2 \rightarrow IMS Conversion
(θ', θ'') are the angles between $\vec{\Lambda}', \vec{\Lambda}''$ and habit plane)	

→

\vec{N}_w	$\vec{\Lambda}$	$ec{\Lambda}'$	$ec{\Lambda}''$	θ', [°]	θ″, [°]
0.48	[1]0]	0.95083	0.915672		
0.39		-1.02181	-1.052355	1.69	0.48
0.78	+	-0.02181	-0.052355		
-0.48	[101]	0.95083	0.983952		
0.78		0.02181	-0.009853	1.69	0.48
0.39	_	1.02181	0.990147		
0.48	$[\overline{1}01]$	-0.95083	-0.915672		
0.78		0.02181	0.052355	1.69	0.48
0.39	+	1.02181	1.052355		
0.48	[110]	0.95083	0.915672		
-0.39		1.02181	1.052355	1.69	0.48
-0.78	_	0.02181	0.052355		
0.48	[11]	-0.95083	-0.881533		
-0.39		1.04362	1.0736067	1.62	0.15
0.78	+	1.04362	1.0736067		
0.39	[]11]	-0.95083	-0.881533		
-0.48		1.04362	1.0736067	1 00	0.51
0.78	+	1.04362	1.0736067	1.89	0.71
-0.48	[111]	0.95083	0.881533		
-0.39		1.04362	1.073607	1.62	0.15
0.78	-	1.04362	1.073607		
-0.39	[111]	0.95083	0.881533		
-0.48		1.04362	1.073607	1.89	0.71
0.78	_	1.04362	1.073607		
0.48	[1]	0.95083	0.949812		
0.78	L J	-1	1.031104	2.24	1
0.39	+	1	-0.968896		
-0.48		0.95083	0.949812		
0.39	[1]11	-1	-0.968896	2.24	1
0.78	L J	1	1.031104		
	_				
0.48		0.95083	0.949812		
0.39	[11]]	1	1.031104	2.24	1
0.78	+	-1	-0.968896		
-0.48		0.95083	0.949812		
0.78	[11]]	1	-0.968896	2.24	1
0.39		-1	1.031104		
L				1	1

Dynamical model of the B2 \rightarrow **R MT.** The evolution of the B2 \rightarrow R instability channel is determined by the observed tension strain ε^{\parallel} of the lattice along one of the symmetry axes $<111>_{B2}$ and by the compression strain ε^{\perp} in the transverse directions. Values of the final strains in the vicinity of M_s are much smaller in comparison with the B2 \rightarrow B19 reorganization. Thus, for example [19], accurate measurements for the aged Ti₄₉Ni₅₁ alloy gave $\varepsilon^{\parallel} \approx 1.1\%$ and $\varepsilon^{\perp} \approx -0.56\%$.

We first assume that the CWP creates the final tension strain ε_1 along the $<111>_{B2}$ direction and the compression strain ε_2 along one of the transverse directions (for example, $<1\overline{2}1>_{B2}$). Then under conditions of low elastic anisotropy, the strain ratio created by the CWP will be $|\varepsilon_1/\varepsilon_2| \approx a^{-2}$ ≈ 1 . Therefore, the observed ratio $|\varepsilon^{\parallel}/\varepsilon^{\perp}| \approx 2$ indicated above cannot be produced directly by the CWP of the chosen type. It seems likely that the final resultant strain contains additional contribution caused by the loss of stability according to an unfinished soft-mode scenario (as indicated above, the B2 \rightarrow R transition is close to the second-order transition). However, here we focus our attention on a less widespread variant of control in which the main role is played by the CWP transferring the threshold strain without tension along $<111>_{B2}$.

In this case, it is natural to consider that the CWP induces the fastest compression of the plane orthogonal to $<111>_{B2}$. The condition $|\epsilon^{\parallel}/\epsilon^{\perp}| \approx 2$ and the relationship $|\epsilon_1^{\perp}/\epsilon_2^{\perp}| \approx \alpha^{-2} \approx 1$ hold both true and are not contradictory. Moreover, the dynamic mechanism can play the key role, because the compression it induces will create quasistatic tension in the direction orthogonal to the compression plane. Then the lattice tension is an indirect consequence of the CWP. Indeed, within the framework of the linear elasticity theory of an isotropic medium, the uniaxial tension ϵ^{\parallel} is expressed in terms of the transverse isotropic compression strain ϵ^{\perp} as follows:

$$\varepsilon^{\parallel} = \frac{2\nu\varepsilon^{\perp}}{1-\nu}.$$
(13)

Then, determining the Poisson coefficient

$$v = \frac{1 - 0.5(C_{11} - C_{12})/(C_{11} + C_{12})}{2},$$
(14)

we can estimate ϵ^{\parallel} considering that the CWP induces the observed strain ϵ^{\perp} . Using the data shown in Fig. 2.6 of [19] (for Ti₄₉Ni₅₁ single crystals cooled in a furnace) and assuming that C₁₁ values for Ti₄₉Ni₅₁ and Ti₅₀Ni₅₀ are close, for the elastic moduli (in GPa) we obtain:

$$C_{11} \approx 155, C_{12} \approx 125, C_{44} \approx 26.$$
 (15)

From Eqs. (15) and (14) we obtain $v \approx 0.4732$. Then for $\varepsilon^{\perp} \approx 0.56\%$ and for the v value calculated from Eq. (13) we obtain $\varepsilon^{\parallel} \approx 1.006\%$. Though this estimate is smaller than the observed value equal to 1.1%, it can be accepted as quite satisfactory with allowance for errors of the employed data and linearity of the employed theory.

We note that the presence of strains of one sign in the CWP is not an obstacle for the CWP application, because at small strains (for the first-order transitions close to the second-order transitions), the role of the habit plane favorable for minimization of elastic distortion energy at the interface between the co-existing phases is not determining. An analysis of the morphological parameters can provide additional arguments for choosing among different CWP variants.

Variant of the habit planes. The habit planes of the R-martensite crystals are close to $\{110\}_{B2}$. Unfortunately, the degree of proximity was not indicated in [19]. Therefore, assuming as previously that the habit planes are determined by the CWP, we now consider their different variants.

In the approximation of the isotropic elastic properties, the pairs of the wave normals can be matched especially simply with the observed habit planes, since in this case we obviate the need for calculating the parameter $\mathfrak{a} = 1$. For a preset orientation of the dislocation line Λ , we can always find a pair of wave normals (that together with Λ form three orthogonal vectors) which describes, according to Eq. (2), any of the family of habit planes parallel to Λ . If the plane is parallel to Λ , the line of its intersection with the plane perpendicular to Λ must be determined first. Then orientations of the normals \vec{n}_1 and \vec{n}_2 are determined by rotating the intersection line through the angles $\pm \pi/4$ about the Λ axis. For a comparison we now consider typical set of orientations Λ corresponding to the symmetry axes of the cubic lattice.

1. Let we have $\overline{\Lambda} \parallel < 10\overline{1} >_{B2}$.

1. 1. The wave beams transferring the tension strain in the $\langle \overline{1} 1 \overline{1} \rangle_{B2}$ directions and the compression strain in the $\langle 121 \rangle_{B2}$ orthogonal directions are excited with wave normals $\vec{n}_1 \parallel \langle \overline{1} 1 \overline{1} \rangle_{B2}$ and $\vec{n}_2 \parallel \langle 121 \rangle_{B2}$. Then from Eq. (2) for $\mathfrak{a} \approx 0.9897 \approx 1$ we obtain the habit planes almost coinciding with $\{414\}_{B2}$ and making the least angles of $\sim 10^{\circ}$ with the $\{101\}_{B2}$ planes. We note that this variant of the wave normals can be used for a combined description of the resultant strain when additional compression in the $\langle \overline{1} 1 \overline{1} \rangle_{B2}$ directions and tension in the $\langle \overline{1} 1 \overline{1} \rangle_{B2}$ directions, providing compression of the $\{\overline{1} 1 \overline{1}\}_{B2}$ planes and the required ratio $|\mathfrak{e}^{\parallel}/\mathfrak{e}^{\perp}| \approx 2$, are observed together with the strain induced by the CWP.

1. 2. We now find \vec{n}_1 and \vec{n}_2 for the $(101)_{B2}$ habit plane given that $\vec{\Lambda} \parallel [10\overline{1}]_{B2}$. Considering that the $(101)_{B2}$ plane is intersected with the $(10\overline{1})_{B2}$ plane along the $[010]_{B2}$ line and rotating the $[010]_{B2}$ vector through the angles $\pm \pi/4$ about the $[10\overline{1}]_{B2}$ axis, we obtain

$$\vec{n}_1 \parallel [\bar{1} \sqrt{2} \ 1]_{B2} \text{ and } \vec{n}_2 \parallel [1 \sqrt{2} \ \bar{1} \]_{B2}.$$
 (16)

It is clear that for $\Lambda \parallel [10\overline{1}]_{B2}$, \vec{n}_1 and \vec{n}_2 can be easily determined formally for the (hkh)_{B2} habit planes. Analogous CWP variants provide the fastest strain of the $\{10\overline{1}\}_{B2}$ planes and incorporation of these planes into the OR.

2. In particular, exact crystallographic orientations of the habit planes $\{011\}_{B2}$ and $\{001\}_{B2}$ can be observed for $\vec{\Lambda} \parallel < 100 >_{B2}$. These habit planes are specially mentioned, since crystals forming polycrystal ensembles are combined along the above-indicated planes. The CWP corresponding to $\vec{\Lambda} \parallel < 100 >_{B2}$ provides the fastest transformation of the $\{100\}_{B2}$ plane and its inclusion into the OR.

3. Let we have $\vec{\Lambda} \parallel <111 >_{B2}$.

3. 1. As a first example, we choose $\vec{n}_2 \parallel [\overline{1} \ 2 \ \overline{1}]_{B2}$ and $\vec{n}_1 \parallel [10 \ \overline{1}]_{B2}$. Then, according to Eq. (2), we obtain

$$\vec{N}_{w} \parallel [1 \pm \sqrt{3} \, a, 1 \mp \sqrt{3} \, a, \bar{2}]_{B2},$$
 (17)

and for $a \approx 1$ we have the family of the habit planes close to $\{413\}_{B2}$ (in the approximation of small integer indices).

3. 2. We now obtain a pair of normals to the $(1 \overline{1} 0)_{B2}$ habit plane for $\overline{\Lambda} \parallel [111]_{B2}$. We consider that the $(1 \overline{1} 0)_{B2}$ and $(111)_{B2}$ planes are intersected along the $[\overline{1} \overline{1} 2]_{B2}$ direction. Then orientations of the normals \vec{n}_1 and \vec{n}_2 in the isotropic approximation (for $\alpha \approx 1$) can be determined by rotation of the vector $[\overline{1} \overline{1} 2]_{B2}$ through the angles $\pm \pi/4$ about the $[111]_{B2}$ axis:

$$\vec{n}_1 \| [1 - \sqrt{3}, 1 + \sqrt{3}, \overline{2}]_{B2}, \vec{n}_2 \| [1 + \sqrt{3}, 1 - \sqrt{3}, \overline{2}]_{B2}.$$
 (18)

It can be easily verified that $(\vec{n}_2 - \vec{n}_1) \parallel [\overline{1} \ 10]_{B2}$, that is, it determines the normal to the habit plane. Speaking about the character of the strain transferred by the CWP, it is pertinent to note two

extreme cases. First, it is possible to assume that the CWP transfers only the compression strain that causes quasi-static tension along the [111]_{B2} direction. It seems likely that this variant is observed in the case of independent formation of individual crystals. The negative volume effect during the transformation, though small, is the evidence in its favor. Second, in the case of the self-consistent formation of polycrystal ensembles, the variants of the CWP transferring strains of opposite signs can be observed, but crystals are combined so that they provide quasi-isotropic resultant strain. In any variant with $\vec{\Lambda} \parallel <111>_{B2}$, the CWP provides the fastest reorganization of the (111)_{B2} plane and its inclusion into the OR.

Orientation relationships. The observed orientation relations, according to [19], are close to the variant

$$\{111\}_{B2} \| (111)_{R}, \\ <\overline{1} \, 2 \, \overline{1} >_{B2} \| [\,\overline{1} \, 2 \, \overline{1}\,]_{R},$$
(19)

$$<\overline{1} 10>_{B2} ||[\overline{1} 10]_{R}.$$

As follows from the consideration in Sections 1 and 2, the OR can be interpreted as a consequence of the tension-compression process that preserves the orientation of the $\{111\}_{B2}$ plane induced by the dynamic strain process of the $\{111\}_{B2}$ plane upon exposure to the pair of wave beams with wave normals from (18). According to [4, 17], it is natural to consider what exactly the plane subject to the fastest strain is involved into the OR, and for the misorientation angle $\Delta \phi = \phi(\alpha) - \phi_0$ of the respective directions where $\phi(\alpha)$ is determined by (12).

When the strains are small, from Eq. (12) we derive the approximate relation

$$\varphi(\boldsymbol{x})^{\circ} \approx \frac{180 \,\boldsymbol{x} \left(\boldsymbol{\varepsilon}_{1} + |\boldsymbol{\varepsilon}_{2}|\right)}{\pi \left(\boldsymbol{x}^{2} + 1\right)} \,. \tag{20}$$

For the B2–R MT, it is natural to expect that the CWP provides only small deviations from formulas (19). Indeed, for the strain $\varepsilon_1 \approx |\varepsilon_2| \approx 0.0764\%$, we obtain from Eq. (20) the rotation angle of the $\langle \overline{1} \ 1 \ \overline{1} \rangle_{B2}$, $\langle 121 \rangle_{B2}$ reference basis vector pair about the $\langle \overline{1} \ 01 \rangle_{B2}$ axis $\varphi \approx 0.044^\circ$. We note also that for the strain $\varepsilon_1 \approx |\varepsilon_2| \approx 0.56\%$ and opposite signs of the strains in the CWP field, reference basis vector pair (18) will rotate about the $\langle 111 \rangle_{B2}$ axis through the angle $\varphi \approx 0.32^\circ$. When the strain signs coincide (we must set $\varepsilon_1 < 0$ in Eq. (20)), the angle $\varphi \approx 0^\circ$, and in this case, the ORs (19) hold true.

Thus, the CWP with wave normals from (18) transferring equal compression strains in the orthogonal directions and providing the fastest strain of the $\{111\}_{B2}$ plane corresponds to the observed strain ratio, orientation of the habit plane, and orientation relations.

Refinement of the data on the dislocation nucleation center in the approximation of the isotropic elastic medium. Till now we have not concretized all the details of the dislocation nucleation center. Suffice it to have known only the orientation of the dislocation line $\vec{\Lambda}$. However, it is easy to perform the necessary refinements useful for vivid geometrical interpretation of the morphological parameters. Setting $\vec{\Lambda} \parallel <111>_{B2}$, we now determine the extra plane from the data on the wave normals and the character of the strain. Recall the description of the strain field of an edge dislocation whose Burgers vector determines the sliding plane and is collinear with a normal to the extra plane. It is convenient to describe the strain field of a rectilinear edge dislocation in the infinite isotropic medium in the plane perpendicular to Λ using cylindrical coordinates [32, 33]. For a fixed distance r to the line $\vec{\Lambda}$, the change of the eigenvalues ε_1 and ε_2 of the strain tensor is characterized by the polar angle θ counted from the shear vector in the half-space comprising the

extra plane. Here $\theta = -\pi/2$ corresponds to points of the extra plane. If we do not require that the strain along the direction $\vec{\Lambda}$ was equal to zero, we obtain

$$\varepsilon_1 = \frac{b(\sin\theta + \cos\theta)}{2\pi r(1 - v)}, \quad \varepsilon_2 = \frac{b(\sin\theta - \cos\theta)}{2\pi r(1 - v)}, \tag{21}$$

where b is the modulus of the Burgers vector \vec{b} of an edge dislocation. The normalized eigenvectors of the strain tensor $\vec{\xi}_i$ determined by projections onto the axes $x_1 \| \vec{b}, x_2 \| [\vec{\Lambda}, \vec{b}]$, and $x_3 \| \vec{\Lambda}$ have the form

$$\vec{\xi}_{1} = \left[\cos\left(\theta - \frac{\pi}{4}\right) \sin\left(\theta - \frac{\pi}{4}\right) 0\right],$$

$$\vec{\xi}_{2} = \left[-\sin\left(\theta - \frac{\pi}{4}\right) \cos\left(\theta - \frac{\pi}{4}\right) 0\right],$$

$$\vec{\xi}_{3} = [0 \ 0 \ 1].$$
(22)

If we require that the strain along the direction Λ was equal to zero, the eigenvalues must be renormalized, and instead of Eq. (21), we obtain

$$\varepsilon_1 = \frac{b((1-2\nu)\sin\theta + \cos\theta)}{4\pi r(1-\nu)}, \varepsilon_2 = \frac{b((1-2\nu)\sin\theta - \cos\theta)}{4\pi r(1-\nu)}$$
(23)

From Eqs. (21) and (23) it follows that the equal negative values $\varepsilon_1 = \varepsilon_2 < 0$ are observed at $\theta =$ $-\pi/2$ in the compression field related to the extra plane. From Eq. (22) it follows that at $\theta = -\pi/2$, the eigenvectors of the strain tensor are at angles of $\pm \pi/4$ to the extra plane. This means that for normals from (18) the orientation of the extra plane of a DNC coincides with the orientation of the habit plane. For vectors $\vec{b} \parallel <100 >_{B2}$ typical of the B2 phase, dislocations with lines $\Lambda \parallel <111 >_{B2}$ are mixed. Hence, the eigenvectors $\vec{\xi}_1$ and $\vec{\xi}_2$ (and hence the wave normals) deflect from the $\{111\}_{B2}$ planes. Recall that for a purely screw dislocation $(\vec{\Lambda} \parallel \mathbf{b})$ in the isotropic medium, one of the eigenvectors (correspondent to the eigenvalue equal to zero) coincides with the radial direction in the plane perpendicular to $\vec{\Lambda}$, and two others (tension and compression axes) form the angle $\pi/4$ with this plane for any arbitrary θ (the tension-compression plane is parallel to $\vec{\Lambda}$). Therefore, in general, 24 variants of the habit planes can be observed rather than six variants (in the degenerate case) when the normals to the habit plane lie in the stereographic orientation triangle. Accordingly, four poles of the normals to the habit planes are grouped in the vicinity of each pole $<110>_{B2}$. Three extra planes (close to the habit planes) and hence six habit planes are associated with each line Λ . The observed accommodation variants of forming packet-pyramidal morphology of crystal ensembles with the R-phase were described in detail in Section 3.4.2 of the monograph [19].

Our analysis [34] has demonstrated that the morphological parameters observed during the B2–R MT within the framework of the dynamic theory [1–4] can provide adequate treatment, despite the proximity of the transformation to the second-order transitions. Small final strains require precise measurements of the OR to compare them with calculated values. When the accuracy of measuring the OR reached 0.01°, the calculated misorientation planes and the corresponding directions included into the OR must be refined considering though small, but still nonzero anisotropy of the elastic properties. In addition, it is clear that taking the anisotropy into account, the fastest strain of the {111}_{B2} plane induced by the CWP cannot be attributed to the DNC having the edge dislocation whose line is oriented strictly along the third-order <111>B2 symmetry axis as a basic segment. This was analyzed in detail in [35].

Additional Notes

A more complicated (than (1)) variant corresponds to the vectors $\vec{n}_{1,2}$ and $\vec{\xi}_{1,2}$ belonging to one and the same symmetry plane. For cubic symmetry crystals these are planes $\{001\}_c$ and $\{011\}_c$. The CWP transports plane deformation of "extension-compression" type that (similarly to static deformation of DNC field) may be characterized by a tensor with the main axes orientations $\vec{\xi}_{1,2w}$ and ratio $k_w^2 \approx |\epsilon_{1w}/\epsilon_{2w}|$. Then it is possible to obtain: $k_w = (\alpha + tg \psi)/(1 - \alpha tg \psi),$ (24)

where ψ is the turning angle (around the axis $\vec{n}_3 \parallel \vec{\xi}_{3w}$) of the vectors $\vec{\xi}_{1,2w}$ regarding the wave normals $\vec{n}_{1,2}$. Depending on the sign of ψ inequalities k> æ (at ψ >0) or k< æ (at ψ <0) may be held true, and at ψ =0 the expression (24) is transformed into (3). It must be underlined that owing to a higher symmetry of the elastic field in the planes {001}_c (as compared with that in {011}_c) for any orthogonal pair of the directions $\vec{n}_{1,2}$ in the plane {001}_c we have v₁=v₂ and, consequently, æ=1. Thus, for the vector pairs $\vec{n}_{1,2}$ and $\vec{\xi}_{1,2}$ in this symmetry plane we have to put æ =1 in formula (2).

In the general case when one can find no pair of parallel vectors from the totalities $\vec{\xi}_{iw}$ and \vec{n}_i (i=1, 2, 3). This means that the planes with the normals $\vec{\xi}_{3w}$ and \vec{n}_3 containing respectively the vectors $\vec{\xi}_{1,2}$ and $\vec{n}_{1,2}$ are not complanar. Nevertheless from the requirement

$$\vec{N}_{w} \parallel \vec{\xi}_{2w} \pm k_{w} \vec{\xi}_{1w}$$
⁽²⁵⁾

it is possible to obtain:

$$\mathbf{a} = |(\vec{\xi}_{3w}, \vec{n}_2)/(\vec{\xi}_{3w}, \vec{n}_1)|, \qquad k_w = |(\vec{n}_3, \vec{\xi}_{2w})/(\vec{n}_3, \vec{\xi}_{1w})|.$$
(26)

In (26) the symbol (,) means the scalar product of vectors that are taken into round brackets. From (26) it follows that:

$$\mathfrak{a} = |(\vec{\xi}_{3w}, \vec{n}_2)(\vec{n}_3, \vec{\xi}_{1w})/(\vec{\xi}_{3w}, \vec{n}_1)(\vec{n}_3, \vec{\xi}_{2w})| k_w.$$
(27)

When DNC characteristics are inherited, the following conditions will be fulfilled: $\vec{\xi}_{1,2w} = \vec{\xi}_{1,2}$, $k = k_w$. The obtained relations allow significant adjustment of the procedure of selection of the most probable DNC, not only for transformations in iron alloys but also for MTs in alloys with the effect of shape memory. It is clear that just for such alloys (having the shape memory effect) the exact inheriting of DNC elastic fields (at $\vec{\xi}_{iw} = \vec{\xi}_i$) is a necessary condition for explanation of the effect of transformation reversibility upon thermocycling.

It is essential that the verification of the compliance between ratios for the threshold and final deformations must be performed on the basis of formula (27).

Summary

Our analysis has demonstrated that within the framework of the dynamic theory based on the synthesis of concepts of the heterogeneous nucleation and wave growth of martensite crystals, the description of morphological parameters is also possible for MTs in alloys with the effect of shape memory. Apparently, the different dislocation nucleation centers can provide conditions for the realization of the fastest variants of transformation of an initial phase into both the final state of martensite and the intermediate states [36]. It is not excluded for example that the B2 \rightarrow IMS \rightarrow B19 reorganization is competitive with the direct channel of the B2 \rightarrow B19 MT.

As for the prospects of the next research it should be noted the necessity of an interpretation within a dynamic theory of the observed variants of transformation twins. Apart from this, it is of urgent interest the carrying out of experiments on MT initiation by a couple of hypersound sources, which would allow to confirm the predictions of the dynamic theory that are based on the information about a deformation tensor relevant to the CWP description. Additional interest is also presented by the dynamic description of the accommodation MT that can occur in the nanocrystalline state.

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Modeling of Deformation and Functional Properties of Shape Memory Alloys based on a Microstructural Approach

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Abstract. This microstructural model of the functional-mechanical behavior of shape memory alloys (SMA) includes a description of the reversible phase deformation, microplastic deformation due to the accommodation of martensite and the evolution of the deformation defects. The laws of these phenomena are formulated in terms of the generalized thermodynamic forces. The microplastic flow rule accounts for isotropic and kinematic hardening, which are related to the accumulation of the deformation defects. The model gives a good description both of reversible and irreversible deformation under one-side or cyclic thermomechanical loading of SMA and opens a way for the fatigue life prediction. The model can be applied for solving of the mechanical problems for SMA parts such as dampers or base isolators used in seismic protection devices.

Introduction

Modeling of the deformation effects in shape memory alloys (SMA) is a quite necessary component of the general knowledge of this class of functional materials. Each particular SMA can undergo either one martensitic transformation or a sequence of transformations. The variety of the transformations and their characteristics stipulates for different types of the mechanical behavior demanding specific theoretical approaches. Consequently, a large number of theories have been developed, so that one can hardly give an exhaustive list of them. All existing models aimed at calculation of the stress and strain evolution of a representative volume under different thermomechanical loading can be roughly divided into two groups: macroscopic and microstructural. Models of the first group [1-5] directly establish relations between the macroscopic (related to a point of the body) stress, strain and internal parameters. One of the first macro-models was the model of Baumgart et al. [1]. It exploits an approach analogous to the classical plastic flow theory and does not comprise any internal parameters specific for the martensitic transformation. The increment of the deformation is split into two parts: a temperaturedriven part proportional to the increment of temperature and the stress-driven part proportional to the increment of the stress, both parts dependent on the current values of the temperature, stress and Odquist parameter. Further developed models announced the use of a set of internal parameters including the volume fraction of martensite [6-12], volume fractions of self-accommodated martensite and detwinned martensite [13]; volume fraction of martensite and the phase strain [14], phase strain as the only parameter [15, 16]. A review and characterization of different macromodels is given in [17].

In microstructural theories [18 - 24] the equations are formulated for the physical processes, producing micro-strain in the micro-regions and the macroscopic strain of a representative volume is calculated by neutralization of strains of micro-regions constituting this volume. As for the primary structural elements of martensite they can be chosen in different ways depending on the choice of the microscopic level. E. Patoor et al. [19] considered them to be different martensite plates bearing the martensitic shift on a habit plane. In works [23 - 26] the primary structural elements of martensite variants (martensite variants) originated from the parent phase in each grain by different but crystallographically equivalent variants of Bain's deformation, i.e. the homogeneous part of the deformation transforming the lattice of the parent austenitic phase into that of the child martensitic phase. The direct and reverse martensitic transformations responsible for the pseudoelasticity and shape memory effects and the reorientation of martensite resulting in the

pseudoplastic deformation of specimens in the martensitic state are described in terms of the evolution of these parameters. An account of the irreversible plastic deformation accommodating the growth of martensitic plates requires an addition of special parameters. This idea was suggested in the microstructural models [20, 23]. The microstructural approach proved to be efficient for simulating the active deformation of a specimen in different states (martensitic, two-phase and austenitic) as well as its straining at cooling and heating under a constant or varying load. It was also suitable for simulating the mechanical behavior of an SMA suspension used as an element of active, semi-active and passive vibration control system [27]; for simulation of structure protection from earthquakes [28]; for modeling of vibration isolation by two helical SMA springs [29, 30]; for solving one-dimensional boundary-value problems [31].

Constitutive equations of the microstructural model

Representative volume and deformation averaging. In the same way as in [23, 24] choose the representative volume *V* of a SMA (Fig.1) consisting of a set of grains, each characterized by the orientation ω of its crystallographic axes and put *V*=1. The orientation can be specified, for example, by Euler angles $\omega = (\varphi, \theta, \psi)$. The rotation tensor $R(\omega)$ transforms the laboratory basis into the crystallographic basis of the grain with the orientation ω .



Fig.1. Scheme of the representative volume of SMA

Apply the A. Reuss hypothesis that the macroscopic strain can be calculated as the average of all micro-strains. As it is very difficult to perform the spatial averaging of the micro-strains, substitute it by the orientation averaging thus expressing the macroscopic strain ε and the volume fraction Φ^{M} of martensite by the formulae:

$$\varepsilon = \sum_{\omega} f(\omega)\varepsilon^{\rm gr}(\omega), \quad \Phi_{\rm M} = \sum_{\omega} f(\omega)\Phi^{\rm gr}(\omega), \tag{1}$$

where the sum is taken on all grains, $f(\omega)$ is the volume fraction of the grains with orientation ω (a discrete analogue of the orientation distribution function), $\varepsilon^{gr}(\omega)$ and $\Phi^{gr}(\omega)$ are the strain tensor and the volume fraction of martensite in a grain with orientation ω (everywhere in this chapter

small deformation tensors are used). Naturally, to perform the summation all tensors $\varepsilon^{gr}(\omega)$ must be referred to the laboratory system of coordinates.

In each grain there can exist N orientational variants of martensite originated from the parent phase by different but crystallographically equivalent Bain's deformations D_n (n = 1, ..., N). The number of variants N depends on the order of the symmetry groups of the parent austenitic phase and of the child martensitic phase. If austenite has a cubic lattice N is one of the divisors of 24, which is the order of the cube symmetry group. For the transformation of face-centered cubic (fcc) lattice into body-centered cubic (bcc) or body-centered tetragonal (bct) lattice N=3; for the transformation of the cubic lattice into rhombohedral lattice N=4, into orthorhombic lattice N=6, and into hexagonal or monoclinic lattice N=12. Thus, we characterize the martensite by parameters Φ_n (n = 1, ..., N), such that $(1/N)\Phi_n$ are the volume fractions of the domains occupied by the orientational variants of martensite. For the total volume fraction of martensite in a grain one then has:

$$\Phi^{\rm gr} = \frac{1}{N} \sum_{n=1}^{N} \Phi_n , \qquad (2)$$

here and everywhere further the argument ω is omitted. With such description of the material structure for the deformation of a grain one can write:

$$\varepsilon^{\rm gr} = (1 - \Phi^{\rm gr})\varepsilon^{\rm A} + \frac{1}{N}\sum_{n=1}^{N} \Phi_n \varepsilon_n^{\rm M} , \qquad (3)$$

the superscripts A and M denoting austenite and martensite, ε^{A} and ε^{M} are the deformations of the austenitic and martensitic phases. In general, each of the strains ε^{A} and ε^{M} can be expressed as the sum of the elastic strain ε^{e} , thermal expansion strain ε^{T} , dislocation slip plastic strain ε^{P} , phase strain ε^{Ph} (strain due to the phase transformation) and the micro-plastic strain ε^{MP} , which is the strain occurring by the localized dislocation slip under the action of the inter-phase stresses. In other words, it is the deformation providing for the plastic accommodation of martensite. In the present work we focus on calculating the phase deformation and micro-plastic deformation, i.e. we consider the case when $\varepsilon^{P} = 0$. Elastic and thermal strains are calculated by commonly known formulae, which we do not write down here. Since the phase strain is the strain, which occurs as the result of the transformation of austenite to martensite we put that for the austenite $\varepsilon^{PhA} = 0$ and for the *n*-th variant of martensite $\varepsilon_{n}^{PhM} = D_{n}$. So, the total phase strain of a grain is

$$\varepsilon^{\rm Ph\,gr} = \frac{1}{N} \sum_{n=1}^{N} \Phi_n D_n \,. \tag{4}$$

Since the micro-plastic strain is connected with the phase deformation and occurs in the regions near the growing martensite variants, one can suppose that it can be expressed by an expansion similar to that for the phase strain:

$$\varepsilon^{\rm MP\,gr} = \frac{1}{N} \sum_{n=1}^{N} \kappa \Phi_n^{\rm p} D_n \,, \tag{5}$$

where Φ_n^{p} are internal parameters – measures of the micro-plastic deformation and the material constant κ establishes the scale of the parameters Φ_n^{p} relative to parameters Φ_n . Similar idea for the description of the micro-plastic deformation was suggested by Q.-P. Sun and C. Lexcellent [20].

Thermodynamic forces of the transformation. Thus, to simulate the variation of the grain deformation one must know the variation of the internal parameters Φ_n and Φ_n^{p} , which occurs when the transformations is going on. It is convenient to formulate the laws of the variation of Φ_n and Φ_n^{p} in terms of the generalized thermodynamic forces. We start from the thermodynamic Gibbs' potential G. For a unit volume one can write

$$G = G^{\text{eig}} + G^{\text{mix}}, \quad G^{\text{eig}} = (1 - \Phi^{\text{gr}})G^{\text{A}} + \frac{1}{N}\sum_{n=1}^{N}\Phi_{n}G_{n}^{\text{M}}, \quad G^{\text{mix}} = \frac{\mu}{2}\sum_{m,n=1}^{N}A_{mn}(\Phi_{m} - \Phi_{m}^{\text{p}})(\Phi_{n} - \Phi_{n}^{\text{p}}), \quad (6)$$

where G^A , G_n^M , G^{eig} are the eigenpotentials of austenite, martensite and of their mixture; G^{mix} is the potential of the interaction between the phases equal to the elastic energy of the internal stresses caused by the incompatibility of the phase deformation. In the work [22] this potential is referred to as the "phase interaction energy function" (PIEF). The eigenpotentials G^{A} and G_{n}^{M} at temperature *T* and stress σ can be expressed by the formula:

$$G^{a} = G_{0}^{a} - S_{0}^{a}(T - T_{0}) - \frac{c_{\sigma}^{a}(T - T_{0})^{2}}{2T_{0}} - \varepsilon^{0a}(T) : \sigma - \frac{1}{2}\sigma : Q^{a} : \sigma \quad , a = A, M,$$
(7)

where T_0 is the temperature of the thermodynamic equilibrium of austenite and martensite at zero stress, G_0^a and S_0^a are the values of the Gibbs' potential and of the entropy at $T=T_0$ and $\sigma=0$, c_{σ}^a is the specific heat (per unit volume), $\varepsilon^{0a}(T)$ is the strain at $\sigma=0$, Q^{a} is the tensor of elastic compliances, symbol ":" denotes double scalar product of tensors.

As the exact calculation of G^{mix} can be done only by solving a very complicated boundary-value problem, one can try to use a qualitative estimation for it delivered by a quadratic form of the internal parameters describing the phase deformation. The matrix A_{mn} of this quadratic form accounts for the interactions between the different variants of martensite.

In one of the most important shape memory alloy TiNi the transformation is from cubic B2 phase into monoclinic B19' phase. For this transformation there exist 12 different Bain's deformations. These variants group into pairs called the Corresponding Variants Pairs (CVP) [32-35]. This martensite structure allows lowering the elastic energy of the interphase stresses. The tendency of the Bain's variants for grouping can be taken into account by the matrix A_{mn} . Enumerating the Bain's variants in a convenient order we propose the following structure of the matrix A_{mn} (all unmarked matrix elements are zeroes):

 $\begin{vmatrix} -\alpha & 1 & 0 & -\alpha \\ -\alpha & 0 & 1 & -\alpha \\ 0 & -\alpha & -\alpha & 1 \\ & & & 1 & -\alpha & -\alpha & 0 \\ & & & -\alpha & 1 & 0 & -\alpha \\ & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ \end{array}$ $\begin{array}{c}
-\alpha \\
-\alpha \\
1 \\
 & 1 \\
-\alpha \\
-\alpha \\
-\alpha \\
0 \\
-\alpha \\
-\alpha \\
1
\end{array}$ A =(8)

where α is a material constant (0 <= α < 1/2) measuring the degree of the interaction between the Bain's variants forming one CVP.

The fact that the plastic accommodation of martensite reduces the elastic energy suggests that the variables of this quadratic form must be the differences $(\Phi_n - \Phi_n^{\rm p})$. The generalized thermodynamic forces F_n and $F_n^{\rm p}$ tending to change the values of Φ_n and $\Phi_n^{\rm p}$ are the derivatives of the Gibbs' potential:

$$F_{n} = F_{n}^{t} + F_{n}^{\text{mix}}, \qquad F_{n}^{t} = -\frac{\partial G^{\text{eig}}}{\partial \Phi_{n}} \approx q_{0} \frac{T - T_{0}}{T_{0}} + \sigma : D_{n}, \qquad F_{n}^{\text{mix}} = -\frac{\partial G^{\text{mix}}}{\partial \Phi_{n}} = -\mu \sum_{n=1}^{N} A_{nm} (\Phi_{n} - \Phi_{n}^{\text{p}}),$$

$$F_{n}^{\text{p}} = -\frac{\partial G}{\partial \Phi_{n}^{\text{p}}} = -F_{n}^{\text{mix}} = \mu \sum_{n=1}^{N} A_{nm} (\Phi_{n} - \Phi_{n}^{\text{p}}). \qquad (9)$$

The full thermodynamic force F_n is dependent on the temperature T and stress σ and it is the sum of the driving force F_n^{t} and the opposing force F_n^{mix} (in the above formula for F_n^{t} we neglect the terms connected with the differences between the thermal expansion coefficients and the elastic constants of the two phases, which is a good approximation for most of the transformations). In its turn the driving force F_n^{t} is the sum of the chemical force F_n^{chem} depending only on the temperature and equal for all the martensite variants and the mechanical force F_n^{mech} depending on the stress:

$$F_n^{t} = F^{\text{chem}} + F_n^{\text{mech}}, \quad F^{\text{chem}} = q_0 \frac{T - T_0}{T_0}, \quad F_n^{\text{mech}} = \sigma : D_n.$$

$$(10)$$

Force F_n^{p} depends on the values of the amount of the *n*-th martensite variant Φ_n and on the measure of the micro-plastic strain Φ_n^{p} ; q_0 is the latent heat of the direct austenite to martensite transformation ($q_0 < 0$); T_0 is the phase equilibrium temperature, i.e. the temperature at which the Gibbs' potentials of the unstressed austenite and martensite are equal; μ is a material constant. Experimental measuring of the temperature T_0 is a very hard task since the transformation usually produces an incompatible phase strain thus occurring in the field of internal stresses. In many cases a good estimate for the temperature T_0 is given by the formula [36]:

$$T_0 = \frac{M_{\rm s} + A_{\rm f}}{2}.$$
 (11)

Here and further M_s , M_f , A_s , A_f are the characteristic temperatures of the martensitic transformation: letters M and A refer to the direct austenite to martensite transformation on cooling and to the reverse martensite to austenite transformation on heating, subscripts "s" and "f" denoting the transformation start and finish. Since a temperature-phase hysteresis exists, one concludes that the transformation proceeds in conditions apart from the equilibrium under an excess thermodynamic force. So we formulate the condition of the transformation in the form:

$$F_n = \pm F^{\rm fr},\tag{12}$$

where F^{fr} is a material constant – the "friction force", which acts similarly to a dry friction force and is responsible for the temperature-phase hysteresis, sign "+" is taken for the direct and "–" for the reverse transformation. Constants F^{fr} and μ are related to the characteristic temperatures and the latent heat of the transformation.

Martensite reorientation. A special approach is used to describe the reorientation (twinning) of martensite. We accept three hypotheses: (1) any variant of martensite can be transformed in any other variant; (2) reorientation occurs along the direction in the space $\Phi_1, ..., \Phi_N$, which corresponds to the fastest decrease of the Gibbs' potential; (3) reorientation starts when the thermodynamic force reaches some critical value. To find the direction of the reorientation we use vector

 $F_n = \left\{-\frac{\partial G}{\partial \Phi_1}, \dots, -\frac{\partial G}{\partial \Phi_N}\right\}$ and take its projection *L* onto plane $\Phi_1 + \dots + \Phi_N = \text{const.}$ If for some *n* it holds that $\Phi_n = 0$ and $L_n < 0$ we substitute *L* for its projection *L'* onto intersection of planes $\Phi_n = 0$ and $\Phi_1 + \dots + \Phi_N = \text{const.}$ repeating this procedure for other components of L_n if necessary. Finally we obtain the direction *l*, which does not lead to a violation of conditions $\Phi_n > 0$, $n = 1, \dots, N$. For this direction we postulate the condition of reorientation:

$$F^{\rm tw}(l) = F^{\rm fr\,tw},\tag{13}$$

where

$$F^{\text{tw}}(l) = -\frac{\partial G}{\partial l} = -\sum_{n=1}^{N} l_n \frac{\partial G}{\partial \Phi_n} = \sum_{n=1}^{N} l_n F_n.$$
(14)

In Eq. 13 F^{frtw} is a constant, characterizing the critical driving force for reorientation. From hypotheses 1 and 2 it follows that the increments $d\Phi_n$ are proportional to l_n :

$$d\Phi_n = l_n \, d\varphi,\tag{15}$$

where $d\phi$ is the proportionality factor.

Micro-plastic flow condition. From Eq. 12 – Eq. 15 one can find the differences $(d\Phi_n - d\Phi_n^p)$ of the internal parameters increments. To find the very increments $d\Phi_n^p$ one needs to formulate the micro-plastic flow conditions. Formulate this condition by analogy with the classic one-dimension plastic flow theory, parameters Φ_n^p acting as the plastic deformation and the force F_n^p – as the stress:

$$|F_n^{\ p} - F_n^{\ \rho}| = F_n^{\ y} \,. \tag{16}$$

The meaning of this condition is that the micro-plastic flow can occurs then and only then when the generalized force F_n^p is equal to the sum of the two opposing factors, one (F_n^y) connected with the isotropic hardening and the other (F_n^{ρ}) – with the kinematic hardening. These two types of hardening we relate to the accumulation of the deformation defects. We assume that the plastic flow caused by the growth of the *n*-th Bain's variant produces defects of two types: reversible b_n and irreversible f_n by deformation. The reversible defects can be related to small dislocation loops, which can expand and shrink in their slip planes, and the irreversible defects – to sessile dislocations, Lomer-Cottrell locks formed in the course of the dislocation interactions and their incomplete annihilation. For the defect densities we propose the evolution equations similar to those in the work [26]:

$$\dot{b}_n = \dot{\Phi}_n^p - \frac{1}{\beta^*} \cdot \left| b_n \right| \cdot \dot{\Phi}_n^p \cdot H(b_n \cdot \dot{\Phi}_n^p), \tag{17}$$

$$\dot{f}_n = \left(1 + q_3 \cdot f_n\right) \cdot \left|\dot{\Phi}_n^p\right| - r(T) \cdot f_n , \qquad (18)$$

where β^* , and q_3 are material constants, r(T) is an Arrhenius-type function of temperature, H is the Heaviside's function. The first term of the right side of Eq. 17 accounts for the increase of the defect density in the course of their movement and formation of the new defects and the second term σ accounts for the decrease of the defect density due to their escape to the outer surface. In Eq. 18 the

first term reflects the accumulation of the irreversible defects in the course of the plastic flow and the second – the annihilation of these defects due to thermoactivated recovery processes.

Eqs. 17, 18 must be supplemented by the closing equations relating their densities to the parameters of hardening. Suppose that the kinematic hardening is due to the reversible defects and the isotropic hardening – to the irreversible ones. For simplicity choose linear relations in the form:

$$F_n^{\ y} = a_y f_n , \tag{19}$$

$$F_n^{\ p} = a_\rho b_n , \tag{20}$$

where a_y and a_p are material constants.

Eqs.12, 13 and 16 make up a set of conditions from which one can obtain the evolution equations for the internal parameters Φ_n and Φ_n^p , thus making possible to simulate the variation of the deformation tensor ε of a shape memory alloy under given variations of the stress tensor σ and temperature *T*, i.e. they establish relations, which formally may be written as:

$$d\varepsilon = f_1(T, dT, \sigma, d\sigma, X), \qquad \qquad dX = f_2(T, dT, \sigma, d\sigma, X), \tag{21}$$

where X denotes the set of internal parameters $\Phi_1(\omega), \dots, \Phi_N(\omega), \Phi_1^{p}(\omega), \dots, \Phi_N^{p}(\omega)$ for all martensite variants in grains with all orientations ω . One of the advantages of this microstructural model is that it accounts for the tension-compression asymmetry without any additional assumptions as this asymmetry is the consequence of the specific structure of the Bain's deformation tensor. The material constants used in this model are the elastic moduli, heat expansion coefficient, Bain's deformation tensor *D*, phase thermodynamic equilibrium temperature T_0 . Constants F^{fr} and μ are calculated from the values of the characteristic temperatures of the transformation and its latent heat. Adjustable constants area, $F^{\text{fr tw}}$, β^* , q_3 , a_y , a_p .

Simulation of the functional-mechanical behavior of shape memory alloys

Active deformation. The values of the material constants specifying the elastic, thermal and phase deformation of SMA were chosen to reproduce the mechanical behavior of the equiatomic TiNi SMA. For a specific TiNi composition they were determined in calorimetric and mechanical tests. For calculation the following values were used: the characteristic temperatures of the transformation $M_f = 317 \text{ K}$, $M_s = 326 \text{ K}$, $A_s = 397 \text{ K}$, $A_f = 406 \text{ K}$, the latent heat of the transformation $q_0 = -160 \text{MJ/m}^3$. The matrix of the lattice deformation D was taken from work [37]. The values of the other constants were chosen $\alpha=0.2$, $F^{\text{fr tw}} = 17 \text{ MPa}$, $\beta^*=0.001$, $q_3=0$, $a_y = 50 \text{ MPa}$, $a_p = 10 \text{ GPa}$. The stress-strain diagrams of SMA deformation in tension for temperatures 273 K, 350 K and 420 K, corresponding to the martensitic, two-phase and austenitic states calculated by integrating the equations are presented in Fig. 2.



Fig.2. Calculated stress-strain diagrams of the SMA in the martensitic (a), two-phase (b) and austenitic state (c).

One can see that the simulation reproduces the typical for TiNi SMA pseudoplastic behavior at 273 K when the alloy is in the martensitic state and pseudoelastic behavior at 420 K when it is in the austenitic state. The lowest level of the stress causing unelastic deformation is for the SMA in the two-phase state. This is completely in agreement with the well-known experimental data (for example, [38, 39]).

Transformation plasticity and shape memory. When an SMA specimen undergoes a direct martensitic transformation under an applied stress it demonstrates the accumulation of reversible and irreversible deformation on cooling. This phenomenon is referred to as the transformation plasticity effect. On the subsequent heating partial recovery of the transformation plasticity strain is observed (shape memory effect). Fig. 3 shows calculated dependences of the TiNi specimen strain on temperature at a thermocycle under different stresses. This alloy demonstrates a very sharp dependence of the irreversible strain on the stress. This happens because the kinematic hardening coefficient $a_{\rho} = 10$ GPa is much bigger than that of the isotropic hardening $a_y = 50$ MPa. At the same time the small value of the constant $\beta^*=0.001$ does not allow a significant growth of the reversible defects density.



Fig.3. Calculated dependences of the strain on temperature due to the direct and reverse transformations under an applied stress 50, 100 and 200 MPa.

Therefore, kinematic hardening hinders the micro-plastic flow only when the applied stress is small. If the applied stress exceeds some characteristic value, the microplastic flow is affected mainly by the small isotropic hardening. This type of behavior was observed experimentally in work [40]. More clearly it is illustrated on Fig. 4c: the irreversible strain is small at the stress less than 100 MPa and grows rapidly with the stress when it exceeds this characteristic (for this SMA) value. Fig.5 shows a comparison of the experimental data [40] and of the simulation.



Fig.4. Calculated dependences of the transformation plasticity strain (a) shape memory strain (b) and the irreversible strain (c) on the stress acting during the direct transformation.



Fig.5. Calculated and experimental [40] dependences of the strain on temperature at cooling and heating under an applied stress 50 and 200 MPa.

Fig. 6 shows the dependence of the M_s temperature (estimated by the strain tolerance 0.01%) on the stress acting in the specimen during the direct transformation. Note the linear dependence, which is in agreement with the Clausius – Clapeyron law for the shift of the phase equilibrium point under an applied stress.



Fig.6. Calculated dependence of the M_s temperature on the applied stress.

For practical applications it is important to know what will be the strain recovery and the irreversible strain, when a specimen after having accumulated a transformation plasticity strain under some stress gets an additional load and then is heated to undergo the reverse transformation. The results of the simulation of this regime of thermomechanical loading are presented in Fig. 7. Note that the irreversible strain in this case is much less than after cooling under stress 200 MPa.