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SHEAR TRANSFORMATION OF AUSTENITE IN STEELS CONSIDERING STRESSES' EFFECTS

The currently known main mechanisms of martensitic transformation of austenite in steel during cooling, physical models, and schemes of shear rearrangement of the iron crystal lattice during $\gamma\rightarrow\alpha$ transformation under the action of internal stresses are considered. An analysis of the available kinetic model of the shear transformation of austenite in steel is carried out considering the influence of stresses. As shown, for the transformation of retained austenite into martensite, two main conditions have to be fulfilled. The first one is thermodynamic condition due to decreasing the temperature of the steel down to the temperature of the end of the transformation of retained austenite. The second condition is kinetic one due to increasing the level of internal stresses in austenite, the cooling rate at the final treatment stage or mechanical impact. To calculate the effect of stresses on the transformation of retained austenite in steel, a new equation is proposed that takes into account the minimum stress required for a crystallogeometrically ordered displacement of Fe atoms during the formation of martensite. As shown, the effect of alloying elements and cooling rate on the temperature of the beginning and end of the austenite transformation can be calculated using the relations given in the article. To calculate the quantity of martensite formed depending on the transformation temperature, an improved Koistinen–Marburger equation is suggested. This equation takes into account not only the temperature of the beginning, but also the temperature of the end of the austenite transformation, *i.e.*, increases the accuracy of the obtained result.

Keywords: austenite transformation, plane shear, stresses, process thermodynamics, martensite crystal, kinetic model.

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Introduction

The study of phase transformations and the development of their models is one of the most important tasks of physics of metals [1–4]. If in steels and cast irons, the kinetics of austenite transformation is determined by carbon diffusion this allows them to be attributed to transformations controlled by diffusion [1–5]. When the rate of transformation is determined by the speed of movement of the interfacial boundaries that differ only in their crystal structure, the transformation is called non-diffusion [3]. Kinetically, a distinction is made between normal polymorphic and martensitic transformation [2–4]. As the temperature of normal transformation decreases, its rate first increases and then decreases. The kinetics of martensitic transformation is characterized by a very high growth rate of individual crystals and a maximum volumetric speed at the initial moment of transformation under isothermal conditions.

According to existing ideas [1] the change in the type of crystal lattice of iron in its polymorphic $\delta\leftrightarrow\gamma\leftrightarrow\alpha$ transformations occurs at the interfacial boundaries, the migration of which is carried out in two ways — ‘diffusion’ and ‘shear’. Accordingly, the mechanisms of phase transformations in steel are conventionally divided into ‘diffusion’ and ‘shear’ or ‘martensitic’.

In the diffusion mechanism of polymorphic transformations, the migration of interfacial boundaries and the rearrangement of the crystal lattice of iron occur because of thermally activated random jumps (fluctuations) of atoms. With the shear mechanism of transformations, the ‘daughter crystal grows in the maternal way by coordinated motion (such as shear) of all atoms of the interface’ [1].

The $\gamma\rightarrow\alpha$ transformation associated with the formation of a polyhedral phase structure by the nucleation of randomly oriented α-grains and their subsequent growth due to the migration of an incoherent boundary without noticeable change in phase composition called ‘massive’ [3] is often given as a practical implementation of the diffusion mechanism of solid-phase transformations, *e.g.*, in low-carbon steels with slow cooling. As known, martensitic transformation leads to the formation of a completely different (oriented-lamellar) structure of the α-phase and does not raise objections about the shear nature of its formation.

In addition to martensite, at least two other structural components are known that are formed with a shear (‘martensitic’) morphology of crystal formation — Widmanstätten ferrite and needle ferrite. In addition, in some alloys there is a course of martensitic and normal transformations at the same temperature [3]. A consistent theory of shear transformation should explain this phenomenon.

The purpose of this work is to review the mechanisms and models of shear transformation of austenite with the role and influence of stresses on this process. The authors believe that this work will be interesting and useful for materials scientists and metal physicists both for understanding the essence of the processes occurring in metals and for the practical use of the equations described in the work.

2. Analysis of the Existing Mechanisms of Martensitic Transformation of Austenite Steels during Cooling

In the works of G.V. Kurdyumov and co-workers, the martensitic transformation is considered as a normal (diffusion) phase transformation in a one-component system further complicated by the influence of strong interatomic interaction, which leads to significant stresses in the martensite crystal and matrix [2, 5].

According to an alternative mechanism, martensitic transformation occurs by means of an instantaneous shear of atomic planes, which does not require thermal activation and is not associated with thermodynamic stimuli of transformation [3, 6, 7]. In this case, the factor that initiates the transformation is considered to be the stresses that occur during abrupt cooling of the sample (quenching) [7].

The diffusion mechanism of $\gamma \to \alpha$ transformation of iron is considered from the standpoint of the phenomenon of self-diffusion of its atoms [3, 8] for the transition of which from the γ-Fe lattice to the new stable positions of the α-Fe lattice requires an energy of thermal oscillations comparable to the energy of self-diffusion of iron atoms.

This transformation, according to Ref. [2], is associated with unregulated shears of atoms, which overcome energy barriers and requires thermal activation. 'The transition from the initial to the newly formed lattice is carried out by repeated of the processes of separation and addition of single atoms. In physical essence, this process is similar to the elementary process of self-diffusion and diffusion [9]. At the same time as noted in Ref. [2], the polymorphic transformation $\gamma \to \alpha$ in non-alloy iron is identified with martensitic transformation because it occurs at a high speed and is not associated with concentration changes. However, not so homogeneous and equally directed as in the case of martensitic transformation, the displacement of atoms during the rearrangement of the crystal lattice of iron, as well as the lack of uniformity in their location at the interfacial boundary γ/α gave grounds to separate the mechanism of polymorphic $\gamma \to \alpha$ transformation to 'martensitic' and 'diffusion', also called 'recrystallization' or 'normal' [2, 3]. The latter term is used in the sense that the mechanism of polymorphic $\gamma \to \alpha$ transformation is traditionally represented by a similar mechanism of phase transformations in crystallization of liquid or condensation with steam by the appearance and growth of the solid phase nucleus. The same mechanism describes the recrystallization of metals and alloys [10].

Traditionally dividing the mechanisms of solid-phase transformations in iron into diffusion and martensitic type, the authors of Ref. [2] however recognized that 'for transformations in a solid body the most typical is the martensitic transformation $\gamma\to\alpha$'.

The information available in the literature on the diffusion mechanisms of solid-phase transformations in iron alloys can be summarized and presented in two groups of data.

The first group consists of the results of theoretical studies of the thermodynamics of phase transformations of metals and alloys. According to these data, the driving force of phase transformations is the system's desire to reduce the free Gibbs energy and their course is considered from the standpoint of Folmer's theory of fluctuation of new phase nucleus and their growth after reaching a critical size. The theory of diffusion phase transformations by the genesis and growth of the nucleus of a new phase, based on the change of free Gibbs energy, has not undergone any significant changes [11] since its inception (30s of XX century) [12]. The principles of this theory are widely covered in the already mentioned literature sources, as well as in educational and reference literature, *e.g.*, [13–17]. It should be noted that often, considering the nucleation and growth of a new phase as processes inherent in diffusion transformations, many authors forget that martensitic transformations also occur by nucleation and growth, and thermal oscillations of atoms play a crucial role in martensite nucleus formation [16].

The second group of literature data is represented by the results of the study of eutectoid (pearlite) transformation in iron-carbon alloys. The theoretical description of the formation of a new phase (ferrite and cementite) in this process is based on data from the first group of literature sources. Further cooperative growth of the two-phase lamellar structure of pearlite is described by the results of theoretical and experimental studies of the kinetics of this type of phase transformations.

The description of the pearlite transformation as a typical diffusion solid-phase transformation is well presented in the literature [1, 3, 4, 17, 18], and the development of ideas on this problem is given in Refs. [19, 20]. It is believed that the diffusion redistribution of dissolved in the iron alloying and impurity atoms, primarily carbon, is a limiting link in the speed of pearlite formation [18]. Characteristic of this group of data on the diffusion transformation of austenite is that they do not consider the mechanism of ferrite and cementite formation, which is replaced by the concept of process kinetics. This was discussed more than 30 years ago in Ref. [16]: '... when we talk about the mechanism of transformation, we mean the method of emergence of the nucleus of critical size. If we consider the growth of a stable nucleus, then this is the kinetics of transformation ... in many works the mechanism and kinetics of polymorphic transformations were considered together, which, of course, did not contribute to the explanation of the physical essence of the phenomenon'. Unfortunately, this situation has not changed...

Paying attention to the thermodynamics and kinetics of austenite decay, improving the mathematical apparatus to approximate theoretical calculations to experimental data, the authors of the said work do not consider the mechanism of $\gamma \rightarrow \alpha$ transformation of iron, even by self-diffusion, and its effect on carbon diffusion in steel. This is confirmed by one of the earliest works in this field [21], which when considering the crystallization of cast iron says that 'there is no data on the shape of the austenite nucleus, as well as other solid phases'. Such data are absent in the literature of recent years [11, 14, 22, 23]. Exploring the crystallization of iron-carbon melts, the authors of Ref. [21], however, found that '... in the early stages of its growth, the austenite crystal develops in the form of an octahedron, that is in the form of an equilibrium crystal faceted with the lowest surface energy'.

The lack of information in the above literature on the mechanism of diffusion transformation of austenite in steel in terms of describing $\gamma \rightarrow \alpha$ rearrangement of the crystal lattice of iron by self-diffusion of its atoms, accompanied by redistribution of carbon atoms, determined further search and analysis of information on this problem in literature specifically devoted to the study of the phenomenon of diffusion [4, 8, 24–30]. The generalization of the information given in these literature sources shows that the process of polymorphic $\gamma \rightarrow \alpha$ transformation of iron can indeed be considered from the viewpoint of self-diffusion of iron atoms, but in a different interpretation.

It is believed that the atom in the process of changing position during phase transformation first passes from the node to the internodal space, is in this less stable state for some time, and thus occupies a more stable position, for example, in a vacant node. This process in its intermediate stage is similar to the formation of a defect in the packing of atoms by the movement of partial dislocations [31].

This assumption does not contradict the existing views, both on the diffusion interpretation of the mechanism of polymorphic $\gamma \rightarrow \alpha$ transformation of iron, and on the shear, because it indicates the commonality of different views on this mechanism. In other words, there is a single mechanism of the elementary act of rearrangement $\gamma \rightarrow \alpha$ of the crystal lattice of iron, and the observed differences in its manifestation are associated with other concomitant factors. The most probable factor that accelerates the self-diffusion of iron atoms, without which it would be impossible to carry out its $\gamma \rightarrow \alpha$ polymorphic transformation by the so-called 'diffusion' mechanism, is microplastic deformation under the action of relaxing internal stresses. In this case, the reason for the formation of a crystal-geometrically ordered structure of the α-phase (ferrite) from γ-phase (austenite) becomes clear.

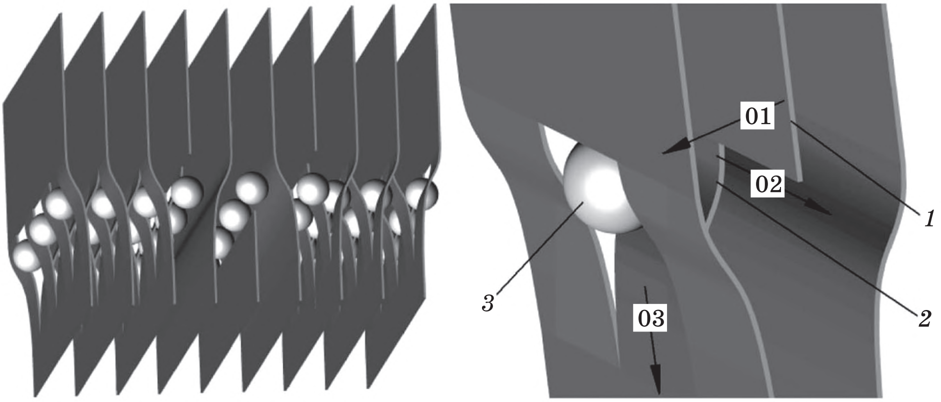


Fig. 1. Schemes of interaction of hydrogen and carbon with inflections at marginal dislocations: *1* — extraplane of marginal dislocation between two atomic layers; *2* — inflection; *3* — impurity atom of introduction or substitution; arrows show possible directions of inflection motion: 01 — traditional sliding of marginal dislocation; 02 — tangential sliding of the inflection; 03 — normal sliding of the inflection [35]

Differences in the morphology of the α-phase, traditionally explained by different mechanisms of its formation, can also be explained by crystallographically ordered rearrangement of iron atoms and features of diffusion redistribution of carbon atoms (heterodiffusion), depending on the level of internal stresses, steel composition and processing conditions [24–35].

In Ref. [35], the process of transfer of carbon atoms during $\gamma \rightarrow \alpha$ transformation of iron is considered from the standpoint of the movement of dislocation inflection (Fig. 1), which plays an important role in plastic deformation by sliding dislocations. The presence of inflections makes it possible to slide dislocations in all directions of polymorphic transformation, capturing carbon atoms with enrichment of the interfacial boundary α/γ, similar to the behaviour of hydrogen atoms with the formation of the H-layer.

When carbon and hydrogen atoms move at dislocation inflections, their diffusion in the crystal lattice of iron accelerates sharply, so this process can be described as the sliding of carbon or hydrogen atoms. An analogue of this type of diffusion is the joint movement of impurity atoms and dislocations, which is called ‘drift’. The higher the concentration of carbon or hydrogen atoms, the more chance they are to interact with the dislocation line by forming inflections.

Since the semi-diameter and binding energies of the impurity atoms differ from the corresponding values of the atoms of the main lattice, this to some extent leads to distortion of the crystal lattice of the solvent, reducing the activation energy of the impurity. Therefore, heterodiffusion, even at the lowest concentrations of impurities (carbon) should occur faster than self-diffusion (iron).

3. Physical Models and Schemes of Shear Rearrangement of the Fe Crystal Lattice at $\gamma\to\alpha$ Transformation under the Action of Internal Stresses

One of the conclusions of the previous stage of the review was that the most probable factor that accelerates the self-diffusion of iron atoms and without which it would be impossible to carry out its $\gamma\to\alpha$ polymorphic transformation by the so-called 'diffusion' mechanism is microplastic deformation under the action of relaxants internal stresses. In this case, the reason for the formation of a crystal-geometrically ordered structure of the α-phase (ferrite) from γ-phase (austenite) becomes clear. The prototype of this process is the martensitic transformation, in which $\gamma\to\alpha$ transformation of the iron is equivalent to the deformation of the original crystal lattice of austenite into the crystal lattice of martensite [1]. Since martensite in Fe–C alloys is a supersaturated with carbon ferrite, the difference between the diffusion mechanism and the martensitic one must be in the processes of redistribution of C atoms between γ- and α-phases and the degree of saturation of the α-phase, which varies from minimal (0.006 wt.% according to the Fe–C diagram) to the maximum corresponding to its content in the alloy. In this case, the shear component, which leads to the restructuring of the f.c.c. of the austenite lattice in the b.c.c. of the ferrite lattice, in both cases must be the same. In this regard, we consider it expedient to consider the process of $\gamma\to\alpha$ transformation from the standpoint of crystallogeometrically ordered shear of iron atoms under the action of internal stresses, which is accompanied by different degrees of redistribution of carbon atoms.

In the case of martensitic transformation, diffusion processes are absent, atomic displacements are comparable to interatomic distances; and in many cases a coherent or semi-coherent connection is preserved between the growing martensitic crystal and the initial phase. Coherent connection is considered an idealized (theoretical) connection in contrast to semi-coherent, which is observed in reality [37].

The formation of a new phase during martensitic transformation is accompanied by macroscopic deformation, which causes an increase in elastic energy (internal stress), which decreases due to additional slight deformation of the lattice without changing its symmetry. Because of the shear at the interphase boundary, there are steps located at a distance l from each other. The occurrence of these steps is associated with reaching the interphase boundary of dislocations because of twinning or sliding in the crystal of the new phase.

The elastic energy resulting from martensitic transformation decreases, if the martensitic crystal formed is a polydomain plate, which consists of a set of parallel plates, which have their own deformations,

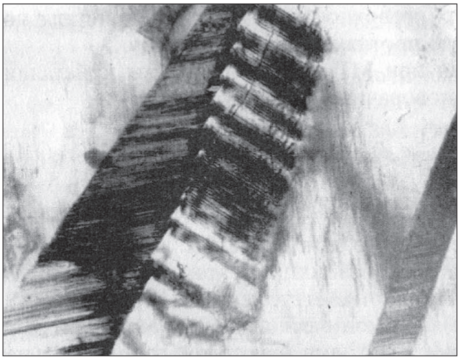


Fig. 2. Intermediate stage of formation of martensite crystals from individual thin plates in Cu–Al–Ni alloy (×20 000) [5]

and are best observed in non-ferrous alloys. Figure 2 shows the stage of formation of a martensite crystal in a Cu–Al–Ni alloy, when one (left) half is already formed and the other (right) half consists of individual plates (twins) separated by sections of the initial phase.

In iron alloys, martensite crystals contain dislocations, twins and packing defects, which indicates the presence of plastic deformation by various mechanisms in the process of martensitic transformation and in this case. As a result, a martensitic crystal with a toothed or stepped interphase boundary is formed (Fig. 3).

We can say that, during the shear transformation, there is not just a growth of the martensite crystal, but its staged formation, which ensures the minimization of stresses, which arise in the process of transformations. It follows that the structure of the martensite crystal is a consequence of the implementation of the peculiarities of relaxation processes at different stages of its formation.

Numerous studies of the microstructure of martensite in iron alloys have shown a wide variety of possible forms, depending on the chemical composition, energy of the packaging defect, cooling rate and transformation temperature. These factors determine the stress state of the undercooled initial phase and affect the way in which the formation of the α-phase from austenite. For example, depending on the manganese or chromium content $\gamma\rightarrow\alpha$ transformation with the formation of martensite is possible in the following reactions: $\gamma\rightarrow\alpha$ (f.c.c.→b.c.c.), $\gamma\rightarrow\varepsilon\rightarrow\alpha$ (f.c.c.→h.c.p.→b.c.c.), $\gamma\rightarrow\alpha$ and $\gamma\rightarrow\varepsilon$. The α-phase occurs in the form of

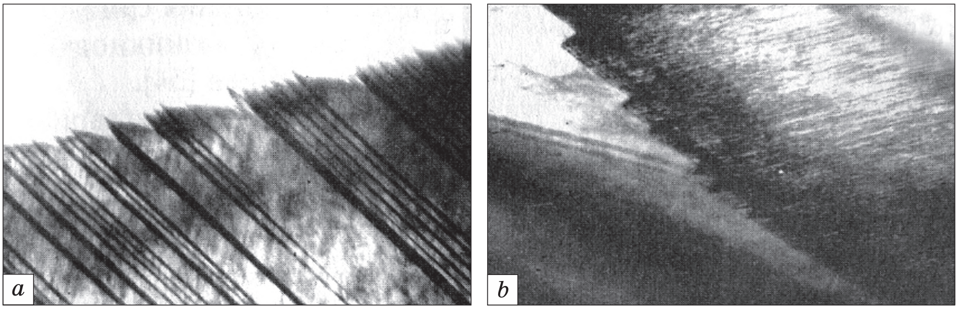


Fig. 3. Toothed (*a*) and stepped (*b*) interfacial boundary of martensite crystals in Cu–Al–Ni alloy (×10 000) [5]

needles, plates or rails, and the ε-phase occurs in the form of strips of different thickness. The α-phase is formed both inside ε-plates and at their intersection or between them [39]. The method of α-phase formation from austenite depends on the transformation temperature, cooling rate and energy of the packaging defect. It is interesting to note the possible shape of the martensitic structure in the Fe–Ni–Mn alloy in the form of packets consisting of strips with a high level of stresses of both the martensitic crystal and the surrounding austenite. At the same time, the density of dislocations in residual austenite during martensitic transformations increases to 10^9–10^{10} cm^{-2}.

Because of stress relaxation, the formed phase and the initial phase are accommodated with the formation of a common interphases boundary. It is believed [38] that accommodation in the martensitic transformation should occur at three levels:

(i) periodic inhomogeneities in martensite;
(ii) by adjusting the positions of the atoms;
(iii) by macroscopic change of shape.

At the first level, accommodation occurs due to periodic imperfections — twins or sliding lines. The second level of accommodation leads to a decrease the deformations of the mismatch localized at the interphase boundaries. Accommodation at this level can occur by elastic or plastic deformation of the initial phase, or martensite, or both phases. At the third level, dilatation and shear deformations occur in the transformed volume. In this case, the deformation by sliding dislocations is more energetically advantageous than twinning, because in the first case there is a lower level of stresses at the interphase boundary.

The interphase boundary has a stepped structure often [38]. This indicates an inaccurate conformity between the crystal structures of the martensitic and initial phases along the habitus plane. The presence of dislocations at the interphase boundary indicates a partial or complete breach of the connection between the phases. With partial coherence, the interphase boundary is a non-interleaved area of complete (coherent) coincidence with areas containing dislocations. Relaxation of stresses arising in the process of transformations also leads to the appearance of dislocation of mismatch at the interphase boundaries of martensitic crystals (Fig. 4).

The distance between dislocations at incoherent interphase boundaries differs by 10–100 times

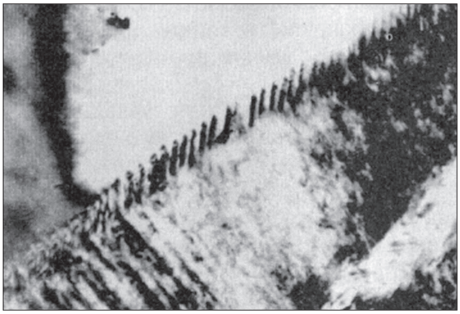


Fig. 4. Dislocations at the interfacial boundary of the martensite crystal of Cu–Sn alloy (×20 000) [5]

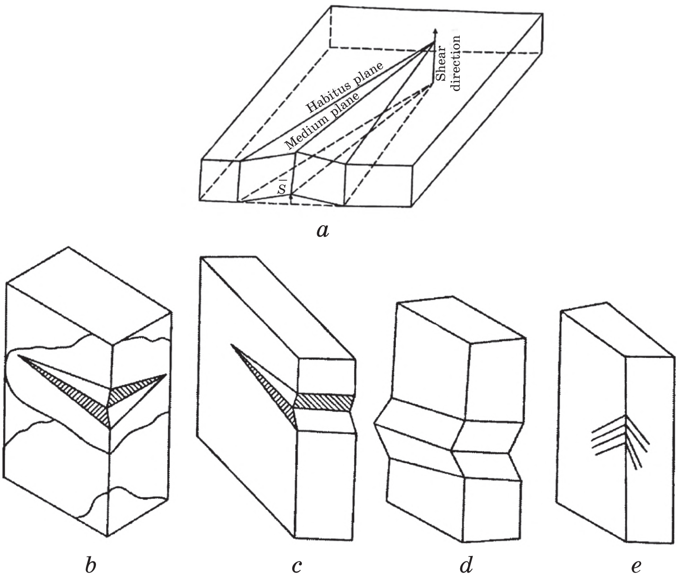


Fig. 5. Scheme of relief (*a*) in the formation of martensite crystal and its possible types (*b*–*e*) in Cu–Al–Ni alloys: *b* — wedge-shaped on two faces; *c* —wedge-shaped layer; *d* — dihedral layer; *e* — lamellar [32]

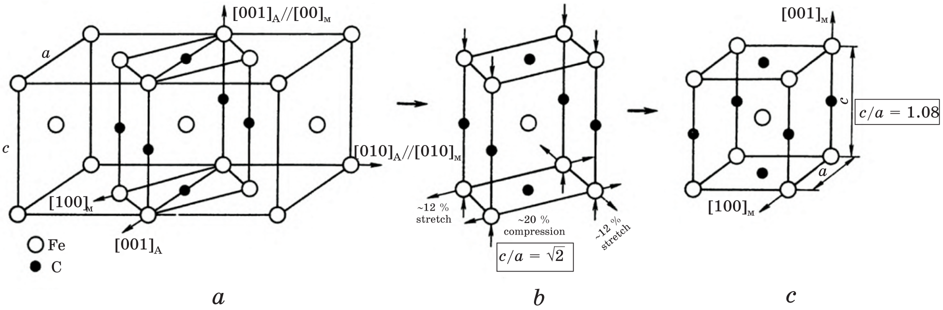


Fig. 6. Bain's scheme: *a* — double f.c.c. lattice of austenite (not all iron atoms are shown, carbon atoms are in octahedral internodes); *b* — selected b.c.t. lattice with $c/a = \sqrt{2}$; *c* — b.c.t. lattice of martensite with $c/a = 1.08$ (carbon atoms occupy only octahedral internodes along the axis $c \parallel [001]$) [40]

of magnitude from the period of the crystal lattice of pure metals that are part of the alloy. The HREM (high-resolution electron microscopy) method (direct observation of the lattice) on the example of Ti–Ni alloy shows the possibility of a continuous (direct) transition of the initial phase planes through the interphase boundary in the martensite plane and then again through the interphase boundary in the initial phase plane [38]. To accommodate the discrepancy between the crystals of the initial and martensite phases due to differences in their interplanar distances at the place of docking, interphase dislocations are formed.

In order to obtain an undistorted habitus plane, defects of the hexagonal type packing must appear on the interphase surface. The scheme of the interphase boundary consisting of coherent sections — steps separated by dislocations (interphase defects) with a certain orientation and distance between them is shown in Fig. 5. Different schemes (models) for different metals and alloys have been proposed to explain the rearrangement of the crystal lattice by the martensitic (shear) mechanism. This structure of interphase boundaries provides a minimum of forces of long-range stress fields, and at certain lengths λ and height h of steps the interphase boundaries can be conservatively moved, ensuring the course of martensitic transformation [34].

The first was Bain's scheme for Fe–C alloys according to which the b.c.c. of the α-Fe lattice is formed from the f.c.c. of the γ-Fe lattice by its direct shear (Fig. 6) [2]. To do this, in two adjacent elementary f.c.c. foci of austenite allocate b.c.t. lattice with the ratio $c/a = \sqrt{2} \approx 1.41$, and then, to obtain the martensite lattice compress, the selected cell along the axis c ([001]) by $\approx 20\%$ and expand along the axes a ([010] and [100]) by $\approx 12\%$. The exact values of deformations depend on the carbon content in the steel, *i.e.* on the tetragonality of the martensite lattice. In carbon steels, the maximum value is $c/a = 1.08$ (Fig. 7).

When Bain's deforms, all the carbon atoms in the austenite lattice are found in the internodes (they are called octahedral because they are surrounded by six Fe atoms) along the [001] axis of the martensite lattice, causing its tetragonal distortion. In such a scheme of crystal lattice rearrangement, the habitus plane is a plane of type $\{100\}\gamma$, and parallel directions in two phases are $\langle 110\rangle\gamma$ and $\langle 100\rangle\alpha$, $\langle 001\rangle\gamma$ and $\langle 001\rangle\alpha$. However, experimental data show the presence of other orientational relations and habitus planes. In addition, according to Bain's scheme, only three different orientations can form martensite from austenite, while 24 orientations have been experimentally identified [39]. In fact, the displacements of atoms during the martensitic transformation are more complex. Based on the above, it was concluded that the martensitic transformation could not be carried out according to Bain's scheme.

In order for the theoretical scheme of lattice rearrangement during the martensitic transformation to correspond to the experimentally observed facts Bain's

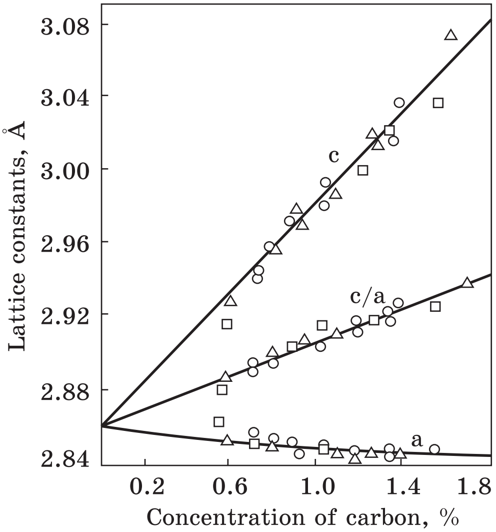


Fig. 7. The lattice constants (c — curve above, a — curve below, and c/a — curve in the middle) of martensite *vs.* the concentration of C in it [39]

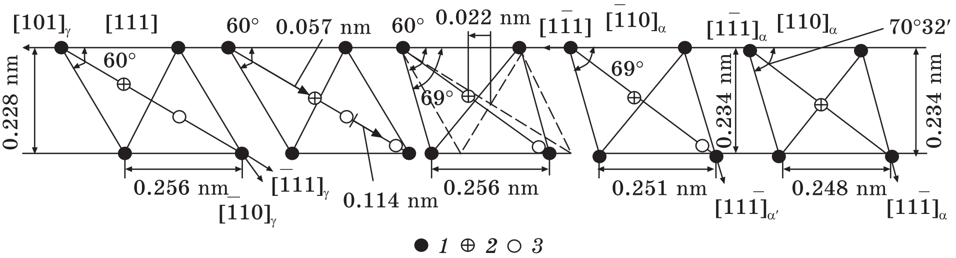


Fig. 8. Reconstruction of the crystal lattice at γ→α transformation according to the Kurdyumov–Sachs scheme: *1* — Fe atoms of the first layer; *2* — Fe atoms of the second layer; *3* — Fe atoms of the third layer [41]

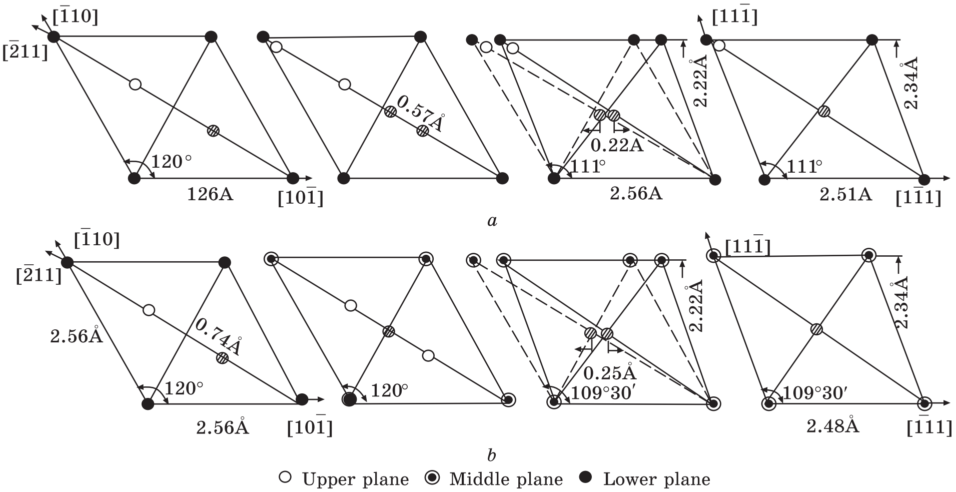


Fig. 9. Comparison of Kurdyumov–Sachs schemes for rearrangement of crystallographic mesh (111) of austenite into mesh (011) of martensite (*a*) and mesh (011) of ferrite (*b*) [39]

scheme must be supplemented by additional deformation, which is carried out either by twinning or dislocation slide. In this case, the experimentally observed orientational relations are explained, and the presence of twins and dislocations in martensite crystals becomes clear. Bain's scheme is usually the first stage of lattice rearrangement in all other proposed mechanisms of martensitic γ→α transformation of iron.

The second scheme that explains the lattice rearrangement during martensitic transformation is the Kurdjumov–Sachs scheme proposed by G.V. Kurdjumov and G. Sachs for martensitic transformation in steel with 1.4% C [40]. This scheme is based on the experimentally established orientation between austenite and the α-phase: families of planes {111}γ || {110}α and directions ⟨110⟩γ || ⟨100⟩α.

The transition from phase to phase according to the Kurdjumov–Sachs scheme is carried out by means of two shifts. The first shift occurs on one of the planes of the type $\{111\}\gamma$ in the direction $[211]\gamma$ (Fig. 8). Atoms located on the first plane of $(111)\gamma$ are shifted by 0.57 nm (shear angle ≈15°15′), and on the second plane by 0.144 nm. The second shift occurs on the plane $(\bar{2}11)\alpha$ in the direction $[11\bar{1}]\alpha$. This shift leads to an increase in the angle at the apex from 60° to 69°. To form the α-phase lattice with the correct parameters (ferrite), it is necessary to reduce the interplanar distances. According to this mechanism, martensitic transformation can occur in low-carbon steels with a carbon content of up to 0.45%, in which the habitus of martensitic crystals corresponds to $\{111\}\gamma$. In this case, the angle at the first shift is 19°28′, and at the second — 70°32′.

According to the Kurdjumov–Sachs scheme, the tetragonal lattice of martensite is intermediate between austenitic and ferritic. The displacements of atoms available in martensitic transformations according to the Kurdyumov–Sachs scheme are slightly smaller than in the case of rearrangement to ferrite (Fig. 9).

It can be assumed that the inhibitory effect for the rearrangement of the austenite lattice into ferrite is exerted by C atoms, which are embedded in the austenite lattice and remain in the lattice during martensitic transformations. It follows that the rearrangement of the crystal lattice of iron during its γ→α transformation with the formation of pre- and eutectoid ferrite occurs in the same way as during martensitic transformation, but is accompanied by carbon diffusion.

The scheme of three-stage stepwise transformation of austenite into martensite or ferrite according to the Kurdjumov–Sachs scheme is conditional. Most likely, the rearrangement of the crystal lattice occurs by a single and continuous shear of atoms, the experimental determination of the trajectories of which, however, today is a difficult problem.

4. Kinetic Model of Shear Transformation of Austenite Considering Stresses Influences

The formation of a new phase during martensitic transformation is accompanied by macroscopic deformation, which causes an increase in elastic energy (internal stress), which decreases due to additional slight deformation of the lattice without changing its symmetry.

Considering martensitic transformation as a thermally activated process B.Ya. Lyubov used the equation of normal transformation and the equation of thermodynamics to describe its kinetics [40]. However, B.Ya. Lyubov in his theory did not take into account the role of internal stresses that can be induced in austenite and arise in the process of γ→α transformation.

The theory of martensitic transformations continues to be developed recently by Ukrainian scientists [41–45]. The role of stresses and strains in the formation of martensite was considered in Refs. [41–43]. A number of problems of thermodynamics of thermally induced thermoelastic martensitic transformations were discussed in Ref. [44]. It was shown that the basic system of equations of balance of thermodynamic forces, which describes the temperature dependence of the volume fraction of martensite, could be obtained directly from the law of conservation of energy, which additionally takes into account the effects of irreversible work against internal dissipative forces. The general balance of thermodynamic forces is carried out between classical (‘chemical’) driving forces, on the one hand, and the so-called non-chemical forces due to elastic, interphase and other energy contributions on the other. In conclusion, the problems of thermoelastic martensitic transformations were discussed on the basis of a microscopic theoretical approach.

A consistent thermodynamic approach for considering martensitic transformations has been proposed in Refs. [40, 42, 44]. Changes in a complex or composite system under constant external conditions can be described as a process of entropy growth. The entropy growth rate σ can be represented by the sum of sets of flows and corresponding forces for all transfer substrates in the amount of N [46, 47]:

$$\sigma = \frac{dS}{dt} = \sum_{k=1}^{N} J_k X_k (k = 1, \ldots, N)\,. \tag{1}$$

In the general case, the flows can be represented as [47, 48]

$$J_i = \sum_{k=1}^{N} L_{ik} X_k (i, k = 1, \ldots, N)\,, \tag{2}$$

where J_i is the flows, X_k is the thermodynamic forces, $L_{ik} = L_{ki}$ is Onsager’s kinetic coefficients [46], i and k are the numbers of charges (transfer substrates).

The change of free energy in a system with variable number of particles and internal stress can be represented as [40]

$$dF = dF_\varepsilon + dF_n = \sigma_{ik} d\varepsilon_{ik} + \varphi_l dn_l; \tag{3}$$

here, dF_ε is the change in free energy in the system associated with the internal stress; dF_n is the change in free energy in the system, which is determined by the variable number of particles of grade l; σ_{ik} is the stress tensor; ε_{ik} is the system deformation tensor; φ_l is the chemical potential of the l-th element of the system; n_l is the number of particles of the l-th element of the system per unit volume ($l = 1, \ldots, N$).

The main driving forces of phase transformations of nonequilibrium thermodynamics are the gradients of chemical potentials [46, 47]. When considering discontinuous systems, the finite differences of chemical potentials ($\Delta\varphi_i$) during the transition from one state to another one are used as thermodynamic forces [48, 49]. If two quantities are used as charges of the process of diffusion-free transformation of austenite — the concentration of α-phase particles and the amount of deformation, then according to (2) the equations of motion take the form [48, 50]:

$$\begin{aligned} J_1 &= L_{11}X_1 + L_{12}X_2, \\ J_2 &= L_{21}X_1 + L_{22}X_2, \end{aligned} \tag{4}$$

where $X_1 = \Delta\varphi$ is the thermodynamic force for iron — change of chemical potential during the transition of particles from γ-phase to α-phase; $X_2 = \Delta\sigma$ is the change of internal stress during the transition from γ-phase to α-phase.

The system of Eqs. (4) describes the contribution of stresses and strains to the diffusion-free transformation of austenite.

In Ref. [50], by solving the system of Eqs. (4) with time-independent coefficients L_{11} and L_{12}, a kinetic equation was obtained for the quantity of martensite formed n_α in time:

$$n_\alpha = \frac{(L_{11}\Delta\varphi + L_{12}\sigma_\gamma)L}{\upsilon}(1 - e^{\frac{\upsilon}{L}t}). \tag{5}$$

According to equation (5), the quantity of α-phase depends not only on the thermodynamic force $\Delta\varphi$, but also on the magnitude of stresses in the γ-phase σ_γ.

Comparing the values of thermodynamic forces, we can classify the types of diffusion-free transformation on the kinetic basis. As noted in Ref. [3], with small deviations of the system from equilibrium, the growth of crystals controlled by self-diffusion is more likely, with large deviations — cooperative growth. The same phase transition in a one-component system under different external conditions can occur at a temperature-independent (or weakly temperature-dependent) growth rate (martensitic kinetics) and at a rate that is exponentially dependent on the temperature at the activation energy close to energy activation of self-diffusion (normal dynamics).

The parameter characterizing the deviation of the system from equilibrium is the undercooling of the alloy $\Delta T = A_{C3} - T_{\text{trans}}$ conversion, where A_{C3} — the end temperature of σ→γ transformation when heated. The scheme of transformations for the constructed model is given in Table.

Therefore, at low ΔT,

$$L_{11}\Delta\sigma > L_{12}\sigma_\alpha > L_{12}\sigma_\gamma, \tag{6}$$

then the growth of α-phase crystals is determined by self-diffusion by a normal mechanism. However, as follows from Eq. (5), in this case the contribution of deformations (and stresses) to the kinetics of transformation is quite significant. In order to comply with condition (6) it is necessary that the stress level in the γ- and α-phases be insignificant, for the α-phase this is possible only in the case of relaxation of internal stresses in the metal at high temperature by the recrystallization mechanism.

With increasing undercooling of the alloy, the thermodynamic stimulus and the rate of normal transformation increase.

At greater ΔT,

$$L_{11}\Delta\sigma \sim L_{12}\sigma_{\alpha} > L_{12}\sigma_{\gamma}. \tag{7}$$

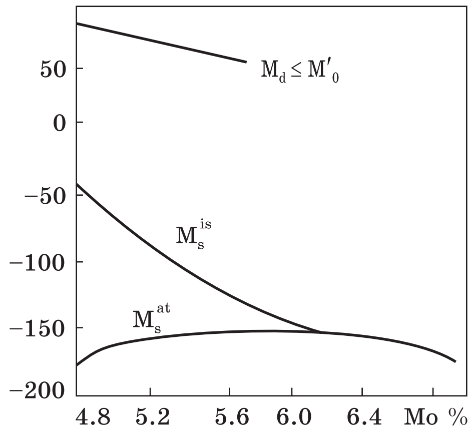
Existing thermal stresses in the γ-phase contribute to the formation of the α-phase by the shear mechanism, while arising in the α-phase on-stresses compensate for thermal stresses in the γ-phase. At a certain quantity of α-phase, there is an equality of stresses $\sigma_{\alpha} = \sigma_{\gamma}$ and further formation of α-phase occurs by a normal mechanism with relaxation of the resulting stress by recrystallization. Thus, condition (7) corresponds to the transformation of the γ-phase by a mixed mechanism, as well as the formation of Widmanstätten ferrite followed by the excretion of the α-phase by a normal or diffusion mechanism [3].

With some undercooling ΔT_i compensation of stresses occurs only when the complete transformation of the γ-phase into ferrite by a shear mechanism, wherein

$$L_{11}\Delta\varphi \sim L_{12}\sigma_{\alpha},\ \sigma_{\alpha} = \sigma_{\gamma}. \tag{8}$$

Table. **Scheme of non-diffusion transformation according to the model constructed in Ref. [51]**

A_{C3}
$L_{11}\Delta\varphi > L_{12}\sigma_{\alpha} > L_{12}\sigma_{\gamma}$, normal transformation
$L_{11}\Delta\varphi \sim L_{12}\sigma_{\alpha} > L_{12}\sigma_{\gamma}$, shear + normal transformation, Widmanstätten ferrite A_{C1}
M_{si} $L_{11}\Delta\varphi < L_{12}\sigma_{\alpha}$, $\sigma_{\alpha} = \sigma_{\gamma}$
$L_{11}\Delta\varphi < L_{12}\sigma_{\alpha}$, $\sigma_{\alpha} < \sigma_{\gamma}$, shear transformation, isothermal martensite, needle ferrite M_{sa}
$L_{11}\Delta\varphi \ll L_{12}\sigma_{\gamma}$, shear transformation, athermal martensite M_f
A_{C1} — the temperature of the start of the α→γ transformation when the alloy is heated; M_{si} — the temperature of the start of the formation of isothermal martensite during undercooling of the alloy; M_{sa} — the temperature of the start of the formation of athermal martensite; M_f — temperature of the finish of the formation of martensite



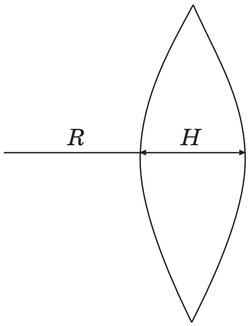


Fig. 10. Temperature intervals of athermal (M_s^{at}) and isothermal (M_s^{is}) kinetics of martensite formation in alloys of the system Fe–24.5% Ni at different Mo contents [3]

Fig. 11. Geometric parameters of martensite crystal

The temperature corresponding to this undercooling is the start point for the formation of isothermal martensite M_{si}, it is close to A_{C1} and below it on the temperature scale (Table). Below the point M_{si}, the formation of the α-phase occurs by a shear mechanism, but the self-diffusion component of the process is still significant affecting the morphology of the formed excretions. When undercooling larger ΔT_i:

$$L_{11}\Delta\varphi < L_{12}\sigma_\alpha,\ \sigma_\alpha < \sigma_\gamma. \tag{9}$$

At temperatures below M_{si}, the formation of isothermal martensite or needle ferrite with ‘rail’ or needle morphology of nucleuses occurs. The temperature range of isothermal martensite formation for alloys of the Fe–24.5% Ni–x% Mo system is shown in Fig. 10 [3]. The temperature M_d of the formation of martensite activated by plastic deformation in these alloys is slightly lower than the thermodynamic equilibrium temperature of austenite and martensite T_0', and the onset temperature of athermal martensite M_{sa} is lower than the onset temperature of isothermal martensite M_{si}.

Finally, at large ΔT (below M_{sa}),

$$L_{11}\Delta\varphi \ll L_{12}\sigma_\gamma. \tag{10}$$

Inequality (10) determines the condition for the formation of athermal martensite, when the self-diffusion component does not affect the formation of the shear structure. The main influence on the rate of γ→α transformation according to expression (10) is exerted by thermal stresses in the γ-phase. The temperature range of creation of this structural component for real alloys is also shown in Fig. 10.

In Ref. [51], the parameters of martensitic crystals in steel formed at the micro-level were established. Microstructural studies show that the martensite crystal has the shape of a plate with a sharp edge, which is visible in the plane of the section in the form of a needle [52]. The shape of the crystal was considered close to the biconvex lens formed by the segments of the sphere (Fig. 11) [40].

When a martensite crystal appears in austenite cooled below the martensite point, the following change in the free energy of the system occurs [40–42]:

(i) change in free energy in the volume occupied by the α-phase crystal (in the range of martensitic transformation, the free energy of the α-phase is less than the free energy of austenite);

(ii) formation of the interface between the α-phase crystal and the surrounding austenite;

(iii) change in elastic energy in the volume of the α-phase crystal and in the initial austenite.

As found in Ref. [50], in the formation of a martensite crystal, the value of ΔF_0 must meet the condition:

$$\Delta F_0 \geq \Delta F_0' = 2\gamma\,, \tag{11}$$

where γ is the energy parameter calculated through the austenite shear modulus [40].

Thermodynamic condition (11) establishes another feature of martensitic transformation and answers the question why it begins at a certain temperature M_s [2–4]. It shows that the difference between the free energies of the austenite and ferrite phases, which increases with decreasing temperature, must be greater than a certain value of 2γ, which is calculated through the shear modulus of austenite. Therefore, relation (11) is fulfilled when austenite reaches a certain temperature M_s during cooling. As the degree of alloy age of austenite increases, its shear modulus increases and the temperature M_s of steel decreases [3].

At a given value of ΔF_0, the parameter R of martensite must take very specific values [50]:

$$R_0 = \frac{2\sigma\Delta F_0}{(\Delta F_0 - 2\gamma)^2}\,. \tag{12}$$

In Ref. [50], we also obtained an equation for the radius of martensitic crystals R_s formed by austenite stresses σ_γ:

$$R_s = \frac{2}{\rho}\frac{F_0^2}{(\Delta F_0 + \gamma)(\Delta F_0 - 2\gamma)} L_{12}\sigma_\gamma \frac{L}{\upsilon}\,. \tag{13}$$

As expected, at $\Delta F_0 \leq 2\gamma$ the formation of martensite crystals does not occur. Thus, the condition $\Delta F_0 = 2\gamma$ determines the start point on the temperature axis for the formation of martensite M_s. At higher temperature than M_s the shear of atomic planes in austenite is energetically unfavourable. As $\Delta F_0 \geq \Delta F'_0$ increases, the martensite crystals that are formed have a well-defined radius R_s of transformation and stresses in austenite. If the radius of the formed particles is $R_s \leq R_0$, then the formation of such α-phase crystals is also not energetically advantageous and they are again converted into austenite. In order for the condition $R_s > R_0$ to be satisfied at a given value of ΔF_0, a certain stresses level in the γ-phase $\sigma_\gamma > \sigma_{\gamma 0}$ is also required.

Thus, to convert residual austenite to martensite requires several conditions: thermodynamic $\Delta F_0 \geq \Delta F'_0$ by reducing the temperature of steel up to the temperature of the end of the transformation of residual austenite and kinetic by increasing the level of internal stresses in austenite $\sigma_\gamma > \sigma_{\gamma 0}$, increasing the cooling rate at the final stage of processing or mechanical impact.

5. Analytical Models of Shear Transformation of Austenite in Steel Considering Internal Stresses

In the field of modelling the kinetics of phase transformations, the most fundamental studies were carried out in the works of A.N. Kolmogorov and M. Avrami, who describe analytical equations where the volume of the newly formed phase depends on the probability of nucleation, linear growth rate and past time [61, 62].

A fundamental review of mathematical modelling of the process of phase transformations is presented in Refs. [1, 39, 40], which indicated that existing analytical models do not explicitly take into account the process of nonstationary nucleation, and this contradicts the physics of the process. As also noted, the analytical models do not allow considering the process of formation of individual grains and their growth.

In addition to analytical models, there is an approach to simulate the process of nucleation and growth based on the model of I.L. Mirkin. He proposed studying the crystallization process using the two-dimensional schemes [17]. The model takes into account the stochastic nature of the process, the incubation period and allows calculating the grain size. At the same time, the stochastic nature of the formation of crystallization centres in the model is not fully realized. In this model, the space of melt and crystals is represented as a set of elementary fragments, such as a raster image in computer graphics, which complicates the implementation of the model in three-dimensional space, as well as a description of the process in continuous space and time.

In Ref. [40], a method for calculating structural transformations under arbitrary cooling according to the isothermal diagram (ITD) was proposed, in which the rule of additivity is applied to the transition from isothermal kinetics of transformations to nonstationary temperature conditions. This rule is valid for isokinetic reactions, *i.e.* those for which the process speed depends only on the cooling rate V and time t, and not on the 'thermal trajectory' at which the system came to this condition. In this case, the isothermal kinetics of the processes of nucleation and growth is usually described by the Avrami equation [40]:

$$V_\alpha = 1 - e^{-(K\tau)^n}, \tag{14}$$

where K and n are coefficients depending on the type of ITD; V_α is the volume fraction of the transformation product.

The Avrami equation, or as it is also called Kolmogorov–Johnson–Meil–Avrami equation [53, 54], is used in many mathematical models describing the decay of austenite [55–58]. A common disadvantage of the above-mentioned works is the neglect of the influence of the stress-strain condition that occurs during the heat treatment of parts on the kinetics of structural transformations, while the available experimental data [41–45, 59–66] indicate a significant effect of stresses and deformations on structural transformations.

Stresses during heat treatment of steel products occur due to volumetric deformations associated with the unevenness of the temperature field and the non-simultaneity of structural transformations. Moreover, the deformations due to structural transitions are comparable to temperature deformations [67]. The description of temperature and structural deformations is usually performed using the total coefficient of linear expansion, which is equal to [59]:

$$a = \frac{d\varepsilon}{dt}, \tag{15}$$

where ε is the free deformation that takes into account temperature and structural changes.

The value of ε can be determined by the dilatograms [59] of steel depending on the structural composition based on the rule of additivity [67].

The studies performed in Refs. [59–66] were carried out in isothermal conditions with uniaxial stretching. It was found that plastic deformation of about 20–30% significantly reduces the incubation period and increases the rate of pearlitic transformation. Bainitic transformation is characterized by acceleration of the process during the deformation, when the strain is removed, the rate of transformation decreases rapidly to its 'normal' value. Thus, the determining factor in accelerating the bainite transformation is the current stresses [40]. Plastic deformation associated with the load has a much smaller impact and cannot be attributed to the accelerating factors.

The maximum rate of bainite transformation in the unloaded condition occurs in the middle of the process, but the transformation under load is characterized by an increase in the rate of decay of austenite in the initial stages of the process [62]. This fact is explained by the acceleration of the crystal lattice rearrangement under stress, which in turn leads to a reduction in the duration of diffusion processes of carbon redistribution required for the transformation, and consequently to slow down the reaction in the final stages. This explains the decrease in the limiting degree of decay of austenite with increasing load. As noted in Ref. [65], the dependence of the kinetic parameters of the bainitic transformation on the acting stress should be ‘strong’ (exponential).

The study of martensitic transformation [67] showed that the applied stress increases the temperature of the start of the transformation and accelerates the process at the initial stage. In the future, the transformation is less intense and ends at a temperature lower than in the unloaded condition. The type of load (tension or torsion) has little effect on the results obtained. The residual austenite content increases with increasing load [67]. These facts indicate the analogous nature of the influence of stresses on bainite and martensitic transformation, which is explained by their identical (shear) mechanism.

In Ref. [68], a mathematical model of steel quenching was proposed considering stresses effects on pearlitic and martensitic transformation. The theory of isokinetic reactions is used to describe the pearlitic transformation in non-isothermal conditions.

For martensitic transformation, the dependence of the quantity of martensite formed V_M on the stress intensity is accepted:

$$V_M = (1 - V_p)\{1 - \exp[-a(M_S - t + b\sigma_i)]\}, \tag{16}$$

where V_P is the volume fraction of pearlite; σ_i is the stress intensity; a and b are obtained experimentally constants.

In Ref. [69], the approach described for the case of successive decay of austenite in the pearlitic, bainitic, and martensitic range. In the mathematical modelling of pearlitic and bainitic transformations, equations similar to those obtained in Ref. [70] for bainitic transformation without load under the assumption of the additive course of the process are used. The volume fraction of bainite at an arbitrary cooling mode V_B is proposed to be found by the equation:

$$V_B = (1 - V_P)\, m \exp\left[-\left\{\int_{\tau_1}^{\tau} Kb(t)^{1/a} \exp(c_B\sigma_0)\, d\tau\right\}^{\alpha}\right]. \tag{17}$$

The multiplier m allows us to take into account the presence in many alloy steels of a limiting degree of bainitic transformation, which at a given temperature and stress-strain condition cannot be exceeded with increasing process duration. The value of m is calculated by the equation:

$$m = (M_{Bs} - t + a_B\sigma_0 + b_B\sigma_i + g_B\varepsilon_i^p)\, d, \tag{18}$$

where M_{Bs} is the temperature of the start of bainitic transformation in steel that is not subject to mechanical impact; ε_i^p is the intensity of plastic deformations [69]; a_B, b_B, g_B, and d are empirical constants.

Equation was used for martensitic transformation [71]:

$$V_M = (1 - V_P - V_B)\{1 - \exp[-a(M_s - t + a_M\sigma_0 + b_M\sigma_0 + g_M\varepsilon_i^p)]\}, \quad (19)$$

where a_M, b_M, g_M, and a are empirical constants.

Due to the lack of experimental data to determine the numerous parameters of the mathematical model, the values of some constants taken equal to zero, others are approximately accepted according to [71–73]. The calculations were performed for quenching on bainite in water of cylindrical parts with a diameter of 1 m with variation of constants. In the course of the numerical experiment, a significant dependence of the established structural composition on the values of the constants was revealed.

The authors of Ref. [74] in the study of the acceleration of the martensitic transformation under the action of tensile stresses, which occurs at low temperatures in chromium-nickel steels, suggested that the decay kinetics depends on both the mean stress and stress intensity.

In Ref. [75], a simple theoretical equation was obtained for calculating the quantity of martensite formed, depending on the average stress in the γ-phase:

$$n_\alpha = n_{\alpha 0} + L_{12}\sigma_\gamma, \quad (20)$$

where $n_{\alpha 0}$ is the quantity of martensite formed in the absence of stresses in the γ-phase; L_{12} is a coefficient constant at the current temperature (Onsager coefficient).

This quantity can be calculated by the Koistinen–Marburger (K–M) Eq. [39], or by the equation proposed in Ref. [76]:

$$n_{\alpha 0} = A_m\left(1 - \exp\left[-K_\alpha \frac{M_s - T}{T - M_f}\right]\right), \quad (21)$$

where A_m is the quantity of austenite preserved to the temperature M_s; M_s is the temperature of the start of the formation of martensite; M_f is the temperature of the finish of the formation of martensite; K_α is a coefficient that characterizes the rate of martensite formation near the temperature M_s

Equation (21) takes into account the initial and final temperatures of martensite formation and describes the various kinetics of its growth [6].

Taking into account the results obtained in Ref. [51], the quantity of martensite formed under the action of stresses in the γ-phase should be calculated by the equation:

$$n_\alpha = n_{\alpha 0} + L_{12}(\sigma_\gamma - \sigma_{\gamma 0}), \quad (22)$$

where $\sigma_{\gamma 0}$ is the minimum stress required for the crystal-geometrically ordered shear of iron atoms in the formation of martensite.

In Ref. [77], by processing experimental data on phase transformations in steels, the combined effect of alloying elements, cooling rate and emerging stresses and strains on the temperature of the start (T_{spt}) and finish (T_{fpt}) of austenite-steel phase transformations in steel was evaluated. According to the dilatograms presented in Ref. [78], two additional parameters were also found: the relative extension of the steel sample before the start of the austenite phase transformation (D_1) and the relative expansion of the steel sample in the austenite phase transformation process (D_2).

Parameter D_1 characterizes the additional deformation (relative elongation) of the steel sample ε_1. It occurs when it is cooled in comparison with the reference sample with a normalized (known) coefficient of linear extension α. According to the basic principles of metal physics and its subfield — the mechanics of a deformed solid — deformations and stresses in a solid are related by the generalized Hooke's law [79].

Parameter D_2 characterizes the stresses created by the phase transformation of austenite. It is known that, during cooling, in austenite, the α-phase is formed with increasing volume of the crystal lattice, which at the micro-level creates a stresses between the phases, which can be estimated by the generalized Hooke's law. Deformation that takes place at the micro-level leads to the formation of defects in the crystal lattice — vacancies, dislocations, interface between phases and crystals. The microdeformation, which passes over the entire volume of the sample, turns into a macrodeformation of the sample, which is characterized by its total relative elongation ε_2 and parameter D_2.

Based on the available data, the regression equations of the start and finish temperatures of the phase transformation of austenite in steel on the chemical composition, cooling rate and parameters of internal deformations D_1 and D_2 were obtained:

$$\begin{gathered}T_{spt} = 883.1 - 42.5\,\mathrm{C} - 157.7\,\mathrm{Mn} + 64.3\,\mathrm{Si} - 11.8\,\mathrm{Cr} - \\ - 46.9\,\mathrm{Ni} - 116\,\mathrm{Mo} - 214.4\,\mathrm{V} - 4484\,\mathrm{P} + 3152\,\mathrm{S} - \\ - 73.2\lg V_{\mathrm{cool}} + 19.3\,D_1,\ R^2 = 0.89;\end{gathered} \tag{23}$$

$$\begin{gathered}T_{fpt} = 586.7 + 98.6\,\mathrm{C} - 197.2\,\mathrm{Mn} + 221.6\,\mathrm{Si} - 102.3\,\mathrm{Cr} - \\ - 51.4\,\mathrm{Ni} - 257.3\,\mathrm{Mo} - 51.8\,\mathrm{V} - 1439\,\mathrm{P} + 2058\,\mathrm{S} - \\ - 137.9\lg V_{\mathrm{cool}} + 5.8\,D_1 - 0.86\,D_2,\ R^2 = 0.85;\end{gathered} \tag{24}$$

The temperature of the start of the phase transformation of austenite T_{spt} all alloying elements, except for silicon and sulphur, as well as the cooling rate had a negative impact. Parameter D_1 characterizes the stresses in the γ-phase and increases the initial and final temperatures of the phase transformation of austenite, which occurs in other models.

The temperature of the finish of the phase transformation of austenite T_{fpt} carbon, silicon and sulphur had a positive impact. Manganese,

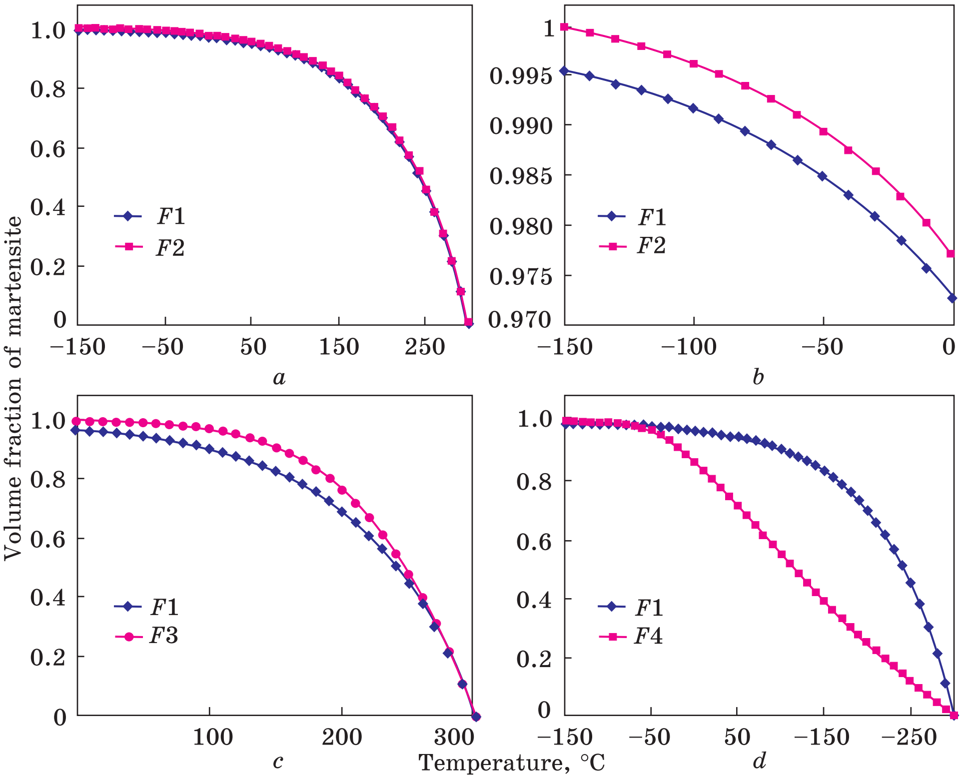


Fig. 12. Calculation of the quantity of martensite from the transformation temperature by different equation: *F*1 — by the K–M equation [40]; *F*2 — according to the modified K–M equation (26); *F*3 — according to Eq. (21) with $K_\alpha = 6.84$; *F*4 — by Eq. (21) with $K_\alpha = 1.0$

chromium, nickel, molybdenum, vanadium, phosphorus, cooling rate and parameter D_2 had a negative impact. Of particular note is phosphorus, the negative impact of which on these temperatures is very strong.

Studies conducted in Ref. [77] also showed that the change in temperature of phase transformations has a different nature for steels with low and relatively high content of chromium and nickel. The latter give nonlinear distortion of the studied values in the temperature range less than 450 °C. Therefore, it is advisable to consider the possibility of creation models for steels with low and high chromium and nickel content, respectively.

The quantity of martensite formed in steel can also be calculated by the Harris–Cohen's equation obtained by processing the experimental results and given in Ref. [6]:

$$n_{\alpha 0} = 1 + K_0(445 - \Delta T)^{5.32}, \qquad (25)$$

where $K_0 = 6.956 \cdot 10^{-15}$, $\Delta T = M_s - T$.

The disadvantage of this equation is that at the temperature of the start of austenite transformation $M_s = 182$ °C and below the calculated temperature of the finish of austenite transformation M_f, it becomes lower than the temperature of absolute zero (−273 °C).

This paper also proposes a modified K−M equation, which takes into account not only the temperature the start but also the finish of the austenite transformation:

$$n_{\alpha 0} = 1 - \frac{\exp k_\alpha (M_s - T) - \exp k_\alpha (M_s - M_f)}{1 - \exp k_\alpha (M_s - M_f)}. \tag{26}$$

Figure 12 shows the results of modelling the transformation of austenite by different equations and comparing them with each other. As can be seen, the difference between the functions $F1$ and $F2$ becomes noticeable only at very low temperatures (Fig. 12, *b*). Equation (21) allows describing the various kinetics of austenite to martensite transformation taking into account temperatures M_s and M_f by changing the parameter K_α, so it is more universal than the K−M equation.

Thus, over more than a hundred years of research on the shear transformation of austenite, scientists around the world have developed significant experimental material on the mechanisms of such transformation and built theoretical models that explain the dependence of the parameters of such transformation on temperature and stress. The analysis of numerous works shows that the accumulated theoretical and experimental results to date allow describing reliably the effect of stresses on the shear transformation of austenite during heat treatment of steels. To increase the accuracy of forecasting the structural condition of steels during heat treatment, it is necessary to conduct a comprehensive study related to the experimental determination of stress on shear transformation and create an adequate physical and mathematical model of austenite transformation based on the obtained influence.

6. Conclusions

In G.V. Kurdjumov's work with colleagues, the martensitic transformation is considered as a normal (diffusion) phase transformation in a one-component system, further complicated by the influence of strong interatomic interaction, which leads to the development of significant stresses in the martensite crystal and matrix. According to an alternative mechanism, martensitic transformation occurs by means of an instantaneous shear of atomic planes, which does not require thermal activation and is not associated with thermodynamic stimuli of transformation. The factor that initiates the transformation is the stresses that occur during rapid cooling (quenching) of the sample.

There is a single mechanism of the elementary act of rearrangement $\gamma \rightarrow \alpha$ of the crystal lattice of iron, and the observed differences in its manifestation are associated with other concomitant factors. The most probable factor that accelerates the self-diffusion of iron atoms without which it would be impossible to carry out its $\gamma\to\alpha$ polymorphic transformation by the so-called 'diffusion' mechanism is microplastic deformation under the action of relaxing internal stresses. In this case, the reason for the formation of a crystal-geometrically ordered structure of the α-phase (ferrite) from γ-phase (austenite) becomes clear.

Rearrangement of the crystal lattice of iron during the $\gamma\to\alpha$ transformation of austenite into steel is carried out by means of regular atomic shifts. The formation of α-phase crystals is associated with the minimization of stresses arising in undercooled austenite and in the process of phase transformation. Different morphology and composition of the α-phase formed are due to the peculiarities of relaxation processes at different stages of its formation. The rearrangement of the crystal lattice occurs by a single and continuous shear of atoms, the experimental determination of the trajectories of which, however, is currently a difficult problem.

The rearrangement of the crystal lattice of iron during its $\gamma\to\alpha$ transformation with the formation of pre- and eutectoid ferrite occurs in the same way as during martensitic transformation, but is accompanied by carbon diffusion. The tetragonal lattice of the carbon-supersaturated α-phase is intermediate between austenitic and ferritic. The shears and displacements of atoms present in the martensitic transformation according to the Kurdyumov–Sachs scheme are of smaller significance than in the case of transformation to ferrite. The inhibitory effect for the rearrangement of the austenite lattice into ferrite is exerted by carbon atoms, which are embedded in the austenite lattice and remain in it during martensitic transformation.

The application of nonequilibrium thermodynamics to the analysis of diffusion-free austenite transformation allowed to obtain a system of equations for the thermodynamic system and to generalize the equations for normal transformation obtained earlier by B.Ya. Lyubov for normal transformation considering internal stresses [49]. The theoretical equation for the growth rate of the α-phase obtained in this work takes into account the influence of stresses on the process of austenite transformation. It is shown that the growth rate of α-phase particles at a constant temperature by a shear mechanism decreases very rapidly (exponentially) in time, determining the incompleteness of the transformation at a constant temperature.

As found in Ref. [50], the formation of martensite crystals does not occur with the difference between the free energies of austenite and martensite $\Delta F_0 \le 2\gamma$. It is assumed that the condition $\Delta F_0 = 2\gamma$ determines the start point of the formation of martensite M_s on the temperature axis. Equations for calculating the radii of the martensitic crystal of critical R_0 and current R_s are obtained. It is shown that a certain stresses level in the γ-phase is required to fulfil the condition $R_s > R_0$ for a given value of the difference between the free energies of the phases ΔF_0.

The literature offers several directions for analytical consideration of the influence of stresses on the kinetics of martensite formation. One of them generalizes the K–M equation with the addition of empirical parameters [67–70], the other uses theoretical calculations of this effect [49, 50, 74] and processing of experimental data on physicochemical models [76].

To calculate the effect of stresses on the transformation of residual austenite, a new Eq. (22) is suggested, which takes into account the minimum stress required for the crystal-geometrically ordered shear of iron atoms in the formation of martensite.

As shown, the influence of alloying elements and cooling rate on the temperature of the start and finish of austenite transformation can be calculated from the equations obtained earlier by the authors [76].

To calculate the quantity of martensite formed from the temperature, a modified K–M equation is proposed, which takes into account not only the temperature of the start but also the finish of the austenite transformation, *i.e.* increases the accuracy of the calculation.

By modelling and comparing calculations by different equations, it was found that Eq. (21) takes into account both the initial and final temperatures of martensite formation and various kinetics of its growth — gradual or rapid, and can be successfully used to calculate the quantity of martensite in real steels.

To increase the accuracy of predicting the structural condition of steels during heat treatment, it is necessary to conduct a comprehensive study related to the experimental determination of stress on shear transformation and create an adequate physical and mathematical model of austenite transformation based on these effects.

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ЗСУВНЕ ПЕРЕТВОРЕННЯ АУСТЕНІТУ В СТАЛЯХ З УРАХУВАННЯМ ЕФЕКТІВ НАПРУЖЕНЬ

Розглядаються відомі на цей час основні механізми мартенситного перетворення аустеніту сталі під час охолодження, фізичні моделі та схеми зсувної перебудови кристалічної ґратниці заліза через $\gamma \to \alpha$-перетворення під дією внутрішніх напружень. Проведено аналіз наявної кінетичної моделі зсувного перетворення аустеніту в сталі з урахуванням впливу напружень. Показано, що для перетворення залишкового аустеніту в мартенсит необхідне виконання двох основних умов: термодинамічної за рахунок пониження температури сталі аж до температури завершення перетворення залишкового аустеніту та кінетичної за рахунок підвищення рівня внутрішніх напружень в аустеніті, збільшення швидкости охолодження на заключному етапі оброблення або механічного впливу. Для розрахунку впливу напружень на перетворення залишкового аустеніту в сталі запропоновано нову формулу, яка враховує мінімальне напруження, необхідне для кристалогеометрично упорядкованого зсуву атомів Fe під час утворення мартенситу. Показано, що вплив леґувальних елементів і швидкости охолодження на температури початку та закінчення перетворення аустеніту можна розрахувати за наведеними у роботі співвідношеннями. Для розрахунку кількости утворюваного мартенситу залежно від температури перетворення в роботі запропоновано удосконалену формулу Коістінена–Марбурґера, яка враховує не тільки температуру початку, але й температуру закінчення перетворення аустеніту, себто підвищує точність одержуваного результату.

Ключові слова: перетворення аустеніту, зсув площин, напруження, термодинаміка процесу, кристал мартенситу, кінетична модель.