ON THE THEORY OF $\alpha-\gamma$-TRANSFORMATION IN IRON AND STEELS

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The fluctuation model of $\alpha-\gamma$-transformation in iron and steels is developed to phenomenologically describe the phase transformation mechanism in terms of the principles of stability loss of one of the phases due to contact interaction. The interphase boundary is treated as a stable highly excited state, in which a low-temperature α-phase becomes unstable and turns into a high-temperature γ-phase during contact. A phase transition is considered to be a collective process. Low degrees of transformation are discussed when lattice rearrangement is a limiting factor. The theory is used for numerical calculations of kinetics of the $\alpha-\gamma$-transformation in iron and U8 steel under rapid heating. The obtained results show fair agreement with experimental data.

As is known, there is still no unified generally accepted theory for perlite-to-austenite transformation in iron–carbon alloys. The most debatable aspects are in the initial stage of transformation concerning the physical causes lying behind the transformation of ferrite, containing almost no carbon ($C \leq 0.06\%$), to austenite at 725 but not at 910°C (the temperature of polymorphous $\alpha-\gamma$-transformation in iron).

At present several mechanisms of austenization are discussed. According to [1], dissolution of 0.02% C in ferrite in conformity with the GP line of the Fe–C diagram results in a decrease of a $\alpha-\gamma$-transformation temperature from 910 to 725°C. Within the frames of such approach the transformation may proceed without participation of carbides or other carbon sources. However, it has not been confirmed experimentally. Investigation of the $\alpha-\gamma$-transformation in technical iron containing 0.02-0.03% C has revealed that the austenization proceeds exclusively at a temperature higher than Ac_3. Only in the case of contact of ferrite with cementite, the austenite nuclei begin to form in the boundary zone independently of the carbon content in the ferrite (0.02% or much less) mainly at the boundaries of perlite grains [1, 4] at the Ac_1 excess.

Generalization of many facts [5] has allowed one to conclude that the effective tensile stresses develop over interphase surfaces which weaken interatomic bonds and thus cause, at perlite heating, the nucleation of a γ-phase at the temperature Ac_1. The stresses are attributed to dimensional inadequacy of the lattices of conjugate phases. As a result, the temperature Ac_1 is interpreted as that of the $\alpha-\gamma$-transformation in the boundary layer of eutectoid ferrite which is displaced relatively to the normal, for iron, the temperature Ac_3 is due to the contact interaction with a substrate, i.e., a surface of cement and then of austenite.

Having revised different theoretical models and a great deal of experimental data, we set forth the following mechanism of the $\alpha-\gamma$-transformation in steels [1, 5]. At the Ac_1 temperature excess, the carbon-free austenite is formed at the ferrite-cementite boundary due to nondiffusional rearrangement of a lattice which is then saturated with carbon and itself becomes an active substrate. Ferrite transformation continues to proceed on this substrate. Then the α-γ-rearrangement of the lattice on the phase boundary and the carbon diffusion proceed simultaneously and cannot be separated from each other.

The present paper is aimed at development of a quantitative fluctuation model of the $\alpha-\gamma$-transformation in iron and steels on the basis of the above qualitative principles and application of the model to interpretation of the available experimental data on austenization at rapid heating of technical iron and U8 steel. The proposed model is based on the thermofluctuation initiation and subsequent motion (growth) of a peculiar boundary which we call an active zone, by analogy with [5]. It is important that motion of the active zone proceeds not atom-by-atom but in a jump-manner. Although the physical metallurgy literature traditionally considers the atom-by-atom mechanism of the new phase growth, the fact that fluctuation processes in metals involve a group of atoms has been confirmed both by theoretical [6, 7] and experimental [8, 9] works. According to [7, 8], $\Lambda \approx 1.5 \cdot 10^{-3}$ μm for technical iron.

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Assuming the collective character of fluctuations and using the considerations of [6] with the main postulates of the theory of absolute reaction rates [10], we may derive the following expression for the interval between subsequent fluctuations:

$$\tau_{ph} = \tau_0 \exp(U/RT)/2\,\mathrm{sh}(n\Delta F/RT) = \tau/2\,\mathrm{sh}(n\Delta F/RT), \tag{1}$$

where $\tau_0 \simeq 2 \cdot 10^{-13}$ sec and $n = \pi\Lambda^3/6v$ is the gain displaying the collective character of the phase fluctuation. Expression (1) differs from the known [11] by the fact that it contains the gain n.

Note, the model is objective only in the case when its main quantities are calculated in closed form proceeding from the properties and the structural condition of the material. Without such a closed form, only those parameters whose reliability criterion is the fitting of the result and the concrete experiment together [12] are mainly used in the calculations. Such an approach is incorrect. We have calculated the main parameters of the model proceeding from the principle of stability of phases and strength of interatomic bonds. The latter are characterized by the iron self-diffusion coefficient D_{Fe}^{γ}.

In order to determine τ, consider the iron self-diffusion at a critical point. In view of cancellation of the factors $\mathrm{sh}(n\Delta F/RT)$, the product $D_{Fe}^{\gamma}\tau$ is believed, to a first approximation, to be independent of a structure. Assume that the condition determining the onset of the phase transformation is

$$(D^{\gamma}_{Fe}\tau)^{1/2} = (\bar{x}_T^2)^{1/2}. \tag{2}$$

For iron, we determine $(\bar{x}_{298K}^2)^{1/2}$ by the formula:

$$(\bar{x}_T^2)^{1/2} = (\bar{x}^2_{298\,K})^{1/2}\,(T/298\,K)^{1/2}\Theta_{298\,K}/\Theta_T. \tag{3}$$

Here $(\bar{x}_{298K}^2)^{1/2}$ is taken from [13], while the Debye temperature Θ_T is taken from [14]. Condition (2) is directly related to the known Lindemann criterion [15] for a phase transition: a phase transition occurs when the amplitude of atomic oscillations attains some critical value for this transition. It implies that the phase fluctuation takes place only after "diffusional collision" of atoms, i.e., only after local loss of lattice stability. It is obvious that the phase fluctuation may become irreversible only in the presence of the appropriate moving force of the transition, i.e., a difference of chemical potentials of phases ΔF.

A new feature in condition (2) is the fact that it refers not to a sole atom but to a phase fluctuation. Therefore, we may write:

$$(D^{\gamma}_{Fe}\tau)^{1/2} = \varepsilon\Lambda. \tag{4}$$

For the α–γ-transformation, $\varepsilon = 2.5 \cdot 10^{-2}$ [13]. In our case the condition (4) means that the diffusion for the time τ_{ph} is sufficient for stresses to relax and thus to provide coherence of the γ-phase growth. From relations (2)-(4), we determine $\Lambda \simeq 1.7 \cdot 10^{-3}\,\mu$m. Knowing Λ, we may evaluate the number n of atoms involved in fluctuations. Calculation yields $n \simeq 2 \cdot 10^2$.

Having obtained Λ and τ_{ph} in closed form, we may calculate the main quantities characterizing the phase transition: rates of growth G and nucleation J. For a velocity of active zone displacement we obtain by virtue of definition

$$G = \Lambda/\tau_{ph}. \tag{5}$$

A nucleation rate may be calculated with an accuracy on the order 1 by the formula

$$J = n_v/\tau_g. \tag{6}$$

Here $n_v = 1/\Delta\Lambda^2$ is the number of potential nucleation sites per unit volume determined as a ratio of an area of interphase boundaries per unit volume to a phase fluctuation cross section; Δ is the structure parameter (for iron $\Delta = \rho^{-1/2} \simeq 10\,\mu$m; $\rho \simeq 10^{10}$ m^{-2} is the density of dislocations, for annealed carbon steels $\Delta \simeq 0.5\,\mu$m is the intercarbide distance [16]; and τ_g is the time of onset of relation:

$$\tau_g = \tau_{ph} \exp(Q/RT) \exp(-S/R). \tag{7}$$

Use of the energy activation of iron self-diffusion in (7) is logically related to conditions (2) and (4). The factor $n_v \exp(-Q/RT) \exp(S/R)$ gives the effective number of nuclei since only those sites of an interphase surface may be considered the nuclei of a new phase which are in an activated state in conformity with (2) and (4).

To evaluate the kinetics of the α–γ-transformation under rapid heating conditions, we use the Kolmogorov equation for a fraction η of the transformed volume. Application of such an approach is motivated in [12, 16, 17]. Let us use the simplified Kolmogorov equation

TABLE 1. Calculated Rates of Nucleation J and Growth G of the Active Zone at Various Carbon Concentrations C in It for Steel U8

C, %	D^{γ}_{Fe}, cm^2/s	τ, s	U, kg/mol	G, mm/s	J, mm^{-3}s^{-1}
	T=725 °C			T=745 °C	
0	$8{,}9\cdot10^{-16}$	$2{,}0\cdot10^{-2}$	207	$1{,}2\cdot10^{-4}$	$1{,}7\cdot10^{4}$
0,4	$8{,}5\cdot10^{-15}$	$2{,}1\cdot10^{-3}$	188	$1{,}1\cdot10^{-3}$	$1{,}0\cdot10^{6}$
0,5	$1{,}5\cdot10^{-14}$	$1{,}2\cdot10^{-3}$	184	$1{,}8\cdot10^{-3}$	$4{,}5\cdot10^{6}$
0,8	$8{,}2\cdot10^{-14}$	$2{,}2\cdot10^{-4}$	170	$9{,}6\cdot10^{-3}$	$7{,}9\cdot10^{7}$

$$-\ln(1-\eta) = \frac{4\pi}{3}\int\limits_0^t J dt' \left(\int\limits_0^t G dt'\right)^3. \tag{8}$$

Such simplification of the Kolmogorov equation, consisting in factorization of time integrals of J and G, leads to some overestimation of the sizes of the new phase areas formed to time t since expression (8) implies that all the nuclei initiated for the time t grow to the same size $\int_0^t G\,dt'$. However, taking into account the exponential dependence of J and G on temperature, we may show that the integrals in (8) to a first approximation with respect to the parameter RT_0/U, are determined by their values on the upper limit that justifies the simplification used. Under the assumption of constancy of the heating rate g, we may substitute T/g for t and pass from time integration in Eq. (8) to temperature integration. As a result, we obtain

$$g = 2\left[-4\pi\Lambda \exp(S/R)/3\Delta \ln(1-\eta)\right]^{1/4} \left\{\int\limits_{T_0}^{T} \operatorname{sh}(n\Delta F/RT) \times \right.$$
$$\left. \times \exp[-(Q+U)/RT]\, dT \left[\int\limits_{T_0}^{T} \operatorname{sh}(n\Delta F/RT) \exp(-U/RT)\, dT\right]^3\right\}^{1/4} / \tau_0. \tag{9}$$

Expression (9) allows calculation of the heating rate g necessary for attaining a prescribed degree of transformation η at any temperature T and thus gives solution of the problem on a shift of the instrumental onset of the $\alpha-\gamma$-transformation in dependence on a heating rate.

To perform calculations by (9), it is necessary to know the iron self-diffusion coefficient D_{Fe}^{γ}. As is known, it highly depends on a carbon concentration [18]:

$$D^{\gamma}_{Fe} = 10^{-C} \exp[-(288 - 29{,}2C)/RT], \tag{10}$$

where C, at. %; Q, kg/mole. Since we have failed, despite numerous attempts, to discover ferrite saturation with carbon at any temperature below the critical one, which is the basis of the carbon-free nucleation hypothesis [1, 5], it should be expected that the carbon exerts no influence on nucleation. However, when an active zone is formed, a role of the carbon changes. Ferrite at the boundary with the active zone is in a "loosened" state, therefore carbon solubility in it may essentially differ from an equilibrium one. Henceforth, we assume that some constant carbon concentration will correspond to the active zone independently of its additional diffusional carbon make-up from dissolvable carbides. From this viewpoint, the possibility of obtaining a larger amount of austenite in steels under hardening is allowed by the Fe–C diagram at the corresponding temperature [1]. Since a carbon concentration in the active zone is not known a priori, we have calculated some carbon concentrations. The results are listed in Table 1. A comparison of the obtained result with experimental data [1] shows that the carbon-free nucleation corresponds to the real nucleation rates. However, after forming the active zone, a carbon concentration in it becomes about 0.5%. This results is in fair agreement with a composition of the first portions of austenite determined in [16]. In calculations, we have determined the moving force of phase transformation from the expression

$$\Delta F = L\Delta T/T_0, \tag{11}$$

where L is the latent heat of a transition which for U8 steel is taken from [1] and for iron from [13]. It should be noted that the expressions used in the present paper are applicable without any changes only for the steels in a structural-equilibrium state. When they are to be used for hardened steels, the metastable character of the latter should be taken into consideration.

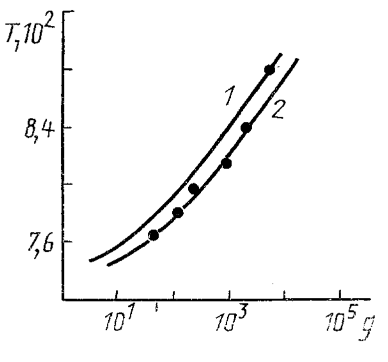

Fig. 1

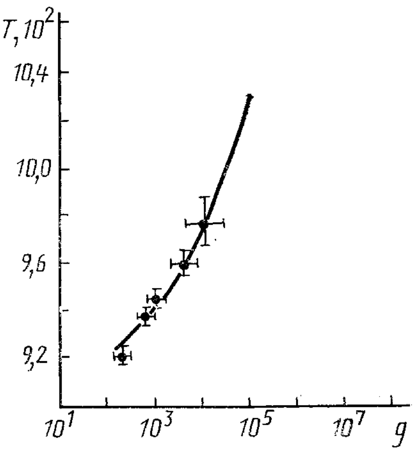

Fig. 2

Fig. 1. Temperature T vs heating rate g for a given degree of $\alpha-\gamma$-transformation, η in U8 steel: 1) $\eta = 4\%$; 2) 0.4. The points stand for experimental data [16]. T, °C; g, deg/sec.

Fig. 2. Temperature T vs heating rate g for the 5% $\alpha-\gamma$-transformation in iron. The points stand for experimental data [16].

The results of numerical calculation by formula (9) for steel U8 are given in Fig. 1. On comparing calculated curves with experimental data, it should be taken into consideration that the latter display the instrumental onset of transformation dependent on the variable sensitivity of a recording device [16] and therefore it is not necessary for them to fall on the constant-degree transformation curves. It follows from Fig. 1 that at small heating rates the instrumental onset of nucleation corresponds to a 0.4% degree of transformation, while at the heating rate $\sim 10^4$ deg/sec, to 4%.

As has been mentioned above, we have performed numerical calculations disregarding the limiting role of carbon diffusion associated with the necessity of additionally saturating the active zone with carbon. The validity of such an approach is confirmed by estimation of the ratio of a carbon diffusion length to an active zone shift path for the same time:

$$(D^C_{\gamma-\mathrm{Fe}}t)^{1/2}/\int_0^t G\,dt' \sim 1, \tag{12}$$

where the carbon diffusion coefficient for austenite $D_{\gamma\text{-Fe}}^C$ is taken from [18]. Since the active zone width Λ is small, any low carbon concentration on the phase boundary is sufficient to saturate it with carbon. Thus, at small degrees of transformation, the carbon diffusion does not limit the process of $\alpha-\gamma$-transformation. However, the carbon diffusion must play the governing part during austenization, i.e., saturation of the formed γ-phase with carbon.

In order to verify the generality of the proposed model, we have made similar calculations for polymorphous transformation in pure iron. In accordance with (2) and (4), the activation energy of growth for iron at 910°C is determined as $U \simeq 180$ kg/mole which is smaller than for steels. To all appearances it is related with "loosening" of a ferrite lattice due to the temperature. The results of numerical calculation for iron (Fig. 2) are in fair quantitative agreement with experimental data [16] for the total heating rate range.

With the purpose of grounding and subsequently developing the fluctuation model of the $\alpha-\gamma$-transformation we consider its structural-geometric aspects. Presently it is established in physical metallurgy that the $\alpha-\gamma$-transformation proceeds through nucleation and a subsequent growth of nuclei. This fact is well demonstrated in [1]. At the same time any fluctuation model in its classical treatment, contradicts this fact because the probability of fluctuation is proportional to the volume, i.e., the number of nucleation sites [12, 19]. As a result, fluctuations are delocalized and cannot be connected with any boundaries. Our proposed model takes into consideration the growth localization in its underlying principles. As is mentioned above, a nucleation event results in formation of a peculiar boundary, i.e., the active zone. Its characteristic feature is the fact that the effective tensile stresses develop in its nearest neighborhood thus reducing the activation energy of growth as calculations show, from 495 to 184 kg/mole for U8 steel ($\Delta U = 311$ kg/mole). We evaluate these stresses as

$$\sigma = \Delta U / n v_\mu. \tag{13}$$

Estimate (13) gives $\sigma \simeq 2 \cdot 10^8$ Pa. Let us compare this value with the value of stress necessary for suppressing the fluctuation delocalization [20]:

$$RT \ln n_v = n v_\mu \sigma. \tag{14}$$

Estimate (14) also gives $\sigma \simeq 2 \cdot 10^8$ Pa. Thus, the effective tensile stresses at the active zone–ferrite boundary lead to localization of the fluctuations at this boundary to provide finally its motion as a whole.

To sum up, the following conclusions can be made:

1. The fluctuation model of the α–γ-transformation in iron and steels is developed which is based on qualitative relations established in physical metallurgy. The model represents phenomenologically the phase transformation micromechanism in terms of the stability loss of one of the phases due to contact interaction. Of particular importance is the consideration of elementary events of a phase transition as collective processes. The main parameters of the model are calculated in closed form proceeding from a structural state and properties of the material.

2. An analysis is made of the carbon effect on growth and nucleation rates. For small degrees of the α–γ-transformation, the carbon diffusion is shown not to restrict the motion of its front. The calculated shift of the temperature of the instrumental onset of the α–γ-transformation as a function of a heating rate at a given degree of the transformation is in fair agreement with experiment.

3. The model is of a general character and may be extended to the phase transformations in other metals.

NOTATION

τ_{ph}, time between subsequent jumps of active zone motion; Λ, shift of the active zone for one jump; τ_0, time of atomic oscillations; U, activation energy of growth; R, gas constant; T, temperature; T_0, temperature of phase equilibrium; ΔT, superheating over the phase equilibrium temperature; n, the number of atoms involved in fluctuation; ΔF, difference of chemical potentials of phases; v, atomic volume; v_μ, molar volume; D_{Fe}^{γ}, self-diffusion coefficient for iron; $\overline{(x_T^2)}^{1/2}$, root-mean-square amplitude of atomic oscillations; Θ_T, Debye temperature; ε, phase dislocation; G, rate of active zone growth; J, nucleation rate of the active zone; n_v, number of potential nucleation sites; ρ, dislocation density; Q, activation energy of iron self-diffusion; S, entropy of iron self-diffusion; η, degree of transformation; t, time of development of transformation; g, heating rate; C, carbon concentration; L, latent heat of a transition; $D_{\gamma\text{-}Fe}^{C}$, carbon diffusion coefficient in austenite; σ, stress.

LITERATURE CITED

1. S. S. D'yachenko, Austenite Formation in Iron–Carbon Steels [in Russian], Moscow (1982).
2. V. N. Svechnikov, V. N. Gridnev, and Yu. A. Kocherzhinskii, Vopr. Fiz. Met. Metalloved., No. 6, 62-65 (1955), Kiev.
3. I. N. Kidin, Fundamental Physical Principles of Electrothermal Treatment of Metals and Alloys [in Russian], Moscow (1969).
4. G. Sheard and J. Nutting, Metals Technol., 7, No. 2, 192-196 (1980).
5. V. M. Zalkin, Nature of Eutectic Alloys and Contact Melting Effect [in Russian], Moscow (1987).
6. S. N. Zhurkov, Fiz. Tverd. Tela., **25**, No. 10, 3119-3123 (1983).
7. K. A. Osipov, New Ideas and Facts in Physical Metallurgy [in Russian], Moscow (1986).
8. J. Harding, Acta Metallurgica, **17**, 949-958 (1969).
9. V. R. Regel', A. B. Slutsker, and V. D. Tomashevskii, The Kinetic Theory of Solid Strength [in Russian], Moscow (1974).
10. S. Glesston, N. Leidner, and G. Euring, The Theory of Absolute Reaction Rates [Russian translation], Moscow (1974).
11. D. Kristian, The Theory of Transformations in Metals and Alloys [in Russian], Part 1, Moscow (1978).
12. G. Yu. Balandina, B. I. Bertyaev, I. N. Zavestovskaya, et al., Kvantovaya Élektron., **13**, No. 11, 2315-2319 (1986).
13. G. V. Samsonov (ed.), Elements Properties PI. Physical Properties (Handbook) [in Russian], Moscow (1975).
14. O. N. Belousov, Izv. Akad. Nauk SSSR, Metally, No. 2, 64-66 (1986).
15. V. V. Pavlov, Solidification and Its Molecular Model [in Russian], Moscow (1985).
16. V. N. Gridnev, Yu. Ya. Meshkov, S. P. Oshkaderov, and V. I. Trofimov, Physical Fundamental Principles of Steel Electrothermal Hardening [in Russian], Kiev (1973).
17. L. N. Aleksandrov, Kinetics of Solid Layers Structurization [in Russian], Novosibirsk (1972).

18. M. A. Krishtal, The Diffusion Mechanism in Iron Alloys [in Russian], Moscow (1972).
19. L. D. Landau and E. M. Lifshits, Statistical Physics [in Russian], Part I, Moscow (1976).
20. V. A. Petrov, Fiz. Tverd. Tela, 25, No. 10, 3110-3113 (1983).

ANALYSIS OF FORMING THE STRUCTURE AND PROPERTIES OF A METAL DURING LASER HARDENING

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A mathematical model of forming the structure and the properties of a metal under laser treatment involving flashing is proposed. The model takes account of the processes in a transient two-phase zone. It is shown that the parameters of a dendritic structure and excess components, a dislocation density, porous structure characteristics, ultimate strength yield stress, and relative elongation nonmonotonically depend on the laser treatment parameters and metal plate dimensions. The calculated results are in fair agreement with experimental data.

Hardening of metals and alloys involving laser treatment is an effective technology of obtaining high-quality materials [1-4]. Thermal processes during laser treatment with internal heat release at phase transitions are studied in [2]. The urgent problem is the analysis of these processes with an account of a two-phase state of a metal and forecasting of its structure and properties under hardening conditions. These aspects are the subject matter of the present article which is the continuation of work [5] concerned with investigation of the thermal state of a metal under hardening.

We shall consider thermal hardening of an aluminum alloy plate of thickness b, which is much less than its longitudinal dimensions. Let the plate move in the direction of the axis z at velocity w and the laser radiation source be immovable. The axis x runs across the plate and the origin of the Cartesian system (x, z) is on its surface. The process scheme and formulation of the heat problem of metal hardening are given in [5].

Consideration was given to hardening by heat treatment of the plate made of aluminum alloy AMg6. In the basic calculations, $b = 20$ mm, $w = 25$ mm/sec, the zone length of laser radiation action was $l_c = 0.5$ mm, the specific heat flux produced by the radiation $q = 6 \cdot 10^8$ W/m², temperatures of a cooling medium on the side of the upper and lower surfaces of the plate $T_{b1} = T_{b2} = 20$°C, and the coefficients of heat transfer from the above surfaces $\alpha = \beta = 100$ W/m²·K. As the temperature of hardening completion, $T_m = 546$°C was assumed, at which a cross section (a portion) of a liquid phase was $S = 0.05$.

After determining the thermal state of the metal [5], we have analyzed the formation of its crystalline structure. The investigation of structured zones by the procedure described in [6, 7] shows that in the course of metal hardening pillar crystals are mainly formed. They are characterized by two main parameters, i.e., a thickness ξ of dendritic axes of the first order and a distance η between the secondary branches of dendrites [8, 9]:

$$\xi = b_0 \left[D (T_L - T_m) v_c^{-1} \right]^{1/2}, \tag{1}$$

$$\eta = a_1 v_c^{-a}. \tag{2}$$

Here D is the diffusion coefficient of an impurity (magnesium); v_c is the cooling rate; a, a_1, b_0 are the numerical coefficients. In calculations, v_c was determined on an isothermal surface of pouring out where a portion of a liquid phase was $S = 0.4$; $b_0 = 1$; $a = 380$, $a_1 = 0.4$ [10].

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