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SYNERGETIC APPROACH TO THE DESCRIPTION OF STRUCTURAL EFFECTS IN METALS UNDER CYCLIC THERMAL ACTIONS

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The question of applicability of the principles of synergetics to the description of the structure formation in nonferrous metals and alloys under thermal cyclic actions is discussed. It is shown that a metal under such actions is a dissipative system whose structure can evolve endlessly, without destruction of the material.

In the last few years, in metal science and the physics of metals a direction in which the principles of synergetics are used for describing the processes of structure formation in metal materials under energetic actions of various nature has been formed. It includes mainly investigations considering the structure evolution in metals and alloys under plastic deformation and destruction [1, 2]. At the same time, in [3] it is noted that the use of the synergetic approach to the description of the structure formation in these cases is incorrect because of the fact that "the deformable crystal is a nonstationary, irreversible, inhomogeneous system whose evolution occurs with increasing configuration entropy and ends in destruction. The above features exclude the possibility that a dissipative structure arises." As an example of a process providing the formation of a dissipative structure, the selective friction transfer (Garkunov effect) is given. Under these conditions, as shown by the authors, a kinetic phase transition from conservative motion of dislocations to their climb occurs and the diffusion microplasticity effect is realized [4]. Putting aside the question of applicability of the principles of synergetics to the description of plastic deformation processes, the authors believe that the dissipative processes in metal materials can be modeled by an example of the structure formation under cyclic thermal actions. In so doing, as we see it, it is possible to avoid incorrectness in interpreting the observed processes, which was discussed in [3].

Thermocycling is a thermal effect which is realized by means of continuous cyclic temperature change and is accompanied by multiple structural or phase transformations upon heating or cooling at a given rate (we mean metal treatment "in the bulk" and not the processes on the surface). The basic diagram of thermocycling is given in Fig. 1.

There is a large volume of experimental data on the structure formation in metal materials under thermocycling, published, in particular, in [6]. For many years the authors of [5] carried out research on the structure formation of aging alloys under thermocycling. The results of the investigations are summarized in [6]. The kinetics and possible mechanisms of the processes of structure formation are described and their specific features are noted. Further investigations are directed toward the development of the concept of structure formation under cyclic energetic actions of different nature. The development of such a concept is possible with the use of the synergetic apparatus.

In the present paper, the authors attempted to show that under thermal cycling a metal is a dissipative system — an open, stationary, reversible, nonequilibrium, endless system whose structure evolves at a nonincreasing configuration entropy without destruction of the material.

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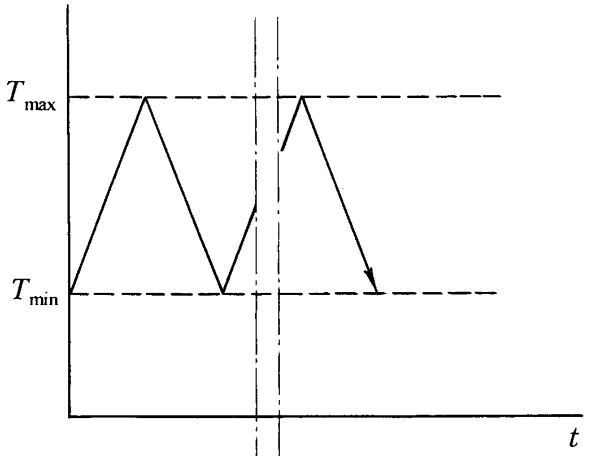


Fig. 1. Basic diagram of thermocycling.

According to [7], such structures can naturally arise in all those cases where the following necessary conditions are fulfilled:

(1) the system is thermodynamically open, i.e., it can exchange substance and/or energy with the environment;

(2) the dynamic equations of the system are nonlinear;

(3) the deviation from equilibrium exceeds the critical value;

(4) the microscopic processes proceed cooperatively.

Below, the structure formation process under thermocycling is analyzed from these positions, taking into account the principles noted in [1–3].

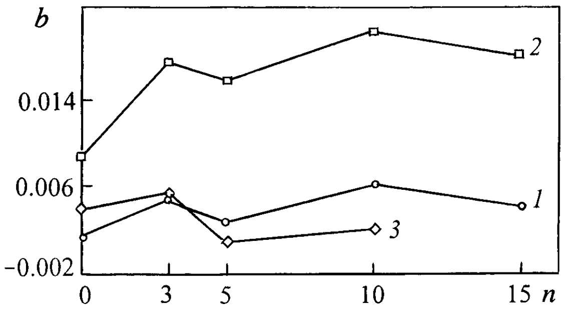
Under thermocycling the *endlessness* of the structure-formation process is provided by the joint action of the "thermal" and "deformation" factors. The terms are put in quotes for the following reasons: when a cyclic energetic action of a different nature (magnetic, laser, ultrasonic) is used, the structural effects are analogous to those observed under thermocycling [8]. The authors suggest that when energy is fed to the metal in the cyclic regime, its unusual "conversion" into thermal and deformation components, which can be immediately accumulated by the metal system, occurs.

The "deformation" factor provides a cyclic "pumping" of the crystalline structure defects into the metal bulk. The presence of a microdeformation and the change in the stressed state of the metal caused by this fact with the superposition of cyclic actions were convincingly shown by many authors [9]; the causes of changes in the stressed state under thermal cycling are presented in [10].

The "thermal" factor provides the realization of relaxation processes with the formation in the defective matrix of substructure fragments having boundaries of the type of granular ones. The structure transformation occurs with the participation of the rotation mechanism of plastic deformation [11] as an alternative to destruction.

The formation of particular structures under cyclic treatment depends on the ratio between the "thermal" and "deformation" factors of action. The prevalence of the "deformation" factor (without relaxation of stresses) leads in the end to the destruction of the material; the prevalence of the "thermal" factor leads to a change in the structure according to the classical scheme with the realization of recrystallization. To afford an endless process, the ratio between both factors of action should be optimum.

In this case, a specific periodic change in the physicomechanical properties of metals and alloys depending on the number of cycles of action is observed. This effect is convincingly shown in [6] on a number of alloys and pure metals in various initial states. In particular, this is illustrated in Figs. 2 and 3, which show the change in the microhardness and physical broadening of interference lines of the D16 alloy [12] and aluminum. Both the microhardness and the physical broadening are structure-sensitive characteristics reflecting



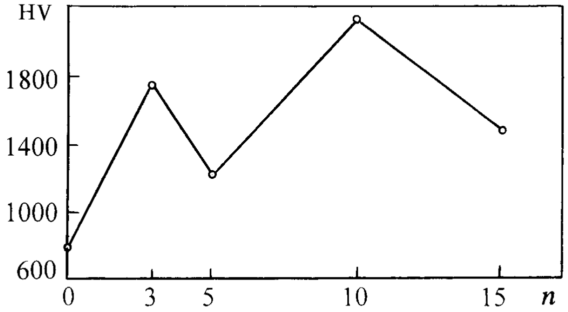


Fig. 2. Change in the physical broadening of interference lines (111) (curve 1) and (422) (curve 2) of the D16 alloy after hardening and low-temperature cyclic treatment at 200 ↔ 20^oC with the use of laser heating (the heating rate is 50 deg/sec) and of (422) of aluminum (curve 3) after deformation by rolling by 50% and thermal cyclic treatment at 300 ↔ 20^oC with the use of furnace treatment (the heating rate is 0.4 deg/sec).

Fig. 3. Change in the D16 alloy microhardness after hardening and low-temperature thermal cyclic treatment at 200 ↔ 20^oC with the use of laser heating.

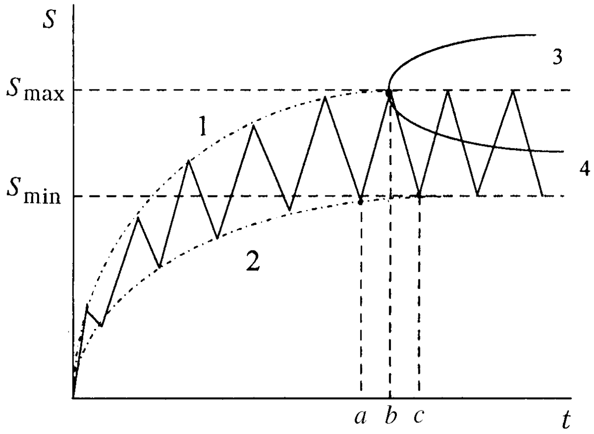


Fig. 4. Scheme of changes in the properties — physical broadening, microhardness, and ultimate stress corresponding to Figs. 2 and 3.

the stressed state of the metal and, consequently, they characterize the structure imperfection level. The periodic change in these characteristics points to the realization of hardening-softening cycles (accordingly, of cycles of accumulation–relaxation of structure defects), which provides the *nonincrease in the configuration entropy and the endlessness of the process*. The *reversibility* of the structure-formation process is associated with the action of the same factors. By properly regulating the "thermal" and "deformation" factors we can realize any structure from the interval $T_{\min} \leftrightarrow T_{\max}$ (Fig. 1).

Figure 4 shows the scheme of the change in entropy corresponding to the change in properties given in Figs. 2 and 3. Line 1 is similar to the cold working with complete hardening when the deformation factor prevails; line 2 — with incomplete hardening when the contribution of the thermal factor is more significant. With such a scheme of change in entropy the conditions

$$\left.\frac{\Delta S}{\Delta t}\right|_{t\to\infty} = \text{const}\,.$$

should be met. In the section *ab*: $S_a > S_b$; *bc*: $S_b > S_c$. For the closed system $dS = 0$.

Under thermocycling, a space-time structure that can keep and circulate indefinitely is formed. The dislocation structure will "vary" within the following limits: chaotic dislocation structure ↔ ordered "fragmented" structure. In so doing, the concentration of crystalline structure defects varies within certain limits; *the configuration entropy of the system does not increase*. Therefore, the system is *stationary* — time-constant, with the difference that the "fragmented" structure is not space-constant, but appears periodically after a certain number of treatment cycles at points *a* and *c*.

Points *a* and *c* do not correspond to the points of the *n*th and $(n+1)$th cycles at $T_{\min}$ on the diagram given in Fig. 1. The "fragmented" structure is not necessarily fixed at the end of each cycle; the interval of treatment between points *a* and *c* corresponds to several cycles (depending on the alloy and thermocycling parameters).

Point *b* in Fig. 4 is identical to the bifucation point at which a change of the deformation mechanism (transition to collective forms of dislocation motion with the participation of rotational deformation modes) and a destruction of the structure formed with the conservative manner of dislocation motion occur. The structural instability at the bifurcation point does not differ fundamentally from that observed for plastic deformations; to describe it, one can use the principles developed by the authors of [1]. When the deformation factor prevails at this point, the structure will evolve with an increase in the configuration entropy (curve 3) in the direction corresponding to the laws of plastic deformation till failure. In the case where the thermal factor prevails, the structure evolves with the participation of relaxation processes (curve 4). The structure formation in the *a*–*b*–*c* interval proceeds in the following direction: an increase in the density of crystalline structure defects with the formation of a weakly disoriented cellular structure inside the "fragmented" structure corresponding to the point *a*; destruction of the weakly disoriented cellular structure (as well as of the "fragmented" structure of the point *a*) followed by the formation at the point *c* of a strongly disoriented "fragmented" structure analogous to the structure at point *a* with the participation of rotational modes of plasticity.

As opposed to the typical deformation when the structure formation is provided by conservative motion of dislocations, under the cyclic action the *kinetic phase transition from the glide of dislocation to their climb is realized.*

The realization of the nonconservative method of dislocation motion is due to the considerable increase in the concentration of vacancies and their increased lifetime. This feature considerably speeds up the diffusion processes [13–15] and, therefore, the processes of structural-phase restructuring of alloys. In particular, in [16] it is shown that the maximum increase in the diffusion coefficient in thermocycling can reach three orders of magnitude. This feature forms the basis for the methods of thermal treatment of alloys [6]. For example, the decay time of the supersaturated solid solution in the operation of aging aluminum alloys reduces from 6–12 h to 0.5 h. When the crystal is supersaturated with vacancies, specific dislocation configurations — Bardeen–Herring sources, dislocation helixes, and tetrahedrons of stacking faults — arise [17].

The presence of dislocation loops and helicoids is evidence that the nonconservative method of dislocation motion prevails. The relationship between the helicoid formation and the nonconservative motion is conclusively shown in [17], where, in particular, the scheme of helicoid formation as a result of the climb of a screw dislocation with thresholds followed by the formation of a screw helix is presented. The dislocation-helicoid transformation is accompanied, depending on the dislocation and helicoid orientation, by the absorption or emission of vacancies (removal or addition of the substance).

Figure 5 shows the dislocation loops and the formation of subboundaries by helicoidal dislocations under thermocycling (the foil for electronic microscopy was made from the middle portion of the sample to exclude surface effects). The helicoid step depends on the kinetics of its formation associated with the alloy thermocycling regime. In particular, for the case of thermocycling of aging alloys the most probable mechanism is the mechanism relating the formation of helicoids to the presence of internal stresses and thermal

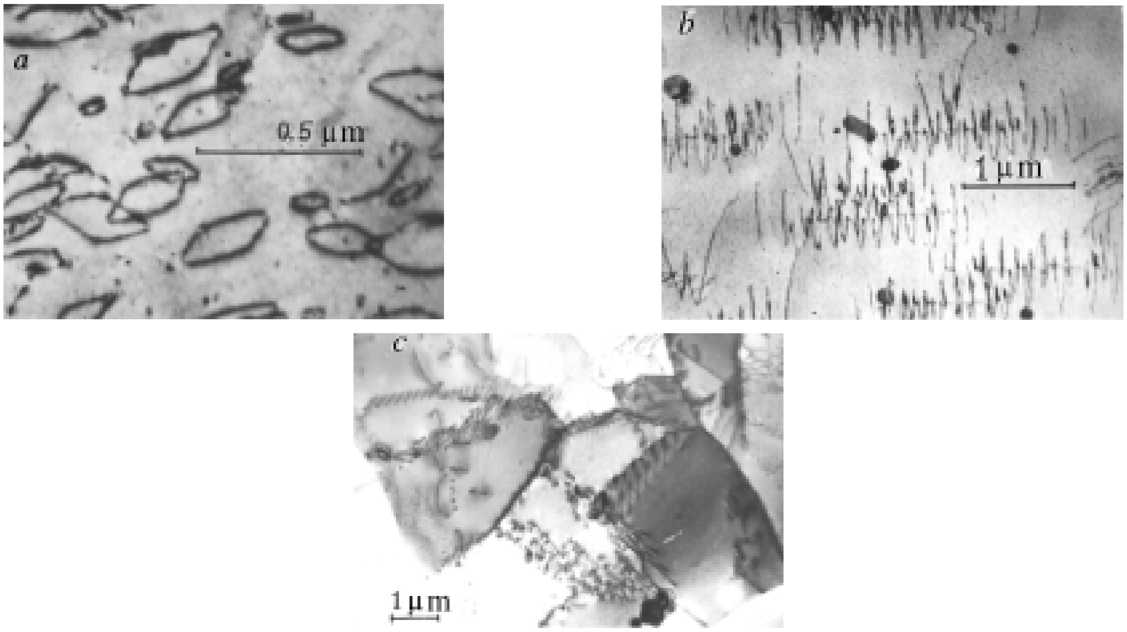


Fig. 5. Dislocation loops (a), helicoidal dislocations (b), and the subboundary formed by helicoids (c) in the AK4-1 alloy as a result of thermocycling: a) and b) 535 ↔ 20°C, 5 cycles; c) 535 ↔ 440°C, 5 cycles + aging at 180°C for 16 h.

fluctuations causing a deviation of the dislocation line from the screw orientation and the appearance of an edge component [6].

To describe the processes of structure formation under thermocycling, the diffusion-dislocation mechanism can be used. Taking into account that under thermocycling an alternating cyclic deformation takes place, the "vacancy pump" model developed in [4] can be used for explaining the increase in the vacancy concentration and helicoid formation. Under the conditions of cyclic stressing of the crystal, in the vicinity of the free surface a gradient of a heightened density of vacancy clusters and dislocation loops, formed due to the diffusion pumping of vacancies from the free surface to the bulk of the crystal with their subsequent condensation is formed. The dislocation loops residing in the crystal bulk and having a size of $5{\cdot}10^{-7}$–10^{-6} m are stable. Dislocation loops of such a size were observed under thermocycling of the D16 alloy in the 250 ↔ 20°C range; the number of cycles was 3–10 [9]. In [4], the condensation model is regarded as one particular form of manifestation of diffusion-dislocation microplasticity. If at the root of the nucleation and evolution of an ensemble of dislocation loops in the crystal under thermocycling are the diffusion processes and the increase in the size of the loops is caused by the processes of their nonconservative motion, we can speak of the realization, under thermocycling, of the diffusion-dislocation mechanism of microplastic deformation. Under thermocycling of metals the condensation of vacancies to loops and their nonconservative motion are possible. In this connection, it is fundamentally important that for a plastic flow to be initiated in realizing the diffusion microplasticity, there is no need for the stress to exceed a certain threshold value. The microplastic flow proceeds with arbitrary small loads. From these positions the considerable decrease in the critical stress of the dislocation multiplication in the metal under thermocycling as compared to the single, more intense stressing is well explained. Under sustained stressing the dislocation loops reach a certain critical size due to the diffusion process and then operate as Frank–Read sources. An increase in the dislocation density is also possible due to the operation of the near-surface sources. According to the data of [18], the mechanism of their action consists of the formation of thresholds due to the climb of the near-surface dislocation segment with the formation of a spiral segment propagating in the glide plane. This is illustrated in [19] for

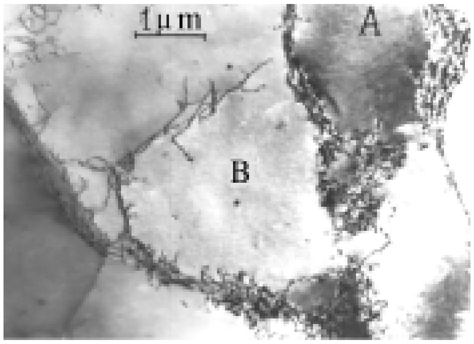


Fig. 6. "Fragmented" structure of aluminum subjected to thermal cyclic treatment in the 300 ↔ 20^{o}C temperature range, 10 cycles with the use of laser heating.

the case of thermocycling of the AMg1 alloy. The realization of this mechanism is also possible at the grain and interphase boundaries that are physically equivalent to the free surface [17].

A metal under the conditions of thermocycling is an *open thermodynamic system* through whose boundaries substance and/or energy flows pass [7]. The system exchanges energy with the environment in the course of treatment.

As a *dissipative structure* of the metal, a special "fragmented" structure with disorientation angles corresponding to the intergranular ones acts [9] (Fig. 6). The axes of the zones of fragments *A* and *B* are, respectively, [130] and [110]. This means that they can be disoriented by angles 26.57^o, 47.87^o, 66.91^o, and 78.69^o. By the term "fragment" the authors mean in this context a section of the substructure separated by the dislocation boundary. The introduction by us of a term with such a meaning is explained by the fact that in electronic-microscopic studies one often observes the formation of strongly disoriented fragments separated on one side by a plane boundary and on the other side by a volume dislocation boundary (which in general is specific of thermocycling). Division of such formations into cells and subgrains is, first, hindered and, second, does not make it possible to trace the trend towards the substructure formations.

The formation of fragments occurs with the participation of rotational plastic deformation modes in the most stressed parts of the metal, mainly near the high-angle boundaries. In this connection, it is necessary to determine what should be regarded as the Benard cell as applied to the structure formation in metals under thermocycling, since a cell in a cellular dislocation structure cannot act as a *Benard cell*, as rightly noted in [3]. Apparently, here there is a terminological incorrectness because of the application of the same term "cell" to different objects. The classical variant of the development of a dislocation cellular structure in the case of deformation or heating [19] involves irreversible transformation of a nondisoriented cellular structure into a weakly disoriented subgranular structure; in this case, only the growth of structural units is possible and the equilibrium state is realized. In the structure obtained under thermocycling the nonequilibrium factor existing in the near- boundary sections of fragments with large angles of disorientation is dominant [20]. The endless development of the structure involves uninterrupted cycles of the formation and growth of disoriented (by angles corresponding to intergranular ones) fragments. The structure (substructure) fragment separated by the large-angle boundary should be considered as an analog to the Benard cell. Therefore, it is the grain-boundary angle, but not the boundary structure as such, that is thereby important. The authors often observed the formation, under thermocycling, of dislocation cells with a disorientation angle of 10–12^o or more. A similar interpretation as applied to a metal material was proposed in [21]: by analogy with the structured liquid a polycrystallized metal in the solid state is regarded as a solidified liquid with "frozen" Benard cells.

Taking into account the foregoing, the investigations of the laws of structure formation under cyclic actions is important for explaining the particular structural state formed in the surface layers of a metal as a result of friction, surface plastic deformation, and cutting.

Characteristic of the structure formation process under thermocyclic treatment is the presence of a *structural hierarchy* that shows up as an interaction of two structural levels — the granular and subgranular ones. The first level is represented by an aggregate of primary (or initial) grains, the second one — by a substructure existing or formed under thermocycling. The granular structure transformation is reduced to the grain growth in accordance with the laws of collective recrystallization. It should be noted that the investigations carried out by the authors in the field of cyclic thermal actions have made it possible to form a special view on the recrystallization processes. The experimental material on the processes proceeding under heating of a deformed metal that has been obtained since the publication of Gorelik's monograph [19] calls for a new phenomenological approach. This topic requires special consideration and is not discussed here. It is only necessary to note that recrystallization seems to be a particular case of the processes realized under thermocycling; it is their initial and incomplete variant.

Refinement is observed only in the case where the development of a substructure competes with the formation of new fragments — micrograins. In the classical description this corresponds to microrecrystallization [22]. The micrograin proper (the new grain) is a large-angle fragment. The structure development at the subgranular level includes all the processes up to the formation of such a fragment. Its appearance at the granular level as a new grain means the formation in this fragment of a large-angle boundary. In this sense, the difference between the grain and the subgrain is only in the disorientation angles.

Practically we can speak of a cooperative behavior of the subsystems. The element of the thermodynamic flow of matter — the atom — can be regarded as a scale-level element determining the formation of a dislocation structure. And the following scale level of the structure determines the changes in the dislocation subsystem.

Thus, integration of the experimental data on the thermocycling of metals and alloys with the use of the principles of nonequilibrium thermodynamics makes it possible to:

(a) provide a single description of the structure formation processes in metal materials under cyclic thermal actions;

(b) widen the range of methods of acting on metal materials to whose description the principles of synergetics are applicable.

NOTATION

$T_{\min}$ and $T_{\max}$, minimum and maximum temperatures of a thermocycle, K; ΔS, change in entropy with a change in temperature upon treatment in the $T_{\min} - T_{\max}$ temperature range, J/deg; t, time, sec; n, number of treatment cycles; b, physical broadening of the x-ray pattern interference line, rad; HV, microhardness, MPa.

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