Nonequilibrium evolution thermodynamics theory

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Alternative approach for description of the non-equilibrium phenomena arising in solids at a severe external loading is analyzed. The approach is based on the new form of kinetic equations in terms of the internal and modified free energy. It is illustrated by a model example of a solid with vacancies, for which there is a complete statistical ground. The approach is applied to the description of important practical problem: the formation of fine-grained structure of metals during their treatment by methods of severe plastic deformation. In the framework of two-level two-mode effective internal energy potential model the strengthening curves unified for the whole of deformation range and containing the Hall-Petch and linear strengthening sections are calculated.

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I. INTRODUCTION

An idea to use an additional variable for account of internal microstructure changes in polycrystalline gases was proposed by Herzfeld and Rice in 1928 [1]. This idea has got development in other numerous researches of that time [2-5]. In 1937 Landau applied it to describe phase transitions in solids [6]. In the post-war years Landau in cooperation with Khalatnikov and Ginzburg for description of phase transitions offered some kinetic equations, describing the evolution of order parameter [7, 8]. In modern science this direction is presented by the theory of the phase fields [9-16]. Unlike the theory of Landau the parameter of order in the theory of the phase fields is not so strict, however, this does not hinder in getting results which rather well coincide with the behavior of the real systems.

To complete the picture, note that another direction in the description of such phenomena was offered in 1967 by Coleman and Gurtin, who complemented the primary idea by the elements of rational mechanics [17]. This direction was continued in Ref. [18–24]. In Ref. [20] an additional variable (order parameter), meaning the scalar density of embryonic microcracks, was introduced to describe the initial stage of destruction of a quasi-brittle solid. Later in the work by Peter Van [21] the application of internal state variables approach to the problem of destruction of cracking materials was examined. For the description of crackness level an additional vector variable $\vec{\alpha}$ is introduced, which is related to thermodynamic conjugated variable $\vec{A}$.

Between both approaches there is no an impenetrable border, they use one and the same fundamental idea. The difference is that the internal state variables approach one comes from the principles and postulates of mechanics of continuous media, while the approach by Landau is based on more general energetic principles, which, however, need further development. Interest which is sometimes shown in comparison of these two approaches is therefore clear [22].

A further approach of mesoscopic non-equilibrium thermodynamics is currently developed for investigation of soft-matter problem with mesoscopic structural elements [25–28]. The method addresses the systems entropy production, which is a detectable quantity at the mesoscopic level of condensed-matter organization; it also reveals effectively the kinetic-thermodynamics properties and peculiarities of the corresponding dynamic matter arrangements.

The present article is devoted to the development of the Landau approach, which in the present version appears under the name of non-equilibrium evolutional thermodynamics (NEET). In part II, the basic postulates of NEET are given, which are grounded by the results attained currently. In part III the approach is applied to the description of defect kinetics during metal treatment by severe plastic deformation (SPD). In part IV summarizing conclusions are given.

II. POSTULATES OF NEET

The first important difference of NEET from the classic scheme treating the problem is the introduction of the set of non-equilibrium thermodynamics potentials [29, 30]. Up to the present, basic, if not unique, stress was laid on the use of the free energy. The free energy is still a major function, which in energetic expression and logarithmic scale is a value inverse to the probability distribution function (PDF) of the system states [31]. A postulate is well known in statistical physics that the most probable states near a maximum of PDF, that is, automatically, near a minimum of the free energy [32] are realized only.

In this context the use of the free energy is very comfortable, because the most probability (stationary) state can be found from the universal principle of a minimum of the free energy. At the same time, in structural physics not for all of the physical systems the PDF is certain,
and, consequently, the free energy on its basis. Mainly, one uses a phenomenological generalization of the free energy, when the application of principle of minimum is not grounded statistically. Applicability of this principle is well proven most strictly for solids with vacancies, at the same time, for solids with other types of defects (dislocations, grain boundaries etc) PDF is unknown, and, consequently, applicability of this principle is not grounded strictly. Therefore a solid with vacancies can be a good model for approbation of ideas, having general character \[33, 35].

If the equilibrium (stationary) state of the system is known, in the case of small deviation of the system from that states, the evolution (relaxation) of the system can be written down as a condition that the system tends to the equilibrium state with a speed the greater the stronger the deviation. In terms of the free energy this condition results in the well known Landau-Khalatnikov evolution equation \([2]\) or in the case of the distributed systems in the Ginzburg-Landau equation \([6]\). At the same time, there is no obstacle to write down the evolution of the system in terms of other thermodynamic potentials, for example, in terms of the internal energy.

The internal energy is the clearest physically determined energy of the system; it is basic in both thermodynamics and physics in general. This energy is included in formulation of the first law of thermodynamics; it is universal for both the equilibrium and non-equilibrium states. In addition, the generalized thermodynamic force is determined through it not phenomenologically, as, for example, for the free energy, but fully strictly within the framework of statistical consideration. Indeed, PDF for a solid with vacancies looks like \([31, 36]\).

\[
f(n) = CW \exp\left(-\frac{U(n)}{k_BT}\right) = C \frac{(N+n)!}{N!n!} \exp\left(-\frac{U(n)}{k_BT}\right),
\]

where \(C\) is a normalizing constant, \(W\) is the thermodynamic probability, \(U(n)\) is the internal energy, \(N\) is the number of atoms in a solid, \(n\) is the number of vacancies, \(k_B\) is the Boltzmann’s constant, \(T\) is a temperature. A pre-exponential multiplier describes combinational, that is entropic, part of the distribution function, related to degeneration of macrostates. The exponent describes a restrictive part of the distribution function, related to overcoming the potential barriers between microstates. The most probable state is determined by a condition \(\partial f(n)/\partial n\), from where, in accordance with (1), most naturally appears a variable

\[
u = \frac{\partial U}{\partial n}, \tag{2}
\]

It has a sense of the average energy of a defect (here a vacancy), or of the chemical potential of defects, on the other side, Eq. (2) is a typical determination of the generalized thermodynamic force. Here it is not, however, postulated, but logically follows from Eq. (1), as a part of the process of determination of the equilibrium state, and, consequently, it must enter relaxation equation, as the equation describing system tendency to the equilibrium state. Now the evolutional equation in terms of the internal energy can be written down as

\[
\frac{\partial n}{\partial t} = \gamma_n \left(\frac{\partial U}{\partial n} - u_c\right), \tag{3}
\]

where \(\gamma_n\) is a kinetic coefficient, \(u_c\) is a value of the vacancy energy in the equilibrium state.

To define the equilibrium value of the vacancy energy and the equilibrium density of vacancies, we all the same must address the condition of a maximum of PDF or a minimum of the free energy, and, it would seem, it is simpler to describe relaxation in terms of the free energy, immediately using the Landau-Khalatnikov equation. However, Eq. (3) is also true, and can also be used. Especially it can be valuable at generalizations to other types of defects, for which phenomenological generalization of the free energy is problematic, and at times speculative, whereas the internal energy is of the universal nature.

The substantial difference of treating the problem in terms of the internal energy is that the generalized force \([2]\) is not equal to zero in the equilibrium state, and, consequently, for the internal energy the extreme principle does not work. This pitfall can be compensated as the generalized force \([2]\) is determined uniformly for both the equilibrium and non-equilibrium states, if the equilibrium energy of the defect is known for us from some sources for the defined values of external control parameters, then it is possible to find its value for other parameters easily. This advantage is for the first time exposed in the present article.

The second postulate, which distinguishes this approach from traditional one, is the use of the density of defects as an independent thermodynamic variable instead of the configuration entropy. Note that this variable is used not in parallel with the configuration entropy, but instead of it. Mutually identical dependence between the density of defects and the configuration entropy, can serve as a foundation for this purpose. In the case of a solid with vacancies this one-to-one dependence follows from the fundamental Boltzmann relationship \(S_c = k_B \ln W\) and from definition of \(W\) in accordance with Eq. (1). For other types of defects this relation is unknown, but it still must be mutually identical. It allows to generalize the 1st law of thermodynamics in the form \([32]\)

\[
dU = V \sigma_{ij} d\varepsilon_{ij} + T dS + \tilde{T} d\tilde{S} + \sum_{l=1}^{N_{def}} \varphi_l dh_l, \tag{4}
\]

where \(V\) is the volume of the system, \(\sigma_{ij}, \varepsilon_{ij}\) are stress and elastic deformations tensors, \(S\) is thermal or, for a solid, oscillation (not configuration) entropy, \(T, \tilde{S}\) are non-equilibrium temperature and entropy, which characterize the dynamic transitional phenomena during the generation and motion of the structural defects \([32]\), \(\varphi_l\),
$H_l$ are energy and density of $l$-kind defects, $N_{def}$ is the number of types of the defects. Thus the internal energy is a function of such independent variables as $\varepsilon_{ij}$, $S$, $\bar{S}$ and $H_l$, that is, $U = U(\varepsilon_{ij}, S, \bar{S}, H_l)$.

The first two terms in Eq. (1) are changes in the internal energy due to contribution of the elastic stress field and equilibrium thermo-motion, the third term characterizes a part of the internal energy, arising due to non-equilibrium transient processes (the necessity of its account is grounded in Ref. [33]), and the last term presents a part of the internal energy concentrated in defect subsystems.

Relation (2) in the case of arbitrary number of defect types can be generalized as

$$\varphi_l = \frac{\partial U}{\partial H_l},$$

and evolution Eq. (3) accordingly

$$\frac{\partial H_l}{\partial t} = \gamma_l(\frac{\partial U}{\partial H_l} - \varphi_{le}).$$

Carrying out transformation of the Legendre type, but with respect to the pair of thermodynamic variables of $\varphi_l$ and $H_l$, we pass to a new thermodynamics potential

$$\tilde{F}_l = U - \varphi_l H_l.$$ (7)

It is not hard to show that for this function a relation

$$H_l = -\frac{\partial U}{\partial \varphi_l},$$ (8)

is just, that is, the new function $\tilde{F}_l$ is related to the internal energies of $U$ in the same way as the classic (thermal or oscillation) free energy [37], if the entropy is formally taken instead the number of defects $H_l$, and the temperature instead of the energy of defect $\varphi_l$. But with the second postulate of NEET such the accountance is recognized, that is, the function $\tilde{F}_l$ can be interpreted, as a modified free energy, when the number of defects of $H_l$ is taken as an independent thermodynamic variable.

If transformation (7) is done for all of types of defects, then such modified free energy will be the function of independent variables $\varepsilon_{ij}$, $S$, $\bar{S}$ and $\varphi_l$, that is, $\tilde{F}_l = \tilde{F}_l(\varepsilon_{ij}, S, \bar{S}, \varphi_l)$. Thus, an own argument for the internal energy is the defect densities, and for the modified free energy the energy of defects, similar to the case of classical thermodynamics, where an own argument for internal energy is the entropy, and for free energy is the temperature.

Classical configurational free energy $F_c = U - TS_c$ is always treated, as one-to-one function of the density of defects, while in obedience to the method of definition (Legendre transformation) it must be the function of temperature. It follows that it is not a thermodynamics potential in a strict sense, and it is only useful as energy reflection of PDF. While the internal energy and the modified free energy, satisfying Eqs. (5), (6) and (8), are real thermodynamics potentials, though dissatisfy extreme principle.

III. TWO-LEVEL TWO-MODE MODEL OF SPD

Now setting the dependence of the internal energy on its arguments, we fully determine our problem in a thermodynamic sense. Let us apply the above approach for solution of a special problem. Producing a fine-grained structure of metals by severe plastic deformation (SPD) is presently urgent. At the initial stage of SPD there goes intensive generation of dislocations, then next the dislocations serve as a building material for the growth of grain boundaries, that results in a finer grain structure. Thus, in the processes of SPD these two types of defects take the main part and predetermine the two-level character of the problem [38].

A. Evolution equations

Let us consider a homogeneous problem, setting the internal energy as a polynomial dependence

$$u = u_0 + \sum_{l=g,D} (\varphi_{gl} h_l - \varphi_{l1} h_l^2 + \varphi_{l2} h_l^3 - \varphi_{l3} h_l^4) + \varphi_{gD} h_g h_D,$$ (9)

where $u_0$, $\varphi_{kl}$, $\varphi_{gD}$ are some coefficients, depending on the equilibrium variables of $S$ and $\varepsilon_{ij}$, as control parameters

$$u_0 = \frac{1}{2} \lambda (\varepsilon_{ij}^c)^2 + \mu (\varepsilon_{ij}^s)^2 + \beta s^2,$$

$$\varphi_{gl} = \varphi_{l1}^c + g \varepsilon_{ii}^c + \frac{1}{2} \lambda (\varepsilon_{ii}^c)^2 + \mu (\varepsilon_{ij}^c)^2 - \beta s,$$ (10)

$$\varphi_{l1} = \varphi_{l1}^s - 2 \varepsilon_{ii}^s.$$

For the sake of convenience we passed from the numbers of defects of $H_l$ to the densities of corresponding variables of $h_l$, and similarly $S \rightarrow s$, $U \rightarrow u$.

The fourth-degree polynomial in parentheses can have at the positive values of coefficients $\varphi_{km}$ two maxima (two modes). The mode which corresponds to the lower value of defectiveness, in the case of dislocations $l = D$, can describe the accidental (homogeneous) distribution of dislocations. The mode, which corresponds to the higher value of defectiveness, describes dislocations belonging to the cell structure in this case. We examine only the simplified case of the homogeneous distribution of dislocations, that is, $\varphi_{3D} = 0$ and $\varphi_{4D} = 0$.

The coefficient of $\varphi_{0g}$ can be considered as a general surface density of the energy of regular (infinity) GB. From data of S.A. Firstov, for cold-roll treatment this energy can equal the doubled energy of a free boundary for same material. For example, it can make approximately $2 \times 2 J/m^2$ for copper. The first term in this context is the own energy of the boundary without a contribution from other factors. It is considered, as a well full-relaxed grain boundary, that is, as a minimum possible surface energy of GB. According to A.S. Firstov, this energy makes $0.15 \div 0.20$ of the energy of
free-surface of the same material. That is, for copper this energy approximately equals 0.2 \times 2 = 0.4 J/m^2.

Contribution of the second term \( gD \varepsilon_D^i \) to the field of compressing hydrostatic stress results in the decreasing of GB energy. It is of great physical importance meaning that the grain boundaries are sites of density lack distributed along some surface. Exactly these sites give the highest contribution to the energy of boundaries. When, due to external pressure, the volume of undensitized sites diminishes, the energy of boundaries diminishes, as well as the potential barriers between the stable neighbor states, that results in growing mobility of the grain boundaries. If elastic deformation is 0.002 that for copper corresponds to the level of tension \( \sim 180 MPa \), the constant \( gD \) is to be taken within the limits of 12 J/m^2. For such value of constant \( gD \) the energy of grain boundaries will diminish within the limits of 10 percents of its value for a relaxed boundary.

The terms in Eq. (10) proportional to \( \lambda_\theta \) and \( \mu_\theta \) must give at the same level of elastic stress of 180 MPa, such contribution, when general effective energy of GB might not exceed the double energy of the free boundary (for copper 4 J/m^2). It gives conditions for choosing constants in the limits \( \lambda_\theta = 0.25 \cdot 10^6 J/m^2 \) and \( \mu_\theta = 0.6 \cdot 10^6 J/m^2 \). The values of these constants are different because the effects of shear are of greater significance for structural rearrangement of the solid.

Other constants are chosen issues from the reasoning that the equilibrium (stationary) values of the density of grain boundaries were in the interval observed in experiments. For the grain boundaries these are two steady states with the density in a region \( h^e_{g^{11}} = 10 mm^{-1} \) and \( h^e_{g^{02}} = 10 \mu m^{-1} \), where the average grain size is 100 \( \mu m \) and 100nm, accordingly.

The same reasoning can be repeated for dislocations. The minimum excess energy of dislocations, in the absence of other factors for copper, equals approximately \( \varphi_D^e = 5 \cdot 10^{-3} J/m \).

Using Eq. (3), which is true for both the equilibrium and non-equilibrium cases, one gets evolution Eqs (11) in the form

\[
\frac{\partial h_D}{\partial t} = -\gamma_D [\varphi_D(h_D - h_D^e) + \varphi_gD(h_g - h_{gD})],
\]

\[
\frac{\partial h_g}{\partial t} = -\gamma_g [\varphi_gD(h_D - h_D^e) + \Phi(h_g - h_{gD})],
\]

where

\[
\varphi = \varphi_Dg - \varphi_2g(h_g + h_{gD}) + \varphi_3g(h^2 + h_g h_{gD} + h_{gD}^2).
\] (12)

As seen, the evolution equations do not directly depend on the parameters \( \varphi_D^e \) and \( \varphi_2^g \), but can depend on them through the equilibrium values \( h_D^e \) and \( h_g \).

For determination of this dependence it is necessary to find position of the maxima of PDF. As for basic defects, participating in SPD, this function is unknown; it creates some difficulties in application of the theory for calculation of specific systems. For overcoming the difficulties let us consider the method of effective potential in terms of the internal energy.

B. Method of effective potential of the internal energy

Let us suppose that the equilibrium energy of defect weakly depends on a current value of the density of defects, and it can be brought under the sign of differentiation in Eq. (6). Then one can introduce the effective internal energy

\[
\tilde{u} = u - \sum_{i=1}^{N_{def}} \varphi_ieh_i.
\] (13)

The evolution Eq. (6) assumes a form

\[
\frac{\partial h_i}{\partial t} = \pm \gamma_i \frac{\partial \tilde{u}}{\partial h_i}.
\] (14)

Here the plus sign is selected in case if an equilibrium value \( \varphi ie \) is in the region of convexity of the internal energy \( u \), the minus sign is selected in the region of its concavity \( u \). In the first case a stationary solution corresponds to a maximum of the effective energy, in the second case a stationary solution corresponds to its minimum. Formally, Eq. (10) realizes an extreme principle, as its stationary points coincide with a maximum or a minimum of the effective potential of the internal energy \( \tilde{u} \).

We take the effective energy in the same form (4) as the initial internal energy \( u \) with the same coefficients of presentation (10), with the only difference that the equilibrium energy of \( \varphi ie \) is included in coefficient of \( \varphi_0g \), that is, \( \varphi_0g > \varphi_0 - \varphi ie \) and \( u > \tilde{u} \). Then, the set of evolution Eqs (11) can be written in the explicit form

\[
\frac{\partial h_D}{\partial t} = -\gamma_D [\varphi_D^e - \varphi_1Dh_D + \varphi_gDh_D^e],
\]

\[
\frac{\partial h_g}{\partial t} = -\gamma_g [\varphi_0g - \varphi_1g + \varphi_2g(h^2 + h_g h_{gD} + h_{gD}^2) + \varphi_gDh_D].
\]

Results got directly from the solution of the set of evolution Eqs (11), and by the method of effective potential of the internal energy (15), coincide, if relations between the coefficients of internal energy expansion \( h_{gD} = (\varphi_0g - \varphi_{ge}) / \varphi_1g \), \( \varphi_1g >> \varphi_2g\) and \( \varphi_1g >> \varphi_3g(h_{ge}) \) are fulfilled.

Coming from the above analysis, such set of parameters and coefficients was accepted for calculations \( \lambda = \mu = 2.08 \cdot 10^{13} Pa \), \( \varphi_D^e = 5 \cdot 10^{-3} J/m^{-1} \), \( \varphi_1D = 10^{-22} J/m \), \( g_D = 2 \cdot 10^{-8} J/m^{-1} \), \( \mu_D = 3.3 \cdot 10^{-4} J/m^{-1} \), \( \varepsilon_D = 6 \cdot 10^{-23} J/m \), \( \varphi_{0g} = 0.4 J/m \), \( \varphi_{1g} = 3 \cdot 10^{-6} J/m \), \( \varphi_{2g} = 5.6 \cdot 10^{-13} J \), \( \varphi_{3g} = 3 \cdot 10^{-20} J/m \), \( \varepsilon_g = 12 J/m \), \( \lambda_g = 2.5 \cdot 10^{5} J/m^{-2} \), \( \mu_g = 6 \cdot 10^{5} J/m^{-2} \), \( \varepsilon_g = 3.6 \cdot 10^{-4} J/m^{-1} \), \( \varphi_{gD} = 10^{-16} J \).

Other coefficients in expressions for the internal energy are considered to be zero. A time step in numerical calculations is \( \tau = 0.67 \cdot 10^{-6} \), kinetic coefficients are \( \gamma_D = 5 \cdot 10^{23} J/ms \), \( \gamma_{hD} = 10^{6} J/m^{-1} s \). The calculation of system evolution with these parameters and coefficients is shown in fig. (1).
From fig. 1 it is evident, that kinetics of grain boundaries and dislocations during the structural phase transition is closely correlated. At the first stage a growth in the number of dislocations initiates growth of grain boundaries and provokes the beginning of the structural phase transition. During the structural phase transition, when the density of dislocations has already gone on a stationary plateau, vice versa, the growth of grain boundaries provokes the growth of the density of dislocations. Thus, in this area, dislocations follow the grain boundaries in repeating the shape of curve of the structural phase transition, but to more weak extent.

C. Strengthening curves

As known the law of strengthening results from dislocation mobility decrease due to braking by different defects, as well as by dislocations from other slide planes. At the dislocation level the law of strengthening is described by Taylor relation \[ \tau = \alpha \mu b \sqrt{h_D}, \] where \( \tau \) is the shear stress; \( \alpha \) is a coefficient, which takes on a value from the interval \( 0.2 \div 1.0 \); \( \mu \) is the shear modulus; \( b \) is the Burgers vector; \( h_D \) is the density of dislocations (Here the modified denotation is used, which is general in a multilevel system of defects).

If GB are formed directly due to an outcoming of dislocations, in this case one can be limited by relations (16), and the Hall-Petch law at the grain level is got, as simple consequence from this relation acting at the dislocation level.

In the theory of NEET deformation is a control parameter which in the case of shear deformation relates to the stress by a simple dependence \( \tau = \mu \varepsilon_e \) so, in terms of the theory the law of strengthening looks like

\[ \varepsilon_e = ab \sqrt{h_D}. \] (17)

This dependence can be used in NEET, as an additional relation to energetic and kinetic relations written above.

In the case of GB, a mode, which corresponds to a lower value of defectiveness, describes a coarse-grained structure, a mode, which corresponds to the greater value of defectiveness, describes a fine-grained structure. A possibility of forming different modes of the same defect is related to the microscopic mechanisms of deformation. In the case of grains they can be related to the circumstance that at the initial stage an increase of the general surface of GB is the effective mechanism of energy dissipation. The contribution of triple junctions can be ignored at this stage. The situation changes substantially, when the average size of grains decreases to 100 nm. In this case, triple junctions can give a considerable contribution to the energy of boundaries, which can result in the formation of a new maximum in this region.

Triple junctions can be considered, as a specific type of defect, but as it is topologically attached to the grain boundaries, they can be integrated and considered, as one defect with a somewhat more difficult dependence of its energy on the number of defects.

The deformation stages during SPD are demonstrated by changes in the character of strengthening law at different stages of the process. At the first stage (area 1, fig. 1b) the law of strengthening can be approximated by the Hall-Petch law, if expressed through elastic deformations

\[ \varepsilon_e = \varepsilon_{e0} - A \sqrt{h_g}, \] (18)

where the constants are \( \varepsilon_{e0} = -0.075 \) and \( A = 0.119 \)mm. The negative sign is taken because at compression that is in conditions typical of SPD the elastic deformation is negative. As seen from the picture, the elastic deformation changes within the limits of \( 0.1 \div 0.5 \) percents, that in view of the value of shear modulus is in region of values for real materials.
In region 2, which corresponds to the most rapid phase of deformation during SPD, the law of strengthening can be approximated by a linear dependence

\[ \varepsilon^e = \varepsilon^{e1} - B h_g. \]  

(19)

with constants \( \varepsilon^{e1} = -0.27 \) and \( B = 0.0059 \text{mm}^2 \). Just the same character of strengthening law change depending on deformation stage was noted in Ref. [40].

IV. FINAL REMARKS

In the article, an alternative approach of non-equilibrium evolitional thermodynamics is considered and all features of the approach are demonstrated by the model example of solids with vacancies. We derive the system of kinetic equations in terms of the internal energy as the most fundamental thermodynamic potential. The generalized thermodynamic force immediately follows from differentiation of the probability distribution function during the procedure of finding the most probable state. In the equilibrium (or stationary) state such force is not zero, and associated with the equilibrium energy of defect in the equilibrium state.

The second feature which distinguishes this approach from traditional one is in using the density of defects as an independent thermodynamic variable instead of the configuration entropy. This allowed to modernize the writing of 1st law of thermodynamics, by adding to it an entropy terms in the form of product of the defect energy and the increment of the defect density (the last term in Eq. (3)). In addition the first law of thermodynamics in this approach is written with dynamical product of the defect energy and the increment of the defect density (the last term in Eq. (4)).

Inclusion in the modified 1st law of thermodynamics of additional terms, describing internal non-equilibrium processes (they can be considered as analogues of the internal variables or the order parameters introduced by Landau), really, extends the dimensionality of the problem. The increase of problem dimensionality makes it simply certain. At the same time, we can introduce the generalized concept of the system state, depending on both equilibrium \( \varepsilon_{ij}^e \), \( S \) and non-equilibrium \( \dot{S} \) and \( H \) variables.

Approach of NEET is applied to simulate the extraordinarily important for practical applications problem, the refining of grain structure of metals by severe plastic deformation methods. Within the framework of the two-level and two-mode approximation the system of kinetic equations, which includes the mutual kinetics of dislocations and grain boundaries, is deduced. For practical calculations the comfortable phenomenological model of the effective thermodynamic potential of the internal energy, which realizes the usual concept of the extreme state, is introduced. Within the framework of this model the unified curve of strengthening, which has stage-like character, is constructed over the whole of the deformation interval. At the initial stage the curve of strengthening can be approximated by square-root dependence close to the Hall-Petch law, and at the finishing stage, it can be easily approximated by linear dependence.

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