A GENERAL ANALYTIC APPROACH TO ANALYSING NONSTATIONARY STOCHASTIC PROCESSES IN THERMODYNAMIC SYSTEMS. PART I: FORMULATION OF THE APPROACH

Igor Tkachenko*, Victoria Miroshnichenko, Boris Drenchev, Boris Yanachkov and Mihail Kolev

Institute of Metal Science, Equipment and Technologies with Hydro- and Aerodynamics Centre "Acad. A. Balevski", Bulgarian Academy of Sciences, 67, "Shipchenski prohod" Blvd, 1574 Sofia, Bulgaria, e-mails: tkachenko@ims.ban.bg; mirovictoria105@gmail.com; bdrenchev@abv.bg; borisya0001@gmail.com; mihail1kolev@gmail.com

Abstract. A novel general analytic approach to analysing nonstationary stochastic processes in thermodynamic systems is proposed based on some well known theoretical notions and experimental results. The approach was developed in detail for the case of the macroplastic deformation of single-phase impurity-free Face-Centred Cubic (FCC)-metal crystals. The relevant basic mathematic relations were deduced including constitutive nonlinear differential equation describing the time evolution of the introduced crystal and dislocation state parameter $s = (\tilde{\sigma}/\sigma)^n$. Two different crystal deformation modes or a transient process in a thermodynamic system $s_j = s_j(t)$ were first revealed by analytical solving the equation. The differences were attributed to various types of the barriers with different dislocation glide resistance $\tilde{\sigma}_j$ or dissociation stress in a deformed crystal. This conclusion was confirmed by an evaluation of the dissociation stress for dislocation barriers under the single and multiple slip conditions in Cu-single crystals.

Keywords: thermodynamic systems, nonstationary stochastic processes, macroplastic deformation of single-phase impurity-free FCC-metals, different crystal deformation modes.

1. INTRODUCTION

As it is well known, a transition of a thermodynamic (macroscopic) system between its energy states may be referenced as a stochastic, nonstationary

*Corresponding author.

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process [1–2]. As examples, the following ones may be particularly considered: emission of electromagnetic radiation, electric conductivity, allotropic phase transformations, plastic deformation, heat transfer etc. Some of the transients are well described by the own specific theory or models, which are based on the corresponding experimental data and reflect effects related solely to the considered phenomenon using the specific parameters, particular, spontaneous and stimulated emission of radiation, as well as normal and super conductivity. Meantime, the most known transient phenomena have not had comprehensive theories to describe wide ranges of their experimental data collected for decades. It concerns especially the plastic deformation of crystalline metallic materials, where some new data were obtained recently, confirming the basic common feature of the phenomenon mechanism, particularly the emission of radiation [3].

So, critical analysis of the current situation concerned with theoretical consideration of nonstationary processes development in thermodynamic systems leads to conclusion about absence of general approach able to be used: (i) to justify and explain some common features of the phenomena mechanisms, namely – two basic regimes of their development; (ii) to describe quantitatively main features of the regimes; (iii) to predict quantitatively the thermodynamic systems performance.

The aim of the whole article is to develop a general approach able to be applied to analyse transient processes in a thermodynamic system together with its physical interpretation and workability verification by comparing some basic model predictions with the corresponding experimental data.

2. BASIC APPROACH PRINCIPLES FORMULATION

Based on the numerous results have been obtained in the course of investigating various transient processes in thermodynamic systems, the following main features of the system behaviour during the processes development were distinguished:

- Composition of the systems by a huge amount of interacting each other atoms (molecules);
- Each of the atoms (molecules) can occupy two degenerated energy states separated by an energy gap;
- Splitting both the energy levels due to the atoms (molecules) interactions;
- Appearance of the energy barriers because of splitting the degenerated energy levels;

– Necessity for each of the atoms (molecule) to overcome the barrier for passing into a nearest energy state;
– Three stage time period of the process development: incubation period, intensive development, saturated stage.

Generalizing the available data, the following basic assumptions may be formulated to describe a transient process in a thermodynamic system:
– a thermodynamic system consists of a huge amount of interacting subsystems each of that can stand in two different degenerated energy states;
– the subsystem transitions between the energy states are spontaneous and independent events;
– the transient processes in a thermodynamic system are of the third order stochastic ones.

Due to big amount of the justification, interpretation and calculation results the whole article is divided in 3 parts to meet the journal requirements to an article volume.

The Part I is devoted to the justification of the novel approach assumptions for the case of the Face-Centred Cubic (FCC) single phase polycrystal macroplastic deformation; to deduce a constitutive equation of the approach based on the above physical assumptions and to analyse some consequences of the obtained mathematic results.

In the Part II, we will conduct the standard linear stability analysis for the obtained analytical solutions of the constitutional nonlinear differential equation and give a physical interpretation of the solutions from the point of view of dislocation mechanisms involved.

The Part III will present some main results of the developed approach application to quantitative description of stress dependence of the dislocation speed, calculation the true stress–true strain curves for some FCC-metal polycrystals and comparison the results with the corresponding experimental data.

3. JUSTIFICATION OF THE APPROACH BASIC ASSUMPTIONS

The justification of the basic assumptions was made based on the known features of both the jerky dislocation glide and interactions of gliding dislocations, taking into account the transient character of a stochastic process of the deformation.

Let us consider a FCC single phase metal polycrystal exposed to an applied uniaxial tensile true stress σ at a constant metal temperature T such as to provide the development of jerky glide of the crystal dislocations. As the

deformation is a stochastic process for the given conditions, the probabilities $P_I(\sigma, t)$ and $P_{II}(\sigma, t) = 1 - P_I(\sigma, t)$ have to be determined to find the above whole crystal at a time t, accordingly, in the state without macroscopic plastic deformation, indicated by low index I and – in the state of macro-plastic flow, indicated with low index II.

According to the commonly accepted notions [4], the macroscopic plastic crystal deformation may be defined as a process developing, if screw components of the majority of crystal dislocations are able to glide in a predominant slip system, and have a mean free path L_p in the glide system, exceeding a mean strongest obstacles spacing λ, $L_p \geq \lambda$. Following to [5], this majority of dislocations is associated with those mixed segments of existing dislocation loops or networks, which are characterized by the most probable value of their length $l_d^* \equiv l_d^*(\sigma, t)$ between the nearest pinning points in a plane of a predominant slip system at a given moment of the deformation. Hereafter these dislocation segments are called the "active" ones.

Considering the known experimental and theoretical results, a mobile dislocation, in order to glide in a plane of a single-phase impurity-free FCC-crystal, has to surmount the resistance offered mainly by obstacles of the following types: (i) individual non-attractive forest and parallel dislocations; (ii) stable dislocation barriers (attractive dislocation junctions, Lomer–Cottrell barriers); (iii) dislocation tangles, cell walls and subgrain boundaries. Though details of the later dislocation configurations are unknown so far, based on the available data the attractive dislocation junctions may be considered as their main components [5]. Besides, Lomer–Cottrell barriers are also formed therein, including the easy glide deformation stage in single crystals as a result of the reactions between moving primary dislocations and a restricted number of segments lying in secondary slip planes [6]. So, the stable dislocation barriers are referred to as the "strongest" obstacles in accordance with [4, 7–9]. Mobile dislocations overcoming these obstacles control the plastic flow of single-phase FCC-metals. The maximum strength of such an obstacle is evidently characterized by a stress $\tau_b(0)$ necessary to dissociate the dislocation barrier at $0K$. According to [4, 9], one can write:

$$\tau_b(0) = \frac{Gb}{4\pi} \cdot \frac{L_p}{l_f^2}, \tag{1}$$

where G is the shear modulus, b is the Burgers vector and $l_f = l_d^*$ is the most probable forest dislocation spacing. According to the just given definition, such a stress should be considered as a threshold one, considerably exceeding the maximum resistance offered by the individual dislocations $\tau_a + \tau_t$, where τ_a

and τ_t are the amplitudes of the athermal and thermally activated resistance associated mainly with the parallel and non-attractive forest dislocations, respectively, $\tau_b(0) > \tau_a + \tau_t$. On the other hand, according to the general synergetic approach [10], a loaded crystal should be considered as a macroscopic system consisting of numerous identical interacting subsystems. Their joint action determines the whole system state at a time t. We identify the subsystems with the active dislocation segments whose collective overcoming the strongest obstacles determines the macroplastic deformation of the whole crystal.

Proceeding from the above, the following scheme of the crystal deformation is proposed as a foundation of the further analysis.

At any stage of the plastic deformation there are active dislocation segments of the length $l_d^* \equiv l_d^*(\sigma, t)$ in planes of a predominant slip system. In some of the planes, they may operate as dislocation sources, if the applied stress σ reaches the value $\sigma_s \approx \overline{M}Gb/l_d^*$, where $\overline{M}$ is the appropriate Taylor factor. For stresses $\sigma_s \geq \overline{M}(\tau_a + \tau_t) \geq \sigma_s$, the segments glide in active planes of a predominant slip system overcoming the resistance of individual as non-attractive forest as parallel dislocations. Under the same conditions, a restricted number of mobile dislocation segments of the length $l_d \gg l_d^*$ also glides in secondary slip planes. As a result of the dislocation reactions, a number of the dislocation barriers appears as components of the dislocation "walls". Further, there are two possible mechanisms for the original dislocation segment to continue its glide: to overcome the barriers with continuing the glide in the initial plane of the predominant slip system (dislocation configuration PMM′P′K′N′NK in Fig. 1); to bypass the barriers according to the cross slip mechanism that includes the gliding in planes of the secondary slip systems (dislocation configuration CA′C′D′B′D in Fig. 1).

Considering only the non-interacting barriers within the dislocation cell walls, different dislocation configurations may be formed in front of them during loading, depending on the distance $S_i \equiv S_i(\sigma, t)$, separating such an obstacle and the nearest dislocation source. Namely, dislocation pile-ups appear in front of those dislocation barriers for which $S_i > l_d^*$. On the other hand, in the case when an unclosed, bowed out active dislocation segment interacts with a corresponding forest dislocation and forms a dislocation barrier, one can write $S_i \leq l_d^*/2$. As a result, no closed dislocation loops are generated later by such a dislocation source. Consequently, there are not dislocation pile-ups in front of those barriers for which $S_i \leq l_d^*/2$. It is natural to consider the active dislocation segments involved in such single barriers as individual ones.

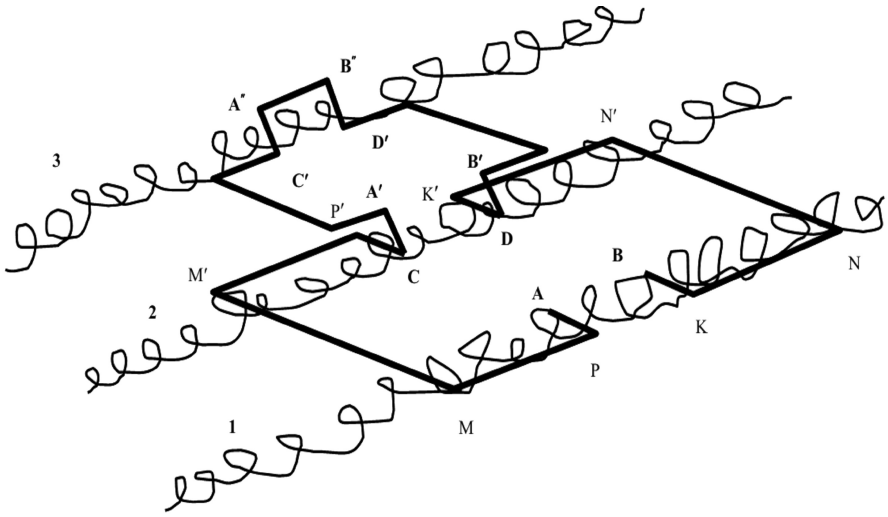

Fig. 1. Schematic representation of the two possible mechanisms of the glide of an active dislocation initially pinned in the points A and B across the strongest obstacles within the dislocation walls 1, 2, 3: overcoming the obstacles with continuing to glide in the initial plane of the predominant slip system (dislocation configuration PMM′P′K′N′NK); bypassing the obstacles by the cross slip mechanism (dislocation configuration CA′C′D′B′D)

The necessary condition for the continuation of the glide in an active slip plane is the dissociation of the dislocation barriers existing in the same plane. Such dissociation is possible under the loading conditions $\overline{M}(\tau_a + \tau_t) < \sigma \leq \overline{M}\tau_b(0)$, according to the thermally activated "unzipping" mechanism [9]. Evidently, the key stage of this dissociation process is the glide of that mobile dislocation segment, which is involved in the barrier and lies in a predominant slip system, where the maximum resolved shear stress acts. Hereafter such dislocation segments are referred to as "driving active" ones. As soon as a dislocation barrier dissociates with assistance of a thermal fluctuation, the driving active segment, together with possibly piled-up mobile dislocation loops, can pass the distance $L_p \approx \lambda$ until it forms the new barrier in the same slip plane. Thus, the glide of a driving active dislocation segment results in: (i) a thermally activated dissociation of the dislocation barrier and (ii) a further athermal long-distance ($L_p \approx \lambda$) dislocation glide through the dislocation forest. Both control the macroscopic slip propagation in an active slip plane.

Based on the described scheme, a particular case is considered in detail: the glide of an individual driving active dislocation segment, i.e. the active segment involved in a single dislocation barrier.

As it follows from the activation energy–displacement curve for a dislocation barrier formation and dissociation [9], an energy of dissociation W may be defined as $W \approx \varepsilon_2 - \varepsilon_1$. Here, ε_2 is the energy of the upper activated state of a driving active dislocation segment. Due to instability of this state, the segment having the energy ε_2 can either be in an immobilized condition or glide through the dislocation forest at a distance $L_p \approx \lambda$ [9]. The quantity ε_1 is the minimum energy of the segment involved in the barrier, i.e. being in the lower, stable immobilized condition for which $L_p \ll \lambda$, i.e. $L_p \approx 0$.

Proceeding from the above, the main assumptions of the approach as applied to the macroscopic plastic deformation may be specified as follows:

(i) The macro-plastic crystal deformation is a result of the glide of mobile mixed dislocation segments of the most probable length (active dislocation segments) with overcoming the strongest obstacles.

(ii) The strongest obstacles to the dislocation glide are non-interacting stable dislocation barriers, the dissociation of which can develop only by the thermally activated "unzipping" mechanism at a critical shear stress $\tau_b \equiv \tau_b(T)$. The control stage of the dissociation is the glide of involved in the barriers active dislocation segments (the driving active segments), which are all equivalent ones due to relaxation of dislocation pile-ups [9] possibly formed in front of the dislocation barriers.

(iii) The macro-plastic deformation of a crystal includes the three, consistently developed in the course of the deformation, stages: independent propagation of primary slip bands; interaction of the slip bands; ultimate strengthening of slip bands resulting in stoppage of the dislocation glide or the crystal fracture.

On the basis of the above first two assumptions, the stress effect on the probability to glide for a driving active dislocation segment was firstly considered.

4. STRESS EFFECTS ON THE ENERGY STATES OF THE SUBSYSTEMS AND A WHOLE THERMODYNAMIC SYSTEM

One of the objectives of the current plastic deformation analysis is to find probabilities $p_I(\tau, t)$ and $p_{II}(\tau, t) = 1 - p_I(\tau, t)$ to detect a driving active dislocation segment at a time t respectively in (I) the immobilized condi-

tion and (II) the state of long-distance glide in a plane of a predominant slip system being under the action of a shear stress $\tau = \sigma/\overline{M}$. In the most general case the probability to find a dislocation segment in an energy state ε is $p(\varepsilon, \tau) \propto q(\varepsilon, \tau) \cdot Q(E - \varepsilon, \tau)$, where $q(\varepsilon, \tau)$is a number of available microstates of a dislocation segment; $Q(E - \varepsilon, \tau)$ is the number of microstates of a reservoir. Evidently, crystal volumes surrounding the considered active dislocation segment may play the role of the reservoir. The quantity $q(\varepsilon, \tau)$includes all kinds of microstates corresponding to the vibrational and configurational contributions to the dislocation entropy. The dislocation energy ε may be considered as a function of two variables $\varepsilon = \varepsilon(\tau, t)$, where x is a coordinate of the midpoint of a dislocation segment along a direction of its displacement. For the defined above two energy states of a driving active dislocation segment one can write $\varepsilon_m = \varepsilon(\tau, x_m)$, where x_m is a midpoint coordinate of the segment in its lower, stable immobilized condition ($m = 1$) and the upper, activated one ($m = 2$). It is obvious that $x_m = x_m(t)$, because of the natural oscillations of a dislocation line caused by thermal fluctuations.

In order to derive expressions for stress dependencies of $p_{I(II)}$, let us consider the changes of $q(\varepsilon_m, \tau)$ in the course of the adiabatic quasi-static increase $d\tau$ of the external parameter $\tau = \sigma/\overline{M}$, since for the reservoir as a macroscopic system $Q(E - \varepsilon, \tau) = \text{const}$. For the considered dislocation segment as a mesoscopic subsystem the following relation must be written [11]:

$$\ln q(\varepsilon_m + \delta A_m, \tau + d\tau) - \ln q(\varepsilon_m, \tau) = -\frac{\partial \alpha_m}{\partial \varepsilon_m} \cdot d\tau, \tag{2}$$

where $\alpha_m = \delta A_m / d\tau$. Here δA_m is a macroscopic work done under the subsystem which is in the energy state ε_m. In general, for the dislocation energy one can also write:

$$d\varepsilon(\tau, x) = \frac{\partial \varepsilon}{\partial \tau} d\tau + \frac{\partial \varepsilon}{\partial x} dx. \tag{3}$$

It is well known that a growth of the external acting stress increases a length of a dislocation being either in immobilized or moving condition due to additional bowing up of a pinned dislocation segment and a growth of a jogs concentration on a moving one. Therefore, for both energy states ε_m, relation $\dfrac{\partial \varepsilon_m}{\partial \tau} > 0$ holds. For a segment displacement in its glide direction ($dx > 0$) at a constant applied resolved shear stress τ, two relations follow from the activation energy–displacement curve [8] $\dfrac{\partial \varepsilon_1}{\partial x} > 0$ and $\dfrac{\partial \varepsilon_2}{\partial x} < 0$. So, let us use below the definitions $V_a \equiv \dfrac{\partial \varepsilon}{\partial \tau}$; $f \equiv \dfrac{\partial \varepsilon}{\partial x}$, where V_a is the activated volume of an active dislocation segment and f is the force acting on the segment. Taking

into account that $V_a = bl_d^* x$ and $f = \tau bl_d^*$, relation (3) for the considered energy states may be rewritten as:

$$d\varepsilon_1 = V_{a1} d\tau + \tau \, dV_{a1}; \quad d\varepsilon_2 = V_{a2} d\tau - \tau \, dV_{a2}.$$

Assuming for simplicity that V_a and f are independent of stress and displacement, respectively, and taking into account that $\delta A_m \equiv V_{am} d\tau$ one yields from equation (2):

$$q\left(\varepsilon_1, \tau\right) \approx q_0\left(\tilde{\tau}/\tau\right), \quad q\left(\varepsilon_2, \tau\right) \approx q_0\left(\tau/\tilde{\tau}\right), \tag{4}$$

where q_0 and $\tilde{\tau}$ are integration constants. As it follows from equations (4), a growth of the applied stress $\sigma = \tau \overline{M}$ leads to a decrease of the number of available microstates for a driving active dislocation segment being in the stable immobilized condition, but increases this characteristic number for the segment in the activated state. This conclusion is in agreement particularly with the commonly accepted dislocation mechanism of the Bordony peak [9]: some of the initially equivalent positions of an immobilized dislocation in a crystal with a certain internal stress become more probable than other ones under the action of an external superimposed stress. It evidently means a decrease of the total number of microstates available for a pinned dislocation due to an increase of the applied stress.

Taking into account the unrealistic particular features of the dependencies (4) $q\left(\varepsilon_1, \tau\right) \to 0$ at $\tau \to \infty$ and $q\left(\varepsilon_2, \tau\right) \to 0$ at $\tau \to 0$, the character of the stress influence on $q(\varepsilon_m, \tau)$ in general case will be described by the scheme shown in Fig. 2. Recalling that $\varepsilon_m = \varepsilon(\tau, x_m)$ and $x_m = x_m(t)$ due to thermal dislocation oscillations, one can write $q(\varepsilon_m, \tau) \equiv q_m(\tau, t)$. For the stress conditions $\tau \geq \tilde{\tau}$ the quantity $q_2(\tau, t)$ may be expressed as:

$$q_2(\tau, t) = q_2(\tilde{\tau}, t) + \frac{dq(\tilde{\tau}, t)}{d\tau} \cdot (\tau - \tilde{\tau}) + \frac{d^2 q(\tilde{\tau}, t)}{2! \cdot d\tau^2} \cdot (\tau - \tilde{\tau})^2 + \cdots,$$

or

$$q_2(\tau, t) = q_2(\tilde{\tau}, t) + q\left(\tau - \tilde{\tau}, t\right). \tag{5.1}$$

As it also follows from the scheme, at a stress $\tau \geq \tilde{\tau}$, $q_2(\tilde{\tau}, t) = q_1(\tilde{\tau}, t) \approx q_1(\tau, t)$, therefore expression (5.1) is rewritten in the form:

$$q_2(\tau, t) \approx q_1(\tau, t) + q\left(\tau - \tilde{\tau}, t\right), \tag{5.2}$$

where $q_2(\tau, t)$, $q_1(\tau, t)$ and $q(\tau - \tilde{\tau}, t)$ are the microstates numbers corresponding to a driving active dislocation segment being at a stress τ respectively

in: the activated condition, the immobilized state and the state of the long-distance glide. According to the probability definition, the following relations flow from the equation (5.2):

$$p_I(\tau,t) \equiv \frac{q_1(\tau,t)}{q_2(\tau,t)}; \quad p_{II}(\tau,t) \equiv \frac{q(\tau-\tilde{\tau},t)}{q_2(\tau,t)}. \tag{6}$$

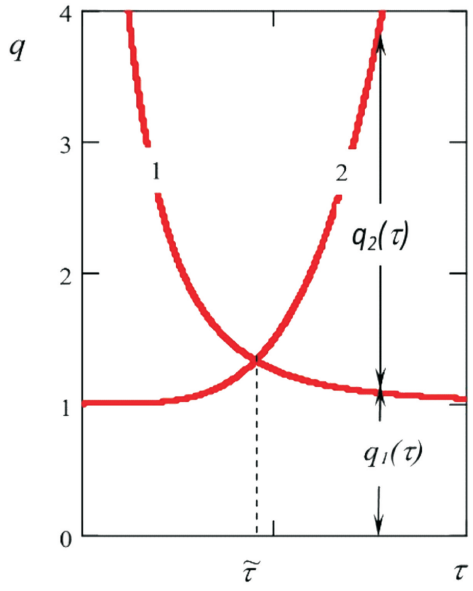

Fig. 2. Schematic representation of the stress influence τ on the number of active dislocation microstates q_j in immobilized $(j=1)$ and mobile $(j=2)$ states

Using equation (5.1) and the probability normalization condition, one obtains:

$$p_I(\tau,t) \approx \frac{q_2(\tilde{\tau},t)}{q_2(\tau,t)}, \tag{7}$$

$$p_{II}(\tau,t) \approx 1 - \frac{q_2(\tilde{\tau},t)}{q_2(\tau,t)}. \tag{8}$$

As it is well known [11], for any thermodynamic system with an unlimited energy spectrum, the number of available microstates $q(\varepsilon)$ is a rapidly growing function of its energy ε, $q(\varepsilon) \propto \varepsilon^F$, where F is the number of degrees of freedom for the system. On the other hand, the energy of a dislocation is a function of an applied stress $\varepsilon = \varepsilon(\tau, x)$. Hence, for a driving active dislocation segment we may write $q_2(\tau,t) \propto \tau^n$; $q_2(\tilde{\tau},t) \propto \tilde{\tau}^n$, where $n = n(t)$ is a non-negative parameter, associated with the dislocation number of degrees of

freedom. Finally, recalling that $\tau = \sigma/\overline{M}$, one finds from the expressions (7) and (8), respectively:

$$p_I \approx \left(\frac{\tilde{\sigma}}{\sigma}\right)^n; \quad p_{II} \approx 1 - \left(\frac{\tilde{\sigma}}{\sigma}\right)^n, \tag{9}$$

where $\tilde{\sigma} \equiv \tilde{\tau} \cdot \overline{M}$. It should be noted that the relations (9) determine the probability of the long-distance glide of an individual driving active dislocation segment exclusively under the conditions of the thermally activated "unzipping" of an attractive dislocation junction followed by the athermal glide of the segment in its original slip plane. According to dislocation theory [9], a stress level providing such a glide of a driving segment is considered as being independent from the presence of a dislocation pile-up in front of the dislocation barrier, due to the internal stress relaxation caused by the dulling of the pile-up. This allows considering all driving active dislocation segments in a crystal as equivalent ones. Using the relations (9) one defines the quantity $\tilde{\sigma}$ as the minimum stress necessary at a given temperature for the thermally activated dissociation of a dislocation barrier in front of which there is or is not a dull dislocation pile-up:

$$\tilde{\sigma} = \tilde{\sigma}(T) \equiv \tau_b(T)\vec{M}.$$

Thus, it may be concluded that the macro-plastic deformation of a whole crystal develops by the joint long-distance glide of all driving active dislocation segments that provides the motion of all the other active segments in a crystal. The total amount of equivalent driving active dislocation segments in a crystal is expressed as: $p_b AN$, where ρ_b is the density of dislocation barriers in an active slip plane; A is an area of such a plane; N is the total number of active planes of a predominant slip system in a crystal. Taking into account the indistinguishability of driving active dislocation segments, the probability to find an arbitrarily chosen one in the moving state is $(1 - s/\rho_b AN)$, where $s \equiv (\tilde{\sigma}/\sigma)^n = s(\sigma, t)$. In view of the independent character of the thermally activated dissociation of the non-interacting dislocation barriers, as well as the fact that $N \to \infty$for real crystals, the probability of the joint glide of all driving active dislocation segments in a crystal is:

$$\lim_{N\to\infty} \left(1 - \frac{s}{\rho_b AN}\right)^{\rho_b AN} = e^{-s} \equiv \exp\left[-\left(\frac{\tilde{\sigma}}{\sigma}\right)^n\right].$$

Thus, the required expressions for the determination of the probability to find a loaded crystal in the state without macroplastic flow $P_I(s)$, and in the

state of macroplastic deformation $P_{II}(s)$, have the following form:

$$P_I(s) = 1 - \exp\left[-\left(\frac{\tilde{\sigma}}{\sigma}\right)^n\right], \tag{10}$$

$$P_{II}(s) = \exp\left[-\left(\frac{\tilde{\sigma}}{\sigma}\right)^n\right]. \tag{11}$$

It should be noted that according to expressions (10) and (11), the parameter $s \equiv (\tilde{\sigma}/\sigma)^n$ completely characterizes the state of a whole loaded crystal with respect to the macroplastic deformation development. On the other hand, as equations (9) show, this parameter also specifies state (energy and number of degrees of freedom) of a driving active dislocation segment with respect to its long-distance glide without leaving the original slip plane.

5. CONSTITUTIVE EQUATION OF A TRANSIENT PROCESS

As it follows from the above, $P_{II}(\sigma, t)$ may be considered as a joint probability distribution of the deforming stress σ providing the macroplastic crystal flow and a delay time t of the flow. Since $P_{II}(\sigma, t) = \exp[-s(\sigma, t)]$, one has to consider the parameter $s(\sigma, t) \equiv (\tilde{\sigma}/\sigma)^n$ as a random variable. So, under the both conditions $\sigma = \text{const}$ or $\sigma = \sigma(t)$, the random function $s(t)$ has to represent the process of the macroplastic deformation. However, the order of the distribution function well defining the considered stochastic process $s(t)$ is not determined so far [1]. It is well known that in the course of the macroplastic flow of a crystal, the following three stages of the deformation are generally distinguished: (i) filling a crystal by non-interacting slip lines, as a result of the slip propagation in planes of a predominant slip system; (ii) interaction of new slip lines with the previously formed ones, leading to strain hardening; and (iii) termination of the plastic flow due to maximum hardening of all the active slip planes, leading to a blocking of dislocation sources and further crystal fracture. Therefore, during the observation of a loaded crystal, it is possible to choose three consistent points of time t_1, t_2, t_3, corresponding to the above three stages of the plastic flow. In terms of the probability distributions for the stochastic process, the following relations are written for the three stages of the crystal deformation, respectively, [1]:

$$\frac{\partial P_{II}}{\partial s_1} \neq 0; \quad \frac{\partial^2 P_{II}}{\partial s_1 \partial s_2} \neq 0; \quad \frac{\partial^3 P_{II}}{\partial s_1 \partial s_2 \partial s_3} = 0. \tag{12}$$

Using the definition $\dot{s}_k \equiv ds\,(t_k)/dt$, the last of the relations (12) may be rewritten as:

$$\frac{\partial^3 P_{II}}{\partial s_1 \partial s_2 \partial s_3} = \frac{\partial^3 P_{II}}{\partial t^3} \cdot \frac{1}{\dot{s}_1 \dot{s}_2 \dot{s}_3} = 0.$$

It is reasonable to assume that a crystal state always changes with a finite rate in time $\dot{s}_k \neq \infty$. It leads to:

$$\frac{\partial\, ^3 P_{II}}{\partial t^3} = 0.$$

Substituting expression (11) in the last relation one obtains a differential equation describing the time evolution of the parameter $s \equiv (\tilde{\sigma}/\sigma)^n$ during the third order stochastic transient of the macroplastic deformation:

$$\frac{d^3 s}{dt^3} - 3\frac{d^2 s}{dt^2} \cdot \frac{ds}{dt} + \left(\frac{ds}{dt}\right)^3 = 0. \tag{13}$$

6. REAL ANALYTIC SOLUTIONS OF THE CONSTITUTIVE EQUATION AND THEIR MAIN PROPERTIES

The analytical solution of the autonomous system (13) leads to the following real time dependencies of the parameter $s \equiv (\tilde{\sigma}/\sigma)^n$:

$$s_1\,(t) = \ln \frac{A_1}{2 - \left(\frac{t}{\widehat{t}_1} - 1\right)^2}, \tag{14}$$

$$s_2\,(t) = \ln \frac{A_2}{2 + \left(\frac{t}{\widehat{t}_2} - 1\right)^2}, \tag{15}$$

where A_j and $\widehat{t}_j$ $(j = 1, 2)$ are integration constants. It is easy to show that relations of the form:

$$s_j\,(t \pm t_{0j}) = \ln \frac{A_j}{2 \pm \left(\frac{t \pm t_{0j}}{\widehat{t}_j} - 1\right)^2}, \tag{16}$$

are also solutions of the main equation (13), where $t_{0j} \neq 0$ are constants. It should be emphasized here that each dependence $s_j(t)$ characterizes the behaviour of an active dislocation segment or the whole crystal volume under

a load. The state of them begins to change at the time $t = 0$. Therefore, the quantity $s(t \pm t_0)$ is used to describe the behaviour of the active dislocation segments or the crystal volumes, with states beginning to evolve at various times $\pm t_0$. The obtained time dependencies $s_j(t)$ and $P_{II\,j}(t)$ are plotted in Fig. 3. As seen, any crystal loaded by the stress σ is characterized by the two different values $s_j (j = 1, 2)$ of the quantity $s(t)$ at the same fixed time. Hence, the time dependences (14) and (15) should be considered as possible different modes of the macroplastic crystal flow or a transient process in a thermodynamic system in general case. According to the definition of s, one finds $s_j = (\tilde{\sigma}_j/\sigma)^{n_j}$. So, the above differences should be associated with two different levels of the each crystal state parameter $\tilde{\sigma}$ and n. Since $\tilde{\sigma}$ characterizes the resistance of a stable dislocation barrier to dislocation glide, one finds in general two types ($j = 1, 2$) of the barriers with different dislocation glide resistance $\tilde{\sigma}_j$ or dissociation stress in a deformed crystal. This conclusion is confirmed by an evaluation of the stress necessary to dissociate a dislocation barrier for single and multiple slip conditions in Cu-single crystals. As it follows from relation (1), the relevant stress is expressed as:

$$\tau_b(0) = \frac{Gb}{4\pi} \cdot L_p \cdot \rho_s, \tag{17}$$

where $\rho_s = 1/l_f^2$ is the density of dislocations lying in planes of secondary slip systems. For single slip conditions ($\rho_s = \text{const}$), such the density for a Cu single crystal is $\rho_s \approx 1.75 \cdot 10^7 \text{cm}^{-2}$, [12–13]. Using the known relation for a mean spacing of attractive forest dislocations [12], one finds $L_p \approx 3.3 \cdot l_f$. For $T \approx 0K$ this yields $\tau_{bs} \approx 2.8 \cdot 10^{-5} G$, in agreement with the experimental values of the critical resolved shear stress for soft oriented Cu-crystals at room temperature $\tau_c \approx (1.9 \ldots 2.6 \cdot 10^{-5})G$, [12–13]. On the other hand, for a dislocation multiple slip conditions $L_p = D/\sin\omega_s$, where D is a nearest spacing of primary slip bands and ω_s is an inclination of the slip bands with respect to planes of the predominant slip system [13–14]. Since $\sin\omega_s \approx \omega_s \approx \gamma_s$, it follows that $L_p \approx D/\gamma_s$, where γ_s is the shear strain in secondary slip systems. Taking into account that $\gamma_s = \rho_s b L_s$ and $L_s \approx D$, equation (17) yields $\tau_{bm}(0) \approx 0.1G$, a value which is essentially exceeding stress levels necessary for real metallic crystals deformation. From the above, the corresponding tensile critical stresses are defined as $\tilde{\sigma}_s(T) \equiv \tau_{bs}(T) \cdot \overline{M}$, $\tilde{\sigma}_m(T) \equiv \tau_{bm}(T) \cdot \overline{M}$ at a given temperature T. So, under the conditions of multiple slip, i.e. continuous generation of secondary dislocations ($\rho_s L_p = \text{const}$), the formed dislocation barriers cannot dissociate under the action of the applied stresses σ, providing the macroplastic deformation of real metal crystals since $\sigma \ll \tilde{\sigma}_m(T)$.

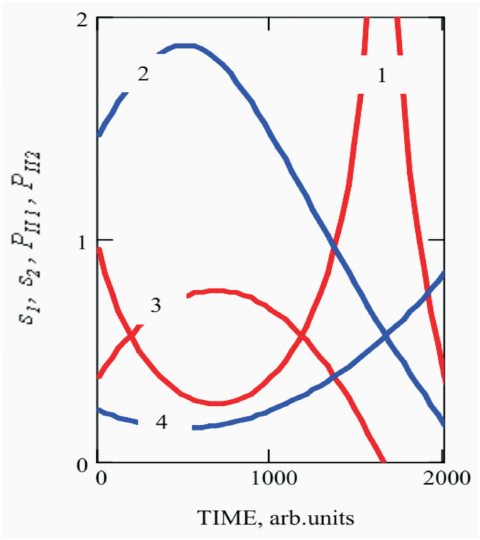

Fig. 3. Calculated time dependencies of the two modes of the approach parameter s_j (lines 1, 3) and the probability P_{IIj} (lines 2, 4) to find a whole thermodynamic system in the final state of its transient process development, specifically – a whole FCC single phase polycrystal in the macro-plastically deformed state

Meantime, for the single slip conditions, i.e. at a constant secondary dislocation density ($\rho_s = \text{const}$), the barriers are able to dissociate with assistance of thermal fluctuations at low stresses $\tilde{\sigma}_s(T) \leq \sigma < \tau_{bs}(0) \cdot \overline{M}$.

Thus, the model results having been obtained show that:

– the macroplastic deformation of single-phase FCC-metals develops heterogeneously on any stage of the flow;
– there are two types of regions with different resistance to the dislocation glide in the deformed FCC-crystals.

These conclusions agree with the composite concept of the plastic deformation of single-phase crystals [14–15] and are confirmed by the experimental data, available for single and polycrystals [16–17].

7. CONCLUSIONS

1. An analytic approach to analysing nonstationary stochastic processes in thermodynamic systems is proposed, which is justified and developed in detail for the case of the macroplastic deformation of single-phase impurity-free FCC metal crystals.
2. Main assumptions making physical ground for the approach for the case of the conducted analysis are as follows:

- the macroplastic crystal deformation is a result of overcoming the strongest obstacles by mixed dislocation segments of the most probable length (active dislocation segments) and their subsequent glide through the “forest”;

- the strongest obstacles for the dislocation glide are non-interacting stable dislocation barriers able to dissociate by the thermally activated "unzipping" mechanism as a result of the glide of involved in the barriers active dislocation segments (the driving active segments), which are all equivalent ones due to relaxation of dislocation pile-ups possibly formed in front of the dislocation barriers;
- the macroplastic deformation of a crystal includes the three stages consistently developing with time: independent propagation of primary slip bands; interaction of the slip bands; ultimate strengthening of the bands resulting in crystal fracture.

3. Based on the assumptions the following basic mathematic relations were deduced: an expression for determination of the probability of the glide of a driving active dislocation segment; formula defining the probability to detect a whole loaded crystal in the macro-plastically deformed state; constitutive non-linear differential equation, describing the time evolution of the introduced crystal and dislocation state parameter $s = (\tilde{\sigma}/\sigma)^n$.
4. As a result of the analytical solution of the constitutive equation, two different crystal deformation modes $s_j = s_j\,(t)$ were revealed. The differences are associated with the presence of dislocation barriers with different dissociation stresses, as confirmed by numerical evaluations and the experimental data.

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