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Non-homogeneous plastic deformation of amorphous metallic alloys under the action of a quasi-static mechanical load

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A hypothesis is formulated and substantiated that quasi-static deformation in an amorphous metal alloy is a complex relaxation multi-stage process, which is a hierarchical sequence of interrelated structural transitions of the first order ordered in time. These nonequilibrium processes sequentially proceed at different scale space-time levels, starting from the lowest level — a cluster of atoms of the first coordination sphere with a relaxation time τ_η, then the middle level - a nanocluster of atoms of the fifth coordination sphere with a relaxation time τ_φ, spatial scale of 10 nm and relaxation time τ, and $\tau \gg \tau_\varphi \gg \tau_\eta$. They are accompanied by transformations of various types of potential energy of atoms (elastic, inelastic, plastic deformation, ZST) into each other. A mechanism and a model of a nonequilibrium transition from an elastic mechanical state to a state with shear transformation zones, a mechanism and a model of localized plastic deformation in an amorphous metal alloy are constructed. In the interval of non-uniqueness, in response to a locally introduced perturbation, a traveling autowave arises, which transfers the slip band from the inelastic deformation regime to the plastic deformation regime. Model parameters are estimated and important physical properties of plastic deformation are calculated.

Keywords: Amorphous metal alloys, mechanical load, plastic deformation, nonequilibrium structural transition, synergetic model, kinetic equations, autowave.

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Introduction

The map of the mechanical states of the amorphous-metal alloys (AMA) in the parameters „temperature-applied stress" σ/μ (μ — the shear modulus) [1–4] shows that within the region from the absolute zero to the room temperature and of the low stresses $\sigma/\mu \ll 10^{-2}$ an elastic-deformation state is implemented. With increase of the stress $\sigma/\mu \leq 10^{-2}$, there is a region of inelastic deformation. The high stresses $10^{-2} < \sigma/\mu < 10^{-1}$ cause heterogeneous plastic deformation of AMA.

Let us note features of the low-temperature deformation of metal glasse [1–3], which have been detected as per strain diagrams (the curves „tensile stress–elongation" plotted using the experimental data) as well as during experimental study of internal friction.

The elastic deformation obeys the Hooke's law, which stipulates that the deformation ε linearly depends on the applied stress σ, i.e. $\varepsilon(\sigma) \sim \sigma$. After load removal the elastic deformation is fully and instantaneously reversible (at the speed of sound).

Within the inelastic deformation region, the dependence $\varepsilon(\sigma)$ becomes non-linear, and the deformation of the sample increases faster than by the linear law. After load removal the decrease of the inelastic deformation is delayed in time. The part of the inelastic deformation is reversible for the time of the observation (experiment). The remaining part of the inelastic deformation is irreversible for the time of observation. However, in case of substantial increase of the observation time the remaining part of the inelastic deformation decreases.

It is believed that inelasticity of the amorphous alloys is related to free volume in their structure: if the free volume is small, then the inelastic deformation is small, too. Therefore, the inelasticity correlates to a degree of relaxation of the structure, at which the free volume is decreased. The inelastic deformation decreases after annealing, at which the structural relaxation occurs and increases with irradiation.

The plastic deformation (PD) is heterogeneous and localized in glide bands. The width of the glide band is up to 10 nm, whereas the distance between the glide bands is up to 10,000 nm. At the same time, the shear bands do not occur spontaneously across the whole volume at an initial stage of the plastic deformation. The band is nucleated at a free surface of the sample to subsequently propagate and surface as a step to another free surface.

In the heterogeneous plastic deformation, plastic flow is localized in the glide bands, while solid body areas between the glide bands are still plastically undeformed. The glide band includes the changes of the atomic structure: the concentration of the free volume is increased, i.e. the average distance between the atoms is increasing.

The propagation speed of the shear bands is very low and it is about $0.3\,\mathrm{mm\,s^{-1}}$ and almost do not depend on a deformation rate within the range $2 \cdot 10^{-4}-10^{-2}\,\mathrm{s}^{-1}$ [5,6]. During annealing, the structure of the shear bands is fully or partially relaxed, but the steps of the shear bands remain, therefore the plastic deformation is irreversible in time.

A synchronous source was used to study the evolution of the structure of the amorphous alloys directly in the process of deformation [7–9]. The [7] has studied the structure under tension *in situ*, thereby detecting the changes of the structure of the zirconium-based metal glasses, which occur in the elastic deformation. It has been found that the single-axis extension result in a small anisotropic change of distances (in fractions of a percent) between the first nearest neighbours.

In [8] the samples were plastically deformed and beside the homogeneous inelastic deformation of the amorphous phase there was the localized plastics deformation (of the shear band). The rolling inelastic deformation results in the small anisotropic increase of the interatomic distance and, hence, the change of the first coordination sphere of the amorphous phase. The work [9] has obtained such the results, wherein the authors also relate the changes of the form of the first coordination sphere to the inelastic deformation.

The study of the deformation processes in the amorphous metal faces some difficulties as it is impossibly to study them by transmission electron microscopy methods used for the study of crystals. Therefore, in spite of a significant number of various models and deformation mechanisms there is no complete theory on the AMA deformation.

The authors in [10] have assumed that the AMA has „shear transformation zones“ (STZ) with excessive free volume and finite lifetime.The „shear transformation zone“ is regarded as a cluster of several dozens of atoms, whose structure is subjected to the shear stress to pass from one state with low energy into another through an activation barrier. This deformation mechanism is developed in a computational model and numerically calculated. The glide process under the STZ mechanism is considered to be thermally activated, with the activation energy of $\sim 1\,\mathrm{eV}$.

The model of „free volume“ in AMA, which is somewhat similar to crystal vacancies, has been suggested in the works [6,11]. However, as there is no crystal lattice, the unit free volume in place of an absence atom is partially distributed across the whole AMA volume. The deformation process is a series of atom jumps into the place of the unit free volume so as the free volume would be transited across AMA. This deformation mechanism is a diffusion-type process, whose activation energy is approximately $0.1\,\mathrm{eV}$.

Both the cases (the mechanisms of [9–11]) should involve consideration both direct and reverse atom jump, and, considering that these mechanisms are studied with defects without the Burgers vector, the motion of these defects should result in the plastic deformation only when there is a stress gradient.

The dislocation flow in AMA within the heterogeneous deformation is conceived in the works [12,13]. In accordance with this model, the Burgers vector of Somigliana two-dimensional dislocations varies in a magnitude and direction along the dislocation line. However, the averaged Burgers vector has a value close to an average interatomic distance. The authors in [13] have suggested that the relaxed linear defects like the dislocations form arbitrary nets in AMA. The defects of this type can affect the low-temperature AMA properties and can be considered as carriers of the plastic deformation.

The works [14–18] have recently constructed a phenomenological description of amorphous plasticity based on physical principles and molecular models. As the usual thermal fluctuations are hardly probable for the temperatures below the glass transition temperature T_g, the configuration disorder state of the deformed system can be characterized by an effective disorder temperature T_{eff} which controls the configuration fluctuations [14]. The work [15] has reformulated the theory on plastic deformation in glass forming materials with STZ taking into account a role of the effective disorder temperature and the entropy flow. The work [16] is dedicated to non-equilibrium thermodynamics of amorphous materials and a role of internal degrees of freedom in the dynamics of such systems. The work [17] has developed the theory of the effective disorder temperature in glass-forming materials which equilibrium is disturbed by external forces. In order to reformulate the theory on the STZ amorphous plasticity, the work [18] has used the thermodynamics of the effective temperature with internal variables as developed in [16,17].

The main thesis of the theory in [14–18] is that the slow configuration degrees of freedom in the amorphous systems are weakly related to fast oscillation degrees of freedom, hence, these two subsystems can be described by various temperatures in the plastic deformation. The systems described by this theory include non-crystal solids at the temperature much less than their glass transition temperature T_g, dense grain materials and soft materials of various kinds, such as foams, colloids. It is caused by the fact that these materials have low thermal conductivity (thermal diffusivity), so the temperature can be localized in the plastic deformation area for the sufficient time. However, the amorphous metal alloys (due to presence of conductivity electrons) have high thermal diffusivity. In fact, for AMA the thermal diffusivity coefficient is of the order of $a \sim 10^{-6}\,\mathrm{m}^2\,\mathrm{s}^{-1}$ and the width of the glide band is of the order of $l \sim 10^{-8}\,\mathrm{m}$, so the time of temperature relaxation for this subsystem (l^2/a) is of the order of $10^{-10}\,\mathrm{s}$.

It is obvious that the physical mechanism of the plastic deformation process is determined by the deformation rate. Assuming that during the quasi-static single-axis deformation with $\dot{\varepsilon} = 3 \cdot 10^{-4}\,\mathrm{s}^{-1}$ the glide band completely passes across the whole width of the sample, we obtain a rate of motion of the glide band front $V \sim 10^{-4}\,\mathrm{m{\cdot}s}^{-1}$. In order to evaluate the time of an elementary event of plastic deformation, we divide the width of the glide band $l \sim 10^{-8}\,\mathrm{m}$ by the speed of motion of the glide band front $V = 10^{-4}\,\mathrm{m{\cdot}s}^{-1}$ to obtain the time of the elementary event of plastic deformation $l/V = 10^{-4}\,\mathrm{s}$. Hence, for the low deformation rates, when the time of the elementary event of plastic deformation is much bigger than the time of temperature relaxation $(l/V \gg l^2/a)$, the energy dissipation of the quasi-static plastic deformation does not result in substantial increase of the temperature within the glide band due to the high thermal diffusivity. Therefore, the control of plastic deformation only by the effective disorder temperature T_{eff} is insufficient in the metal amorphous alloys.

The plastic deformation of the crystal solid bodies is described by a suggested scale approach [19]. It is believed that the plastic deformation can develop as local structural transformation in areas of variously-scaled stress concentrators. The excessive free volume in these areas results in emergence of virtual points of a new structure in the interstice space. It results in undergoing local structural transformation by means of collective configuration excitations.

Due to insufficient experimental data on the AMA deformation it is difficult to distinguish the main mechanisms of deformation and to coherently describe its complexity (elastic, inelastic, plastic) and its space&time hierarchy. In order to develop the unified theory on AMA deformation, it is necessary to consider the relation of processes of macroscopic deformation to the nanostructural change of the structure.

The works [20,21] have recently formulated the physical mechanism and the microscopic mode of the inelastic deformation undergoing in the amorphous metal film, as stimulated by an external mechanical impact. This process is conditioned by nanostructural elements of the amorphous medium: nanoclusters with an additional free volume, which contain two-level systems. In glass deformation the two-level systems are excited, so that they significantly contribute to the inelastic deformation, the structural relaxation and the formation of nanoclusters and nanocrystals. Under mechanical impact, beside the mechanism of local thermal fluctuations, the physical mechanism of inelastic deformation of the metal glass also includes an athermal mechanism of quantum tunneling of atoms or atom groups, as stimulated by shear stress.

The analytically obtained results for the non-equilibrium phase transitions of the first kind have been verified by calculation modelling using the method of molecular dynamics [22–24]. The method of molecular dynamics can be used to directly compute various integral parameters of the entire modelled system or its separate parts. The ongoing state of the system and its changes have been analyzed by calculating the kinetic temperature. The study of the crystal-liquid phase transition and vice versa included calculation of the various structural characteristics which can be used to determine the beginning of the phase transition and its duration. In particular, calculation of an orientation parameter of the order makes it possible to distinguish the state of the liquid-crystal system. The results of [20–24] qualitatively and quantitatively describe relationships of non-equilibrium structural transformations in the amorphous metal alloys, as stimulate by the thermomechanical processing. It is planned to numerically illustrate the relation of kinetics of transitions by two parameters of the near- and mid-order to the kinetics of the relaxation equation for AMA's plastic deformation.

The present work is presented in an attempt to formulate the unified theory on plastic deformation: a hypothesis of physical nature, physical mechanisms, and a synergetic model of localized plastic deformation in the amorphous metal glasses, as stimulated by the quasi-static (low-rate) mechanical load.

The features of the low-temperature deformation [1–9] have been analyzed to show that a complex phenomenon (the localized plastic deformation) could be fully described based on conceptions about non-equilibrium structural transitions in self-organizing systems (the synergetics) [25] and it requires to solve the following tasks: 1) formulation and justification of the hypothesis on the physical nature of the AMA's quasi-static deformation; 2) the description of the mechanism and formulation of the kinetic model, which relate the near atom order to the mid atom order and describe nucleation and development of the STZ ensemble; 3) description of the mechanism of, and the formulation of the synergetic model of nucleation of the structural defect of a higher scale level — the glide band; 4) the description of the mechanism, the kinetic model of the autowave development of the glide band; 5) the findings and the conclusion. The tasks have governed formation of the structure of the work presented.

1. Formulation and justification of the hypothesis on the physical nature of quasi-static deformation

Based on the results and findings of the studies of [1–24], it is usable to formulate and justify the hypothesis on the physical nature of the AMA's quasi-static deformation. The AMA's quasi-static deformation is a complex relaxation multi-step process, which is a time-ordered hierarchial sequence of interrelated structural transitions of the first kind. These non-equilibrium processes consequently undergo at the various scaled space&time levels, starting from the lowest level — the cluster of the first nearest neighbours with the time of relaxation τ_η, then the mid level — the nanocluster of the fifth coordination sphere atoms with the relaxation time τ_φ, and, finally, the highest level — the atoms of the glide band with the space scale of 10 nm and the time of relaxation τ, whereas $\tau \gg \tau_\varphi \gg \tau_\eta$. They are accompanied by transformations of various kinds of the potential energy of atoms (the energy of elastic, inelastic, plastic deformation, ZST) into each other.

Let us consider the quasi-static single-axis deformation with $\dot{\varepsilon} = 3 \cdot 10^{-4}\,\text{s}^{-1}$, the loading time of $t_{\text{load}} = 100\,\text{s}$ for the AMA samples of 1 cm wide with the lengthwise elasticity (the Young's modulus) $E = 100\,\text{GPa}$. For the time $t_{\text{load}} = 100\,\text{s}$, the sample deformation reaches the value

$\varepsilon_3 = 3 \cdot 10^{-2}$, while the stress reaches the yield point $\sigma_3 = 3\,\text{GPa}$. It has been experimentally found that the propagation speed of the shear bands weakly depended on the deformation rate within the interval $2 \cdot 10^{-4}$–$10^{-2}\,\text{s}^{-1}$ [5]. The average propagation speed of the bands is very small is about $0.3\,\text{mm}\cdot\text{s}^{-1}$ [6].

Let us consider the solid sample of an amorphous metal alloy, which is initially in a non-equilibrium state of metal glass in a cubic form. Under single-axis tension, the sample is deformed to be shaped as a rectangular parallelepiped. During the deformation, the system gets the work $|A| = \int \sigma(\varepsilon)d\varepsilon$, which transforms into the potential energy of atoms U.

Let us evaluate the density of accumulated potential energy of deformation under the quasi-static single-axis deformation with $\dot{\varepsilon} = 3 \cdot 10^{-4}\,\text{s}^{-1}$, the loading time $t_{\text{load}} = 100\,\text{s}$ for the AMA sample of 1 cm wide with the lengthwise elasticity (the Young's modulus) $E = 100\,\text{GPa}$. For the time $t_{\text{load}} = 100\,\text{s}$, the sample deformation reaches the value $\varepsilon_3 = 3 \cdot 10^{-2}$, while the stress reaches the yield point $\sigma_3 = 3\,\text{GPa}$. Assuming that the glide band completely passes across the whole width of the sample, we obtain the rate of motion of the glide band front $V = 10^{-4}\,\text{m}\cdot\text{s}^{-1}$.

It is known that the density of the potential energy of the homogeneous longitudinal elastic deformation is $e = E\varepsilon^2/2$. When attaining the proportionality limit $\sigma_1 = E\varepsilon_1$ and the deformation $\varepsilon_1 = 1 \cdot 10^{-2}$, the density of the potential energy of the elastic deformation per one atomic volume (atom) is $v_{\text{el}} \sim 0.85 \cdot 10^{-3}\,\text{eV}$. The internal potential energy of the atomic system is increased by the value of the work done to the body. It is clear that v_{el} is much less than the kinetic energy of the atom $e_{\text{kin}} \sim 0.025\,\text{eV}$ per atom at the room temperature. During removal of external load, the sample is instantaneously (with the speed of sound) reshaped to its original form. That is, the systems does the work to the external medium and returns its elastic energy to it, whereas the potential energy of system atoms takes its original value. The elastic deformation is instantaneously reversible.

With the stress above the proportionality limit σ_1, but below the elastic limit $\sigma_2 = E\varepsilon_2$, $\varepsilon_2 = 2 \cdot 10^{-2}$, along with the elastic deformation the medium undergoes the structural transition of the first kind to form a new near order η oriented along the direction of the applied stress, i.e. the inelastic deformation occurs. In order to overcome the potential barrier between the states of the initial and new near order, it is necessary for the system to accumulate a critical value of the density of the potential energy of the elastic deformation $e_{\text{el}}(\sigma_1) = E\varepsilon_1^2/2$ ($v_{\text{el}} \sim 0.85 \cdot 10^{-3}\,\text{eV}$ per the atomic volume), and it also requires the loading time which exceeds the time of relaxation τ_η. The work done to the system is spent for increasing the internal potential energy: the elastic energy and the energy of inelastic deformation (of the new near order) $|A| = U_{\text{el}} + U_{\text{anel}}$. During removal of load, the samples is restoring its form, i.e. it instantaneously does the work to the external medium, which is equal to the elastic energy accumulated therein. The medium state is moving away from the equilibrium, as the internal structure has the new near order. The medium temporarily accumulates this energy of inelastic energy U_{anel}, but relaxes within a finite time. The inelastic deformation related to the new near η order is reversible, but is still delayed with the small time of relaxation τ_η.

With the stress below the elastic limit σ_2, along with the elastic deformation, the inelastic deformation of the first nearest neighbours, there is additional inelastic deformation of the atoms of nanoclusters with the average time of relaxation τ_φ. This deformation can be described by emergence of the mid order φ (or the STZ concentration — n, which accumulate the additional potential energy U_{def}). In order to overcome the potential barrier between the state with the new oriented near order η and the STZ state, it is necessary for the system to additionally accumulate the critical value of the density of the potential energy of the elastic deformation $e_{\text{el}}(\sigma_2) - e_{\text{el}}(\sigma_1) = E(\varphi_2^2 - \varphi_1^2)/2$,and it also requires the loading time which exceeds the time of relaxation τ_φ. At $\varphi_2 = 2 \cdot 10^{-2}$ the additionally accumulated energy is $v_{\text{el}} \sim 0.85 \cdot 10^{-3}\,\text{eV}$ per the atomic volume. The work done to the system is spent for increasing the internal potential energy: the elastic energy and the energy of inelastic deformation U_{anel}, the STZ energy $|A| = U_{\text{el}} + U_{\text{anel}} + U_{\text{def}}$. During removal of load, the samples is restoring its form, i.e. it instantaneously does the work to the external medium, which is equal to the elastic energy accumulated therein. The medium state is further moving away from the equilibrium, as along with the new oriented near order the internal structure additionally exhibit STZ'es. The medium temporarily accumulates the STZ energy U_{def} and relaxes within a finite time. The inelastic deformation related to STZ is reversible, but is delayed with the average time of relaxation τ_φ.

With increase of the stress to the elastic limit σ_3, along with elastic and inelastic deformation the sample is also subjected to the plastic deformation. The plastic deformation manifests itself in an irreversible change of the sample form (formation of the steps on the surface, which occurs when the glide plane is surfing). The work done to the system is accumulated as the potential energy of elastic deformation, the energy of inelastic deformation U_{anel}, the STZ energy U_{def} and the energy of the additional surface of the sample U_{pl} (the energy of plastic deformation). In order to overcome the potential barrier between the STZ state and the state of plastic deformation, it is required for the system to additionally accumulate the critical value of the density of the potential energy of inelastic deformation $e_{\text{el}}(\sigma_3) = E\sigma_3(\varepsilon_3 - \varepsilon_2)$, whereas the additionally accumulated energy is $v_{\text{el}} \sim 1.7 \cdot 10^{-3}\,\text{eV}$ per the atomic volume. During removal of load, the plastically deformed sample is restoring its form only partially. The energy of elastic deformation fully and instantaneously returns into the external medium. The energy of inelastic deformation U_{el} returns during the time of relaxation τ_η. The STZ potential energy of defects U_{def} only partially returns to the external medium during the time of relaxation τ_φ, as its remaining part transforms into the energy of plastic deformation U_{pl} (the additional energy of the surface). That is why the plastic deformation is irreversible and its time of relaxation τ is large.

Let us evaluate the increase of the local temperature within the glide band provided that the energy of plastic deformation has partially (20%) passed into heat. The work done to the system when attaining the elastic limit is of the order $v_{\text{el}} \sim 1.7 \cdot 10^{-3}$ eV per the atom, which is much smaller than the average kinetic energy of the atom at the glass transition temperature $v_{\text{kin}} \sim 5 \cdot 10^{-2}$ eV per the atom. Therefore, if the imparted energy is uniformly distributed across the system volume, then the increase of the system temperature is insignificant (approximately by $0.2 v_{\text{el}} \sim 0.34 \cdot 10^{-3}$ eV, i.e. by 5 K). But the energy of plastic deformation is heterogeneously distinguished in the glide bands. The width of the glide band is of the order of $l \sim 10^{-8}$ m, whereas the average distance between the glide planes is of the order of $l \sim 10^{-6}$ m. Therefore, the local increase of the temperature within the glide band is of the order of the glass transition temperature $\sim 100 \cdot 5 \sim 500$ K.

However, the amorphous metal alloys (due to presence of conductivity electrons) have high thermal diffusivity. In fact, for AMA the thermal diffusivity is of the order of $a \sim 10^{-6}\,\text{m}^2{\cdot}\text{s}^{-1}$ and the width of the glide band is of the order of $l \sim 10^{-8}$ m, so the time of temperature relaxation for this subsystem (l^2/a) is of the order of 10^{-10} s.

Assuming that during the quasi-static single-axis deformation with $\dot{\varepsilon} = 3 \cdot 10^{-4}\,\text{s}^{-1}$ the glide band completely passes across the whole width of the sample, we obtain a rate of motion of the glide band front $V \sim 10^{-4}\,\text{m}{\cdot}\text{s}^{-1}$. In order to evaluate the time of an elementary event of plastic deformation, we divide the width of the glide band $l \sim 10^{-8}$ m by the speed of motion of the glide band front $V = 10^{-4}\,\text{m}{\cdot}\text{s}^{-1}$ to obtain the time of the elementary event $l/V = 10^{-4}$ s.

Hence, for the low deformation rates, when the time of the elementary event of plastic deformation is much bigger than the time of temperature relaxation $(l/V \gg l^2/a)$, the energy dissipation of the quasi-static plastic deformation does not result in substantial increase of the temperature within the glide band due to the high thermal diffusivity.

It is obvious that the physical mechanism of the plastic deformation process is determined by the deformation rate. Therefore, it is possible to use the transformations only of the potential energy of the system atoms to qualitatively describe the process of the low-rate AMA's quasi-static deformation.

Thus, it is justly hypothesized that the AMA's quasi-static deformation is a complex multi-phase relaxation process, which is a time-ordered hierarchial sequence of interrelated structural transitions of the first kind at the various scaled space&time levels, which are accompanied by the transformations of the various kinds of the potential energy into each other. Based on this hypothesis, it is possible to construct the mathematical model of the AMA's quasi-static deformation.

2. Mechanism and model of the non-equilibrium transition „the elastic mechanical state–the state with the shear transformation zones“

The absence of long-range order in the mutual arrangement of atoms is a defining feature of amorphous bodies [1–3], so the description of their complex structure based on the conception of a long-range order parameter only, like for the crystals, is insufficient. It is experimentally found that the metal glasses with strong topological disorder often exhibit a rather perfect local order with accuracy to elastic distortions, coinciding with the local order in stable or metastable crystalline bodies of the same composition [1–3].

The spatial structure of the metal glass is formed of structural units, which are connected so as to avoid formation of the crystal structure, but elements of some order exist. The structural unit defines the near order (from a selected atom), has the radius of up to $\sim 3-5$ Å and includes about $1-1.5$ of the tetrahedron, whose vertices comprise the atoms [1–3].

The mid order means the radius from $\sim 3-5$ to 10 Å [1–3]. In this region the AMA atoms are slightly displaced in relation to the positions of the ideal crystal, but there is still correlation the positions of the atoms. At the distances above ~ 15 Å the displacements of the atoms in relation to the positions of the ideal crystal increase, the correlation in the atomic positions disappears, so there is no long-range order in AMA. The near- and mid-order is well defined from the experimental data and numerical calculations using the method of molecular dynamics [1–3,22–24]. The changes of the near- and mid-order well correlate to the changes of an atomic structure at the transitions of the various type [1–3,22–24].

When mechanically loaded, AMA is subjected to homogeneous inelastic deformation [1–3], which at an atomic level results in the anisotropic change of the distances between the atoms, i.e. to the change of the near- and mid-order.

In order to describe the relaxation of an amorphous structure from the elastic mechanical state into the inelastic state, let us introduce a dimensionless magnitude characterizing the structural state of the medium that is called the mid-order parameter η. Physically, the parameter of the order η is a volume fractions (normalized to the volume fraction of saturation) of inelastically-deformed atoms with the near order within a unit volume. In the elastic state the order parameter η is zero, while in the inelastic state the order parameter η is unity. The process of structural relaxation is viewed as a time sequence of the structural states of the medium described by the order parameter variation in time, i.e. $\eta = \eta(t)$ [26]. We assume that in terms of the parameter η the elastic state is locally stable, i.e. it is separated from the locally stable inelastic state by the energy barrier. The structural relaxation of the deformed non-equilibrium homogeneous structure from the elastic to inelastic state is described by the Landau-Khalatnikov equation [20,26,27] for the order parameter η:

$$\frac{\partial\eta}{\partial t} = -\alpha_\eta(T,\sigma)\eta(\eta-\eta_2)(\eta-1),\ \ \eta_2 = 1-\frac{E_{\text{el}}}{E^*_{\text{el}}}, \quad (1)$$

$$\alpha_\eta(T,A) = \omega_0\left[e^{-\frac{(E_\eta-\sigma V_\eta)}{kT}} + \Theta(\sigma-\sigma_1)e^{-\frac{a}{a_{dB}}}\right], \quad (2)$$

where $\alpha_\eta(T,\sigma)$ is the relaxation rate containing two terms of a different physical nature. The first, „thermal" one is related to the local thermal fluctuation of the first nearest neighbours from the initial near order (the elastic deformed one) to the new inelastically-deformed near order. The second „athermal" one is related to two-well potential's tunneling of the first nearest neighbours from the initial near order (the elastic deformed one) to the inelastically-deformed near order (as stimulated by the local stress). E_η — the energy of activation of atomic rearrangement, σ — the mechanical stress, V_η — the activation volume of the atomically-rearranged cluster. Here $a_{dB}(\sigma)$ — the de Broglie wavelength, a — the width of the potential barrier in the two-well potential [20,21], $\omega_0 \approx 10^{13}$ Hz. $\Theta(\sigma-\sigma_1)$ — the theta-function, which is non-zero when the value of the stress σ causes the inelastic deformation, σ_1 — the proportionality limit. $E_{\text{el}}(\sigma)$ — the density of the energy of elastic deformation, $E^*_{\text{el}}(\sigma_2)$ — the critical value of the energy density of elastic deformation, σ_2 — the elastic limit. In the poorly-deformed state of the medium $\frac{E_{\text{el}}}{E^*_{\text{el}}} \ll \frac{1}{2}$ the elastic state of the medium is globally stable, while the inelastic state of the medium is locally stable. When attaining the proportionality limit $\frac{E_{\text{el}}}{E^*_{\text{el}}} \approx \frac{1}{2}$ the elastic and the inelastic states of the medium are locally stable and they are around an indifferent equilibrium. When attaining the elastic limit $\frac{E_{\text{el}}}{E^*_{\text{el}}} = 1$ the elastic state of the medium becomes absolutely unstable, and the inelastic state of the medium is globally stable. If the density of the energy of elastic deformation attains the value E^*_{el}, and the time of mechanical impact exceeds the time of relaxation α_η^{-1}, then the medium completely relaxes to the inelastic state.

The classical phase transition of the first kind gas-liquid is implemented through the formation of a critical nucleus of a new phase directly in the initial phase [26,27]. However, the STZ formation within the volume of the amorphous phase is greatly hampered by additional factors. For example, the density of the STZ structure differs from that of the amorphous matrix, so the STZ formation requires taking into account the elastic stresses occurring in both the STZ and the amorphous structure. At the room temperature, the AMA are characterized by low mobility, thereby slowing down the STZ formation.

So, the elastic energy and other factors increase the energy of the STZ formation directly in the amorphous structure, and this heterogeneous state ceases to play the role of the activated complex for the structural transition of the first kind. Therefore, during the process of load-stimulated relaxation, the medium first passes to another homogeneous state (the inelastic state), which is a pre-transition state, from which the STZ state will be formed thereafter.

To describe the process of non-equilibrium transition of the first kind from the elastic state of the medium to the STZ state, let us introduce another dimensionless magnitude characterizing the structural state of the medium that is called the mid-order parameter φ. In case of the STZ state, the order parameter is selected to be the normalized volume fraction of the STZ-located atoms (normalized to the volume fraction of saturation) within a unit volume. In the elastic state the order parameter is zero, while in the STZ state the order parameter is unity. The process of structural transformation is viewed as a time sequence of the structural states of the medium described by the order parameter variation in time, i.e. $\varphi = \varphi(t)$. We assume that in terms of the parameter φ the elastic state is locally stable and it is separated from the locally stable STZ state by the energy barrier. In deformation, the structure first relaxes from the elastic to inelastic state in terms of the order parameter η, while the potential energy of local displacements of the first nearest neighbours is accumulated in the medium (the potential energy of inelastic deformation of the medium). Therefore, the energy barrier separating the elastic state and the STZ state in terms of the parameter φ decreases. If the density of the energy of elastic deformation attains the value E^*_{el}, and the tie of mechanical impact exceeds the time of relaxation α_η^{-1}, then the medium completely relaxes to the structure in the inelastic state. At $\eta \to 1$, the energy barrier in terms of the parameter φ becomes very small or even zero. The medium becomes unstable with respect to the STZ formation.

The structural relaxation of the deformed non-equilibrium amorphous medium from the elastic to the STZ state is described by the Landau–Khalatnikov equation [20,26,27] for the order parameter φ:

$$\frac{\partial\varphi}{\partial t} = -\alpha_\varphi(T,\sigma)\varphi(\varphi-\varphi_2)(\varphi-1),\ \ \varphi_2 = [1-\eta], \quad (3)$$

$$\alpha_\varphi(T,\sigma) = \omega_0\left[e^{-\frac{(E_\varphi-\sigma V_\varphi)}{kT}} + \Theta(\sigma-\sigma_1)e^{-\frac{a}{a_{dB}}}\right], \quad (4)$$

where $\alpha_\varphi(T,\sigma)$ is the relaxation rate containing two terms of a different physical nature. The first, „thermal" one is related to the local thermal fluctuation of the medium, while the second, „athermal" one is related to two-well potential's tunneling of the atom group, as stimulated by the local stress σ. E_φ — the energy of activation of STZ emergence, V_φ — the activation volume of the cluster atomically rearranged with the STZ formation. If the time of the mechanical impact exceeds the time of relaxation α_η^{-1}, the medium completely relaxes to the structure in the inelastic state $\eta \to 1$, while the energy barrier in terms of the parameter φ becomes zero and the STZ formation starts. If the time of mechanical impact exceeds the time of relaxation α_{φ}^{-1}, the medium completely relaxes to the STZ state.

As the formation of the STZ state is suppressed directly in the amorphous structure, then the non-equilibrium transition of the first kind has to pas through the pre-transition state — the inelastic state and is described by the two parameters (η, φ) obeying the equations (1), (3). From the inelastic state, the system enters the STZ state via a saddle point in the space of the coordinates of the structural transition (η, φ).

Let us construct a model potential of this phase transition $F(\eta, \varphi)$ in the space of the coordinates of the structural transition (η, φ). The analysis conducted (1), (3) shows that the transition with the two coordinates (η, φ) can be described by the following dependence of the model potential:

$$F(\eta, \varphi) = \frac{\eta_2}{2}\eta^2 - \frac{(1+\eta_2)}{3}\eta^3 + \frac{\eta^4}{4} + \frac{1}{2}\varphi_2\varphi^2 - \frac{(1+\varphi_2)}{3}\varphi^3 + \frac{\varphi^4}{4}, \tag{5}$$

$$\eta_2(E_{\mathrm{el}}) = 1 - \frac{E_{\mathrm{el}}}{E_{\mathrm{el}}^*}, \ \varphi_2(\eta) = 1 - \eta. \tag{6}$$

With $\frac{E_{\mathrm{el}}}{E_{\mathrm{el}}^*} = \frac{1}{2}$ and $\varphi = 0$ the potential $F(\eta, 0)$ — is double-well and symmetric. With $\eta = \frac{1}{2}$ and $\varphi_2(\frac{1}{2}) = \frac{1}{2}$, the potential $F(0, \varphi)$ — is double-well and symmetric.

Let us consider the transition only along the coordinate η, and $\varphi = 0$. Then the potential takes the form

$$F(\eta, 0) = \frac{\eta_2}{2}\eta^2 - \frac{(1+\eta_2)}{3}\eta^3 + \frac{\eta^4}{4}. \tag{7}$$

With the fixed parameter $0 < \eta_2 < \frac{1}{2}$, the function $F(\eta, 0)$ has two minimums $(\eta_1 = 0)$, $(\eta_3 = 1)$ and one maximum at $(\eta = \eta_2)$, whereas $F(0, 0) = 0$, $F(\eta_2, 0) = \frac{\eta_2^3}{6}(1 - \frac{\eta_2}{2})$, $F(1, 0) = -\frac{(1-2\eta_2)}{12}$, i.e. $F(1, 0) < F(0, 0)$. Thus, using the potential $F(\eta, 0)$ makes it possible to describe the structural transformation of the first kind from the elastic state $(\eta_1 = 0)$ to the inelastic state $(\eta_3 = 1)$ through the potential barrier of the height $F(\eta_2, 0)$.

Let us consider the transition only along the coordinate φ, and $\eta = 0$. With the fixed parameter $0 < \eta_2 < \frac{1}{2}$ the function $F(0, \varphi)$ has one minimum $(\varphi_1 = 0)$ and an inflection point $(\varphi_2 = \varphi_3 = 1)$, whereas $F(0, 0) = 0$, $F(0, \varphi_2 = 1) = \frac{\varphi_2^3}{6}(1 - \frac{\varphi_2}{2}) = \frac{1}{12}$, $F(0, 1) = -\frac{(1-2\varphi_2)}{12} = \frac{1}{12}$, i.e. $F(0, 1) > F(0, 0)$. Thus, it follows from the form of the potential $F(0, \varphi)$ that the direct structural transformation of the first kind from the elastic state $(\varphi_1 = 0)$ to the STZ state $(\varphi_3 = 1)$ is impossible.

With the fixed parameter $0 < \eta_2 < \frac{1}{2}$ the function $F(\eta, \varphi)$ within the area of determination of the variables $0 \leq \eta \leq 1$, $0 < \varphi < 1$ has nine special points: the four minimums $(0, 0), (1, 0), (0, 1), (1, 1)$; one maximum $(\eta_2, 1 - \eta_2)$; and the four saddle points $(\eta_2, 0), (\eta_2, 1 - \eta_2), (0, 1 - \eta_2), (1, 1 - \eta_2)$. The potential $F(\eta, \varphi)$ in the points of minimum takes the following values: $F(0, 0) = 0$, $F(1, 0) = -\frac{(1-2\eta_2)}{12}$, $F(0, 1) = \frac{1}{12}$, $F(1, 1) = -\frac{1}{6}(1 - \eta_2)$. It is obvious that the global minimum is in the state $(1, 1)$.

When attaining $\eta = 1$,the function $F(1, \varphi)$ has one inflection point $(\varphi_1 = \varphi_2 = 0)$ and the point of minimum $(1, 1)$. The potential barrier separating the elastic state $(\varphi_1 = 0)$ and the STZ state $(\varphi_3 = 1)$ disappears.

With the fixed small deviation η from zero, it is possible to leave the initial state $(\eta, 0)$ and to directly enter the final state $(\eta, 1)$, whereas it has to overcome the quite large barrier (almost equal to the maximum), which separates these states. This is a classical mechanism of the structural transition of the first kind.

In the direct transformation „the elastic state–the STZ state“, the transition barrier is too large due to the elastic energy of the STZ formation. But it is possible to make a transition over the pre-transition state $(\eta \to 1, 0)$. In this state $\varphi_2 = [1 - \eta]$ tends to zero, therefore the barrier to be overcome to get to the STZ state tends to zero as well. It is much more beneficial to first make a transition along the coordinate η from 0 to 1, thereby resulting in a sharp decrease of the barrier along the coordinate φ. And only afterwards to make the transition along the coordinate φ from 0 to 1.

Now, it is possible to construct the synergetic model of the localized plastic deformation (formation of the shear band, the new higher structural level of deformation), in which the mid order φ or, which is the same, the STZ concentration (the number of the areas within a unit volume) n plays the role of a control parameter.

3. Mechanism and synergetic model of the localized plastic deformation in the amorphous metal glass

The relaxation behavior of the deformed amorphous metal glass can be described within a linear model of the viscoelastic medium [28]. The evolution of the deformation ε under the constant stress σ is described by the Kelvin–Voigt equation, which can be integrated

$$\frac{\partial \varepsilon}{\partial t} = -\frac{1}{\tau}\varepsilon + \frac{\sigma}{\eta} = \frac{1}{\eta}\left[-\mu\varepsilon + \sigma\right],$$

$$\varepsilon(t) = \frac{\sigma}{\mu}\left[1 - \exp\left(-\frac{t}{\tau}\right)\right], \ \mu = \frac{\eta}{\tau}. \tag{8}$$

Here, the first summand characterizes the relaxation of the shear component of deformation in time τ, the second one — the flow of the viscous liquid under impact of the shear component of the stresses σ, η — the dynamic shear viscosity, μ — the shear modulus.

During system unloading, when the stress σ is zero, the equation (8) is integrated to output an expression for deformation relaxation

$$\varepsilon(t) = \varepsilon(0)\exp\Big(-\frac{t}{\tau}\Big). \tag{9}$$

Thus, the linear model of the viscoelastic medium (8) predicts a deformation nature which is undergoing in time, i.e. relaxing. As ε relaxes to zero, the deformation obtained is reversible in time, hence, it is not plastic. It is caused by the fact that the shear stress in included in the deformation relaxation equation as an external constant parameter. The phenomenon of plastic deformation is complex, so the process of transition of the mode of inelastic deformation to the mode of plastic deformation is ensured by self-organization of the shear component of deformation, the shear component of stresses on the one hand and STZ on the other hand.

Let us formulate the synergetic model of plastic deformation (formation and propagation of the glide band), in which the STZ concentration n plays the role of the control parameter [25].

The change rate of the control parameter n is specified, on the one hand, by the intensity of dissipation processes characterized by the time of relaxationτ_n, so is on the other hand by impact of the collective mode, which is determined by its amplitude ε and the conjugate field σ:

$$\dot{n} = -\frac{1}{\tau_n}(n - n_e) - g_n\varepsilon\sigma, \tag{10}$$

where $n_e = n_e(T, \hat{\sigma}_{\text{ext}})$ — the equilibrium value n specified by the external conditions, $\hat{\sigma}_{\text{ext}}$ — the tensor of external stresses, g_n — the coupling constant, T — the temperature. The last summand in (10) describes the decrease of the concentration n during plastic deformation in the stress field.

Due to the viscous friction in the medium, the shear stress obeys the relaxation equation

$$\dot{\sigma} = -\frac{1}{\tau_\sigma}\sigma + g_\sigma\varepsilon n, \tag{11}$$

where τ_σ, g_σ — the constants. The first summand in (11) describes the process of relaxation of the shear stress to the equilibrium value $\sigma = 0$. The second summand in (11) takes into account a positive feedback between the shear deformation and STZ, which results in the rise of the shear stress and, thus, it causes the self-organization process.

The order parameter is selected to be a value of the shear plastic deformation ε, while the conjugate field is selected to be a shear component of the tensor of stresses σ.The equation defining the behavior of the collective mode ε is reduced to the Kelvin–Voigt equation for the viscoelastic medium (8). Thus, in the simplest case the change rates of the magnitudes ε, σ, n are described by the Lorentz system (8), (10), (11) [25].

The obtained system is featured by a linear character of the equation (8) for the change rate of the order parameter ε and non-linearity of the equations (10), (11) for the values n, σ, whose change obeys the behavior of ε. The negative nature of the non-linear coupling in the equation (10) means reduction of the concentration n when the collective mode ε increases. Accordingly, the non-linear summand in the equation (11) describes the positive feedback, which is exactly the reason resulting in the qualitative rearrangement of the system as a result of the self organization in the STZ ensemble.

The said equalities form the full system of the equations, which determined a self-consistent behavior of the collective mode of plastic deformation and STZ. The dissipation nature of plastic deformation is implemented at the ratio of the relaxation times $\tau_\sigma, \tau_n \ll \tau$, which governs that the slow order parameter $\varepsilon(t)$ „dominates“ the fast magnitudes $\sigma(t), n(t)$. Then, the equations (10), (11) can use an adiabatic approximation $\dot{n} = 0$, $\dot{\sigma} = 0$. As a result, the magnitudes σ, n are expressed through ε as follows:

$$n = n_e\left[1 + \Big(\frac{\varepsilon}{\varepsilon_m}\Big)^2\right]^{-1}, \ \varepsilon_m^{-2} = A_nA_\sigma,$$

$$A_n = \tau_n g_n, \ A_\sigma = \tau_\sigma g_\sigma, \ \sigma = A_\sigma n_e\varepsilon\left[1 + \Big(\frac{\varepsilon}{\varepsilon_m}\Big)^2\right]^{-1}. \tag{12}$$

Taking into account that in the stationary state $\dot{\varepsilon} = 0$ the equality (12) in the limit $(\varepsilon^2 \ll \varepsilon_m^2)$ must pass in the Hooke's law $\sigma = \mu\varepsilon$, we obtain the critical value of the parameter n_c:

$$n_c^{-1} = \frac{A_\sigma}{\mu} = \tau\tau_\sigma\frac{g_\sigma}{\eta}. \tag{13}$$

The time dependence of the order parameter $\varepsilon(t)$ is determined by the Landau–Khalatnikov relaxation equation [26,27]

$$\tau\dot{\varepsilon}(t) = -\frac{\partial V}{\partial\varepsilon}, \tag{14}$$

where the synergetic potential V in the dependence on the order parameter $\varepsilon(t)$ is determined by inserting the equalities (12) into the evolution equation (8). With the constant values of τ, η the dependence V in the limit $(\varepsilon^2 \ll \varepsilon_m^2)$ is reduced to the Landau expansion [26]:

$$V(\varepsilon) = \frac{A}{2}\varepsilon^2 + \frac{B}{4}\varepsilon^4, \ A = 1 - \frac{n_e}{n_c}, \ B = \varepsilon_m^{-2} = A_nA_\sigma. \tag{15}$$

As per (14), (15), the nature of the stationary state conforming to the condition $\frac{\partial V}{\partial\varepsilon} = 0$ is determined by a ratio between the value of the parameter n_e as specified by the external states and the critical value n_c determined by the equality (13). In the sub-critical mode $n_e < n_c$ we have the stationary values $\varepsilon_0 = \sigma_0 = 0$, and there is no plastic deformation. In case of $n_e > n_c$, when in the dependence (15) the parameter $A < 0$, the synergetic potential $V(\varepsilon)$ has the minimum $\varepsilon_0 = (\frac{|A|}{B})^{\frac{1}{2}}$, and the system spontaneously passes into the excited state with plastic deformation ε_0:

$$\varepsilon_0 = \varepsilon_m\sqrt{\frac{n_e}{n_c} - 1},$$

$$\sigma_0 = \mu\varepsilon_m\sqrt{\frac{n_e}{n_c} - 1}, \ n_e = n_c, \quad \text{at} \ n_e > n_c. \tag{16}$$

It is clear that the increase of ε results in the decrease of n and the increase of σ as per the dependence (16) looking like the Hooke at $\varepsilon \gg \varepsilon_m$ and outputting to saturation when reaching the limit degree of plastic deformation ε_m. In this regard, we can say that the transition of the system to the excited state as defined by the spontaneous plastic deformation $\varepsilon \neq 0$ results in transformation of a part of the STZ potential energy to the work done by the shear stress component $\varepsilon\sigma$.

At the low loads σ_{ext}, when $n_e(\sigma_{\text{ext}}, T)$ is below the critical value n_c, the STZ concentration is so small that there no collective coupling (interaction) therebetween. $V(\varepsilon)$ (15) is monotonically increasing and the system is relaxing to the stationary values $\varepsilon_0 = \sigma_0 = 0, \ n = n_e$. With the increase of the load σ_{ext} the condition $n_e > n_c$ is ensured, there is attraction appearing between the STZes and the STZ condensate is formed — a new structural state of the medium with plastic deformation. $V(\varepsilon)$ (15) gets the minimum in the point $\varepsilon_0 = \varepsilon_m\sqrt{\frac{n_e}{n_c} - 1}$, which corresponds to the stationary value of plastic deformation, which occurs at the new scaled (structural) level (the formation of the glide plane). As per (16), the time of formation of this new structural level of deformation $\tilde{\tau}$ and the value of partial viscosity $\eta(\tilde{\tau}) = \mu\tilde{\tau}$ defined thereby look as follows

$$\tilde{\tau} = \tau\left[\frac{n_e}{n_c} - 1\right]^{-1}, \ \eta(\tilde{\tau}) = \eta\left[\frac{n_e}{n_c} - 1\right]^{-1}, \ \eta = \mu\tau. \tag{17}$$

As the viscosity is determined by the equality $\eta^{-1} = \frac{\partial\dot{\varepsilon}}{\partial\sigma}$ and the include of the new structural level of deformation results in contribution of $\dot{\varepsilon} = \frac{\varepsilon_m}{\tau}$ to the rate of plastic deformation, then the effective viscosity is $\eta_{\text{eff}}^{-1} = \eta^{-1} + \eta(\tilde{\tau})^{-1}$. Taking into account (17), at $n_e > n_c$ we obtain therefrom: $\eta_{\text{eff}} = \frac{n_c}{n_e}\eta < \eta$, i.e. the formation of the new structural level of deformation reduces the effective viscosity of the medium.

Above, we have considered the plastic deformation as continuous non-equilibrium structural transformation. But in reality it proceeds as per the mechanism of the first kind [1,2]. For this we will take into account a non-linear nature of the dissipation process, which includes reduction of the shear modulus $\mu(\varepsilon)$ with increase of the plastic deformation. It is convenient to use the simplest approximation:

$$\mu(\varepsilon) = \frac{\mu}{1 + (\frac{\varepsilon}{\varepsilon_\tau})}, \tag{18}$$

where the positive parameter ε_τ determines a characteristic scale of the plastic deformation at which the dispersion exhibits. At the same time, the dependence $V(\varepsilon)$ exhibits a barrier separating the initial and the new stationary state, which characterizes the transitions of the first kind [25]. As a result, the synergetic potential (15) and the relaxation equation (14) look as follows:

$$V(\varepsilon) = \left(1 - \frac{n_e}{n_c}\right)\frac{\varepsilon^2}{2} - \frac{1}{\varepsilon_\tau}\frac{\varepsilon^3}{3} + \left(\frac{1}{\varepsilon_\tau^2} - \frac{n_e}{n_c\varepsilon_m^2}\right)\frac{\varepsilon^4}{4},$$

$$\tau\dot{\varepsilon}(t) = -\frac{\partial V(\varepsilon)}{\partial\varepsilon} = -(\varepsilon - \varepsilon_1)(\varepsilon - \varepsilon_2)(\varepsilon - \varepsilon_3), \tag{19}$$

$$\varepsilon_1 = 0, \ \varepsilon_2 = \frac{\frac{1}{\varepsilon_\tau} - \sqrt{D}}{2\left(\frac{1}{\varepsilon_\tau^2} + \frac{n_e}{n_c\varepsilon_m^2}\right)}, \ \varepsilon_3 = \frac{\frac{1}{\varepsilon_\tau} + \sqrt{D}}{2\left(\frac{1}{\varepsilon_\tau^2} + \frac{n_e}{n_c\varepsilon_m^2}\right)},$$

$$D = \frac{1}{\varepsilon_\tau^2} - 4\left(1 - \frac{n_e}{n_c}\right)\left(\frac{1}{\varepsilon_\tau^2} + \frac{n_e}{n_c\varepsilon_m^2}\right). \tag{20}$$

It is clear from (19), (20) that at the small n_e the discriminant $D(n_e) < 0$, so there is only one physical stable state with the plastic deformation $\varepsilon_1 = 0$, the complex roots $\varepsilon_2, \varepsilon_3$ — non-physical. When attaining the critical value $n_e = n_c^*$ (the discriminant $D(n_e^*) = 0$) the physical state with the plastic deformation $\varepsilon_1 = 0$ is still absolutely stable, but the physical (noncomplex) roots $\varepsilon_2, \varepsilon_3$ appear:

$$\varepsilon_2 = \varepsilon_3 = \left[2\varepsilon_\tau\left(\frac{1}{\varepsilon_\tau^2} + \frac{n_e}{n_c\varepsilon_m^2}\right)\right]^{-1}, \ n_c^* \simeq \frac{7}{8}n_c, \tag{21}$$

whereas the new physical state with non-zero plastic deformation $\varepsilon_2 = \varepsilon_3$ is absolutely unstable. With further increase of n_e, it is clear from (20),(21) that the root ε_2 decreases and starts tending to the root $\varepsilon_1 = 0$. When attaining the supercritical value $n_e = n_c$, the discriminant $D(n_c) = \frac{1}{\varepsilon_\tau^2}$, and the physical state with the plastic deformation $\varepsilon_1 = 0$ becomes absolutely unstable.

$$\varepsilon_1 = \varepsilon_2 = 0, \ \varepsilon_3 = \left[\varepsilon_\tau\left(\frac{1}{\varepsilon_\tau^2} + \frac{1}{\varepsilon_m^2}\right)\right]^{-1}, \ n_c = \frac{\mu}{A_\sigma}. \tag{22}$$

The new physical state with non-physical ε_3 becomes absolutely stable.

In other words, if the parameter n_e does not exceed the critical value n_c^*, then $V(\varepsilon)$ is of a monotonically increasing nature. At $n_e = n_c^*$ the plateau appears to be transformed to a minimum with increase of n_e. The state with plastic deformation becomes synergetically beneficial starting from the value $n_e = n_{**}$, at which the condition $V(0) = V(\varepsilon_3)$ is attained to ensure the equality of the potential values without deformation $\varepsilon = 0$ and at the stationary value $\varepsilon = \varepsilon_3$. When attaining the supercritical value n_c, the barrier separating the states $\varepsilon = 0$ and $\varepsilon = \varepsilon_3$, disappears and $V(\varepsilon)$ takes the form inherent to the transitions of the second kind.

Let us discuss some important properties of the deformed medium. It is non-linear which is manifested by a complex nature of the dependence „stress–deformation“ [1,2]. During loading the deformed medium changes its structure, i.e. it is structurally unstable [20,25], for example, in relation to the STZ formation. The deformed medium is active [20,25], as it contains local sources of potential energy and shear (STZ), which are distributed across the volume. As per conceptions of the nature of self organization in open systems [25], such an active non-linear structurally-unstable medium can generate autowave processes.

The medium non-linearity results in emergence of non-uniqueness of stationary homogeneous solutions of the relaxation equation of plastic deformation (the deformation modes). In the transition region $n_c^* > n > n_c$, the distributed system can originate a running autowave [25], which transfers the sample from one (inelastic) mode of deformation to another (plastic) one.

The heterogeneity of the amorphous medium results in heterogeneous STZ distribution, so in some area of the sample surface the STZ concentration can become above the critical one n_c^*. The STZes start interacting, attracting and, finally, condense to a nucleus of the new structure with plastic deformation. It is followed by an undergoing relay process of propagation of plastic deformation along a direction of maximum tangential stress (propagation of the shear band) selected along the direction of the axis x, which obeys the autowave equation [25]:

$$\dot{\varepsilon}(t) = -\frac{1}{\tau}(\varepsilon - \varepsilon_1)(\varepsilon - \varepsilon_2)(\varepsilon - \varepsilon_3) + D\frac{\partial^2 \varepsilon}{\partial x^2}, \tag{23}$$

where D — the mobility coefficient of plastic deformation.

For the initial conditions, let us set a deformation profile changing in some arbitrary point of the X by hopping from $\varepsilon_1 = 0$ to ε_3. During the transition period, the initial profile will be rearranged to become a stationary front of the wave propagating along the axis x with the constant speed V. The coordinate system related to the moving front of the wave from right to left will have the equation (23) of the autowave propagation process as follows:

$$D\frac{d^2\varepsilon}{dx^2} - V\frac{d\varepsilon}{dx} + \Phi(\varepsilon) = 0,$$

$$\Phi(\varepsilon) = -\frac{1}{\tau}(\varepsilon - \varepsilon_1)(\varepsilon - \varepsilon_2)(\varepsilon - \varepsilon_3). \tag{24}$$

Here $\varepsilon(x)$ — the deformation, x — the coordinate along the axis x, V — the linear speed of movement of deformation modes. The boundary conditions will be specified as

$$\varepsilon(+\infty) = \varepsilon_3,\ \ \varepsilon(-\infty) = \varepsilon_1. \tag{25}$$

Here, ε_1 and ε_3 — stationary deformations of the samples, which correspond to the mode with inelastic deformation and plastic deformation, respectively. The problem is solved by finding the value V, which is an eigenvalue of the equation (24), (25), which corresponds to the stationary solution of the autowave equation.

The autowave speed can be obtained by inserting to reduce the order of the equation (24), (25) and integrating within the limits from ε_1 to ε_3:

$$V = \left[\int\limits_{\varepsilon_1}^{\varepsilon_3} \Phi(\varepsilon)d\varepsilon\right]\left[\int\limits_{\varepsilon_1}^{\varepsilon_3} P(\varepsilon)d\varepsilon\right]^{-1},\ P(\varepsilon) = \frac{d\varepsilon}{dx}. \tag{26}$$

This expression can not exactly calculate V until solving the equations (24), (25) and finding the function $P(\varepsilon)$. But the expression (26) describes the main qualitative relationships of the phenomenon we are considering. The function $P(\varepsilon)$ has a constant plus sign across the entire width of the front, so the expression (26) provides the information about the direction of the wave motion (i.e. about the sign of V). Furthermore, the expression(26) can also be used to determine a condition at which the direction of this motion can change. If the integral $\int_{\varepsilon_1}^{\varepsilon_3} \Phi(\varepsilon)d\varepsilon > 0$, then the wave moves towards the filling the sample with the mode of the plastic deformation ε_3. The equality $\int_{\varepsilon_1}^{\varepsilon_3} \Phi(\varepsilon)d\varepsilon = 0$ is a critical condition of a changed direction of the front motion, at which the speed of wave propagation becomes zero. This condition corresponds to the stationary state of the system, at which the sample can stably and stationarily have coexisting areas with plastic deformation and inelastic deformation. There is a critical value of the concentration n_{**}, at which the speed of autowave motion is zero. The medium part subjected to the non-equilibrium transition to the state with the plastic deformation (formation and propagation of the glide band) is a quasi-static structural defect of the new scaled level with large time of relaxation. The plastic deformation is irreversible, so the autowave front can not propagate toward the opposite side.

Using a specific form of $\Phi(\varepsilon)$ (24), we obtain the expression for $\frac{d\varepsilon}{dx}$:

$$\frac{d\varepsilon}{dx} = \sqrt{\frac{1}{2D\tau}}(\varepsilon_3 - \varepsilon)(\varepsilon - \varepsilon_1). \tag{27}$$

Using (27), we obtain the expression for the wave speed V:

$$V = \sqrt{2\frac{D}{\tau}}\left(\frac{[\varepsilon_3 + \varepsilon_1]}{2} - \varepsilon_2\right). \tag{28}$$

It is clear from (28) that the speed of autowave propagation of the plastic deformation is proportional to the square root of the product of the mobility coefficient to the inverse time of relaxation of plastic deformation.

The width of the autowave front can be determined as the ratio of the maximum drop of plastic deformation to the maximum gradient of deformations $P_{\max}$ at the front

$$\delta = \frac{(\varepsilon_3 - \varepsilon_1)}{P_{\max}\sqrt{2D\tau}\,\frac{1}{(\varepsilon_3 - \varepsilon_1)}}. \tag{29}$$

Thus, the width of the front is proportional to the square root of the product of the mobility coefficient to the time of relaxation of plastic deformation.

Then, the equation (24) is solved by as follows:

$$\varepsilon(x) = \left[\varepsilon_3 + \varepsilon_1 \exp\left(\frac{4x}{\delta}\right)\right]\left[1 + \exp\left(\frac{4x}{\delta}\right)\right]^{-1}. \tag{30}$$

It follows from (30) that the deformation profile is symmetrical and $P_{\max}$ corresponds to the value of deformation equal to $\frac{[\varepsilon_3+\varepsilon_1]}{2}$. It should be noted that as δ, V, ε_3 are macro-magnitudes which can be measured experimentally, then the relationships (28), (29) provide a means of calculating the mobility coefficient, the time of relaxation and the maximum gradient of plastic deformation, which are important physical properties of the plastic deformation. The characteristic experimental values are $\delta \sim l \sim 10^{-8}\,\mathrm{m}$, $V \sim 10^{-4}\,\mathrm{m{\cdot}s^{-1}}$, $\varepsilon_3 \sim 10^{-2}$ [1,2,5,6], then it is possible to use (28), (29) to calculate $\tau \sim 10^{-8}\,\mathrm{s}$, $D \sim 10^{-12}\,\mathrm{m^2{\cdot}s^{-1}}$, $P6_{\max}\,\mathrm{m}^{-1}$.

Thus, the process of formation (on the free surface), progression and surfacing of the shear band to another free surface of the sample is a process of nucleation and propagation of the autowave of the plastic deformation.

4. Findings and conclusion

The results obtained in Sections 2–4 can be used to make the following conclusions:

– the AMA's quasi-static deformation is a complex relaxation multi-step process, which is a time-ordered hierarchial sequence of interrelated structural transitions of the first kind. These non-equilibrium processes consequently undergo at the various scaled – space&time levels, starting from the lowest level — the cluster of the first nearest neighbours with the time of relaxation τ_η, then the mid level — the nanocluster of the fifth coordination sphere atoms with the relaxation time τ_φ, and, finally, the highest level — the atoms of the glide band with the space scale of 10 nm and the time of relaxation τ, whereas $\tau \gg \tau_\varphi \gg \tau_\eta$;

– when stressing from the proportionality limit to the elastic limit, the process of formation of the STZ state directly in the amorphous structure is suppressed, as the elastic energy and other factors substantially increase the energy of STZ formation.

– the non-equilibrium structural transition of the first kind from the elastic state to the STZ state undergoes through the pre-transition state (the inelastic state) and is described by the two parameters: of the near order and the mid order, which obey the related Landau-Khalatnikov relaxation equations;

– the relaxation rate contains two terms of a different physical nature. The first, „thermal" is related to local thermal fluctuation of the cluster atoms from the elastic deformed state to the new state with inelastic deformation. The second, „athermal" is related to two-well – potential's tunneling (as stimulated by the local stress) of the cluster atoms from the elastic deformed state to the new state with inelastic deformation;

– the physical cause and the condition of instability of the state with the initial near order in relation of transition to the STZ state is accumulation of the density of potential energy of elastic deformation to the critical value of $\upsilon_{\mathrm{el}} \sim 1.7 \cdot 10^{-3}\,\mathrm{eV}$ per the atomic volume, and it also requires the loading time which exceeds the time of relaxation of the mid order;

– when stressing from the elastic limit to the yield point, the process of formation of the STZ state directly in the amorphous structure is suppressed, as the elastic energy and other factors substantially increase the energy of its formation;

– the non-equilibrium structural transition of the first kind from the STZ state to the state of plastic deformation is ensured by self organization of the shear component of deformations, the shear component of stresses, on the one hand, and STZ, on the other hand, and described by the system of the Lorentz equations;

– if during load increase the STZ concentration exceeds the critical value, the behavior of the STZes exhibits collective effects (attraction interaction), and they can condense;

– due to attraction of the STZes with accumulated potential energy, an elementary shear and excessive free volume, a condensed nucleus of plastic deformation is forming. The collective mode of plastic deformation spontaneously occurs to result in a „plastic" addition to the initial value of the elastic and inelastic deformation;

– a new structure level of deformation appears, i.e. macroscopic plastic deformation. At the same time, the collective component is added to the initial shear stress, and the STZ concentration decreases. With increase of the value of plastic deformation, the shear stress and the time of relaxation of the new structural level of deformation increase, while the STZ concentration and the effective viscosity of the medium decrease;

– the physical cause and the condition of instability of the STZ state in relation of transition to the state of plastic deformation is additional accumulation of the density of potential energy of inelastic deformation (the STZ energy) to the critical value of $\upsilon_{\mathrm{el}} \sim 1.7 \cdot 10^{-3}\,\mathrm{eV}$ per the atomic volume, and it also requires the loading time which exceeds the time of relaxation of plastic deformation;

– as the AMA is a heterogeneous medium [1,2], then the STZes are characterized by non-homogeneous distribution. It results in localization of establishment of the collective coupling (attraction) in the STZ ensemble and in autolocalized formation– the autowave. Its nucleation and propagation forms a structural defect (the glide band) at the higher scaled – space&time level [1,2];

– only the structurally unstable, active non-linear medium can generate autowave processes. During loading the AMA medium changes its structure, i.e. it is structurally unstable in relation to the STZ formation. The deformed AMA medium is active, as it contains local sources of potential energy, shear and excessive free volume (i.e. STZes), which are distributes across the volume. The AMA medium non-linearity results in emergence of non-uniqueness of stationary homogeneous solutions of the relaxation equation of plastic deformation.

The theoretical consideration has been carried out to disclose an autowave nature of the effect of plastic deformation and to analytically calculate the speed of propagation of the autowave of switching from the mode of inelastic deformation to the mode with plastic deformation. In response to the locally imparted disturbance, the interval of non-uniqueness originates the running autowave forming the glide band. As the experimental value of the front width $\delta \sim l \sim 10^{-8}\,\mathrm{m}$, the front speed, $V \sim 10^{-4}\,\mathrm{m{\cdot}s^{-1}}$, plastic deformation$\varepsilon_3 \sim 10^{-2}$ are determined [1,2,5,6], then it is possible to calculate the important physical properties of the plastic deformation: the time of relaxation $\tau \sim 10^{-8}\,\mathrm{s}$, the mobility coefficient $D \sim 10^{-12}\,\mathrm{m^2{\cdot}s^{-1}}$, the maximum gradient $P6_{\max}\,\mathrm{m}^{-1}$.

Thus, the proposed hypothesis, the kinetic and synergetic models can formulate the physical picture, cause, condition, macroscopic mechanism of the quasi-static inelastic and plastic deformation as the complex relaxation multi-step process, which is the time-ordered hierarchial sequence of interrelated structural transitions of the first kind. They explain the localized nature of the plastic deformation appearing in AMA and qualitatively and quantitatively describe the results and the relationships obtained experimentally [1–9]. The space&time structures (autowaves) of localization of microscopically-scaled deformation, which originate in the sample at this time, are spontaneously generated in deformation with the low constant speed. During the plastic deformation, the deformed medium is spontaneously delaminated into small (in terms of the width of the glide plane) and large (in terms of the width) plastically undeformed areas between the glide planes.

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Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] K. Sudzuki, K. Khudzimori, K. Khasimoto. *Amorfnye Metally* (Metallurgiya, M., 1987), 328 p. (in Russian).

[2] A.M. Glezer, N.A. Shurygina. *Amorfno-nanokristallicheskiye splavy* (Fizmatlit, M., 2013), 452 p. (in Russian).

[3] G.E. Abrosimova. UFN, **181**, 1265–1281 (2011) (in Russian). DOI: 10.3367/UFNr.0181.201112b.1265

[4] F. Spaepen. In: *Houches Lectures XXXV on Physics of Defects* (North Holland Press, Amsterdam, 1981), p. 133–174.

[5] G. Neikhauzer, R.P. Shtossel'. V sb.: *Bystrozakalennye metallicheskie splavy*, pod red. S. Shtiba, G. Varlimonta (Metallurgiya, M., 1989), p. 247–252 (in Russian).

[6] F. Spaepen. Acta Metall., **25**, 407–415 (1977). DOI: 10.1016/0001-6160(77)90232-2

[7] M. Stoica, J. Das, J. Bednarcik, H. Franz, N. Mattern, W.H. Wang, J. Eckert. J. Appl. Phys., **104**, 0135222008. DOI: 10.1063/1.2952034

[8] G.E. Abrosimova, A.S. Aronin, N.S. Afonikova, N.P. Kobelev. FTT, **52** (9), 1763–1768 (2010) (in Russian).

[9] T.C. Hafnagel, J.A. Wert, J. Almer. Phys. Rev. B, **73** (6), 064204 (2006). DOI: 10.1103/PhysRevB.73.064204

[10] A.S. Argon, H.Y. Kuo. Mater. Sci. Eng. A, **39** (1), 101–109 (1979). DOI: 10.1016/0025-5416(79)90174-5

[11] D.E. Polk, D. Turnbull. Acta Metall., **20**, 493–498 (1972). DOI: 10.1016/0001-6160(72)90004-1

[12] J.J. Gilman. J. Appl. Phys., **46**, 1625–1633 (1975). DOI: 10.1063/1.321764

[13] M.F. Ashby, J. Logan. Scripta Met., **7**, 513 (1973). DOI: 10.1016/0036-9748(73)90105-1

[14] E. Bouchbinder. Phys. Rev. E, **77**, 051505 (2008). DOI: 10.1103/PhysRevE.77.051505

[15] J.S. Langer. Phys. Rev. E, **77**, 021502 (2008). DOI: 10.1103/PhysRevE.77.021502

[16] E. Bouchbinder, J.S. Langer. Phys. Rev. E, **80**, 031131 (2009). DOI: 10.1103/PhysRevE.80.031131

[17] E. Bouchbinder, J.S. Langer. Phys. Rev. E, **80**, 031132 (2009). DOI: 10.1103/PhysRevE.80.031132

[18] E. Bouchbinder, J.S. Langer. Phys. Rev. E, **80**, 031133 (2009). DOI: 10.1103/PhysRevE.80.031133

[19] V.E. Panin, V.A. Likhachev, Yu.V. Grinyaev. *Strukturnye urovni deformatsii tverdykh tel* (Nauka, Novosibirsk, 1985), 255 p. (in Russian).

[20] E.E. Slyadnikov, I.Yu. Turchanovskiy. ZhTF, **91** (11), 1662 (2021) (in Russian). DOI: 10.21883/JTF.2021.11.51526.35-21

[21] Y.Y. Slyadnikov. Izv. vuzov. Fizika, **64** (12), 27 (2021) (in Russian). DOI: 10.17223/00213411/64/12/27

[22] S.Yu. Korostelev, E.E. Slyadnikov, I.Yu. Turchanovskiy. Izv. vuzov. Fizika, **65** (8), 49 (2022) (in Russian). DOI: 10.17223/00213411/65/8/49

[23] S.Yu. Korostelev, E.E. Slyadnikov, I.Yu. Turchanovsky. AIP Conf. Proc., **2509**, 020113 (2022). DOI: 10.1063/5.0084375

[24] S.Yu. Korostelev, E.E. Slyadnikov, I.Yu. Turchanovskiy. *Tez. dokl. mezhdun. konf. „Fizicheskaya mezomekhanika materialov. Fizicheskite printsipy formirovaniya mnogourovnvoy struktury i mekhanizmy nelineinogo povedeniya“* (Tomsk, Rossiya, 2022), p. 300–301 (in Russian). DOI: 10.25205/978-5-4437-1353-3-183.

[25] G. Khaken. *Synergetics* (Mir, M., 1980), 406 p. (in Russian).

[26] L.D. Landau, E.M. Lifshitz. *Statisticheskaya fizika*. Ch. I (Nauka, M., 1976), 584 p. (in Russian).

[27] L.D. Landau, I.M. Lifshits. *Fizicheskaya Kinetika* (Nauka, M., 2001), 528 p. (in Russian).

[28] L.D. Landau, E.M. Lifshitz. *Teoriya uprugosti* (Nauka, M., 1987), 247 p. (in Russian).