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The mechanism of the anomalous behavior of the plastic flow of materials with high crystal relief caused by the dynamic impurity subsystem

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A model of dynamic interaction of dislocations with an impurity subsystem of crystals with a high potential relief of the crystal lattice (Peierls barriers) is developed. Such materials include metals with body-centered cubic structure, semiconductors, ceramics, and many others. It is shown that the modification of impurity migration barriers near the dislocation core significantly affects the segregation of impurities on the moving dislocation. The presence of a substantially nonequilibrium initial stage of segregation kinetics leading to anomalies of dislocation dynamics and yield strength of materials is substantiated.

Keywords: dislocation dynamics, segregation of impurities in the dislocation core, synergetics of dislocation and impurity subsystems, stable and unstable regimes, plastic flow anomalies.

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1. Introduction

Range of anomalous modes of behavior of mechanical properties is observed at crystal materials studying or application. In initially low-defect crystals the plastic flow instabilities can appear, as presented in the work [1], as a result of catastrophic multiplication of dislocations with formation of their density waves. In materials, containing significant number of impurities, another anomalous behavior mechanism is possible, caused by dynamic interaction of dislocation and impurity subsystems. Impurities influence on dislocations dynamics significantly modifies the mechanical properties of crystal materials and is subject of comprehensive study, both experimental and theoretical [2-5]. There are several dynamic modes in various areas of values of temperature and strain rate. One corresponds to static impurities, sort of "embedded" into crystal lattice and creating individual obstacles for dislocations moving. Under other conditions the impurities diffuse to dislocations and create enriched atmospheres around them, modifying the dynamic characteristics of dislocations with its collective influence, resulting in their so called "ageing". Forced dragging of low-mobility impurities by dislocations is also possible [6]. On a macroscopic level it results in "dynamic strain ageing" of material in general. At comparable mobilities of dislocations and impurities the plastic flow instability is often formed, appearing as jumps on strain curves (Portevin-Le Chatelier effect [7-11]). Another mode corresponds to high-mobility impurities, which atmosphere easily follows the dislocations moving, without creation of high additional deceleration [12].

For the first time the impurities interaction with uniformly moving dislocation of edge type was examined in the work [13] and then in [14–19] and many others. In these works the formation of continuum impurity cloud around dislocation, called Cottrell atmosphere, was calculated. At this point the dynamic interaction of impurities and dislocations is well-studied for materials with face-centered cubic (FCC) structure of crystal lattice. The situation for crystals with body-centered cubic (BCC) structure, semiconductors, ceramics and other materials, in which dislocations movement is limited with a high potential relief of crystal lattice, also called as Peierls barriers, is studied much less. The laws of dislocations dynamic ageing depend on their movement mechanism and are different for two mentioned types of materials. In materials with FCC structure the crystal relief is low, and dislocations move with passing the barriers, created with "forest dislocations" or any other local centers. In materials with high crystal relief there is a so called kink mechanism of dislocations movement [20], and kinetics of impurity subsystem perturbation, induced by moving dislocations, is completely different [21]. In such materials, beside formation of continuum Cottrell atmosphere, the effects, caused by impurities redistribution on a short scale near dislocation core, are also possible. For instance, in the work [22] the situation is studied, when dynamic ageing in niobium with oxygen in temperature range of 423-448 K is caused by impurities redistribution at atomic spacing near dislocation core, that the authors called the Snoek dynamic ageing.

At traditional continuum approach the impurities interaction with screw dislocations is often neglected, since they do not create a long-range field of hydrostatic pressure.



Figure 1. Location of E_1 nodes with maximum bond energy of H impurity atoms with screw dislocation in *W*.

However, at the same time many other types of interaction, appearing at interatomic scale in dislocation cores, e.g. of chemical nature, are not considered. As opposed to this, the atomic calculation reveal the presence of rather high energy of impurities bond with screw dislocations. For instance, the interaction of hydrogen impurities with screw dislocation in *W* in various positions was calculated in the work [23], and for the most favorable position the rather significant bond energy was observed, equal to 256 ± 32 meV. Six such equivalent positions, designated as E_1 , are shown in Fig. 1.

For calculation of effects, related to short-range action, the continuum approach can not be used and the discrete description is required. It is often considered [24,25], that it can be done only by numerical simulation due to large difficulties in description of co-evolution of two multi-particle systems: solute atoms and dislocations. In its entirety it is indeed true, but, if we set the less ambitious task of qualitative clarification of mechanisms of phenomena and trends, related to influence of various material parameters, the simplified approach, presented in this work, can be useful.

The key aspect of materials dynamic strain ageing theory is a variation of impurities content on dislocation lines. But this aspect is not consistently addressed in the existing works and the kinetic law is often simply postulated as [19]:

$$c(t_a) = c_0 + (c_{eq} - c_0) \{ 1 - \exp[-(t_a/\tau_D)^n] \}.$$
 (1)

Here c_0 — average concentration of impurities in crystal volume, c_{eq} — equilibrium concentration of impurities in dislocation core, t_a — time spent by dislocation in front of a barrier, while waiting for transition, equal to h/V, h distance between barriers (for Peierls barriers h is a period of crystal lattice a), V — average dislocation speed, τ_D characteristic time scale of impurity subsystem relaxation, exponential factor n changes within $1/3 \div 1$. Equation (1) is a simple extrapolation between initial exponential kinetics of impurities segregation on dislocation line and final yield of equilibrium. But in some cases the growth of impurities concentration on dislocations is observed with their movement speed increase, that contradicts the law (1). Such behavior indicates the significant supplement of diffusion processes with direct dragging of impurities by dislocation core. Also, for better understanding of the phenomenon, it would be more helpful not to postulate the formulas like (1), but to derive a kinetic law from the underlying physical mechanisms, at least within a simple model. Development of the corresponding theory is the purpose of this work.

2. Short-range impurities model

At various dislocation movement speeds, compared to impurities mobility, the various spatial scales of their interaction are observed. In the examined case of rather fast movement the small scales of an order of several periods of crystal lattice around dislocation become significant. The special importance of short-range interaction with impurities in the scale of dislocation core is given by discreteness of dislocations movement on atomic scale — between valleys of periodic crystal lattice - that is happened, as known, with thermally activated jumps [20]. Jumping change of dislocation position results in redistribution of impurity atmosphere on each stage, kinetics of which depends on potential relief arrangement for impurities migration to dislocation core surroundings. For complete quantitative description of such processes the microscopic pattern is surely important, but for revealing the phenomenon mechanism it is useful to fully disengage from details and concentrate on its universal features.

Schematically simplest one-dimensional view of the migration relief is shown in Fig. 2. Any arrays of equivalent cells, filled with impurities, can be understood as the examined states of impurity content in the core and around it, as it is shown in Fig. 1 with three states for clarity.



Figure 2. Scheme of impurities migration relief near dislocation core. States directly in the core (d) and adjacent previous (-) and following (+) ones are highlighted with notification of impurities transition times between these states and crystal volume.

Away from dislocation the migration relief is periodical, and time τ_0 of impurity displacement by lattice period has an unperturbed value. Near the core the potential relief is distorted with interaction, so there is a deep minimum, corresponding to the most energetically favorable location of impurity relating to dislocation, designated on the figure with letter d. Attraction to this position reduces the barrier of E for impurity transition to it and reduces the time of the corresponding thermally activated jump $\tau = \tau_* \exp(E/kT)$ compared to reverse transition time $\tau_1 = \tau_{*1} \exp(E_1/kT)$ or time of migration away from the core $\tau_0 = \tau_{*0} \exp(E_0/kT)$, therefore $\tau \ll \tau_0, \tau_1$. Here $\tau_*, \tau_{*1}, \tau_{*0}$ — pre-exponential factors, taken as constants. Meaning of activation energies $E_0, E_1, E = E_1 - \Delta E$ is explained in Fig. 2. Presence of reduced barrier E for impurities transition into dislocation core compared to transition barriers E_0 in crystal volume results in necessity of separating the processes of impurities redistribution around the core into a special class and requires separate examination, as noted in [21,22]. The similar approach was used in the works [23,24], where only redistribution of impurity hydrogen atoms between the closest interstices was considered at dislocation movement to α -Fe without new impurities inclusion. Thus. the total number of impurities in the core surroundings was considered constant, unlike this work, where new impurities inclusion and their content growth in the core with dislocation movement will be considered.

Impurities in the energy-lowest state d are hardest to remove from dislocation, and, therefore, they are of the most interest for pinning force calculation. For that reason the main attention will be paid to calculation of d state filling, while other states in the simplest approximation will be considered low-perturbed and interpreted as some reservoir with constant concentration c_0 . This is with the exception of states, adjoint to d during movement of +, -,since due to dislocation movement with possible dragging or retardment of impurities between these states the significant redistribution of impurity concentration is happened. Since it is considered, that dislocations are moved with sufficiently high speed V, time $t_a = a/V$, spent at a single valley of crystal relief, in the examined simplified model is assumed non-sufficient for inclusion of impurities of farther crystal lattice nodes.

Let's examine an evolution of impurity content in dislocation core, characterized with concentration c_d per one lattice period along dislocation line. Let's also introduce the designation c for concentrations of impurities in the adjacent states. It is considered, that dislocation movement has a cyclical pattern and most of the cycle time t_a is accounted for a waiting time before the barrier. Kinks propagation time over the whole dislocation segment after their nucleation is to be neglected. Due to large difference of times of impurities transition into dislocation core τ and into the adjacent lattice nodes τ_1 , τ_0 the evolution of impurity content in a single cycle happens in two stages, significantly different in terms of duration. For time of about τ only the fastest process of impurities transition from the adjacent states (\pm) into the core (d) happens, almost without participation of farther impurities. And only after, for time, including τ_0 , the exchange with impurities from the reservoir happens and equilibrium content is established. If time of waiting of dislocation transition through the barrier t_a is relatively small, the equilibrium content is not reached and quantity of segregated impurities has the significantly non-equilibrium pattern. Behavior at initial stage, for which we will provide an analytical description, is of special interest for studying the conditions of appearance of dislocation dynamics anomalous modes.

Let's write the equation for redistribution of impurity concentrations for a time t_a , when dislocation resides in one of the crystal relief valleys, waiting for the jump to the next valley

$$\frac{dc_d}{dt} = c(1-c_d)/\tau.$$
 (2)

The right part of the equation (2) describes the impurities flow from the adjacent states into the core (d) per unit time. It is considered, that transitions are possible into unoccupied states only, therefore, for instance, frequency of transition into state d is proportional to probability $1-c_d$, that node is free, etc. Due to maintenance of the total number of impurities $c_d + c$ within one cycle this sum is equal to its initial value $c_d + c = c_{d0} + c_{c0}$, allowing to exclude c from (2). The observed closed-form equation

$$\frac{dc_d}{dt} = (1 - c_d)[-c_d + c_{d0} + c_{c0}]/\tau, \qquad (3)$$

is easily solved by means of variables separation

$$c_d(t) = \frac{(c_{d0} + c_{c0})(1 - c_{d0})\exp[(1 - c_{d0} - c_{c0})t/\tau] - c_{c0}}{(1 - c_{d0})\exp[(1 - c_{d0} - c_{c0})t/\tau] - c_{c0}}.$$
(4)

3. Impurities dragging at stationary movement of dislocations

Stationary from macroscopic point of view movement of dislocation over the periodic relief of crystal lattice on a micro-scale is performed by means of successive thermally activated jumps by one lattice period with single jump waiting time t_a , so the average dislocation speed is $V = a/t_a$. Change of dislocation position is accompanied with the corresponding transformation of impurity subsystem. At dislocation jump through barrier it falls within a new state with unperturbed concentration c_0 , and impurities $c_d(t_a)$, accumulated by the moment of jump, are reset. Impurities, left in the crystal relief valley, abandoned by dislocation, strive to relax to a new dislocation position. At the same time, the values of impurity content, reached at the previous stage by the moment of dislocation jump t_a , will act as initial conditions for concentration relaxation at a new stage $c_{c0}^{(2)} = c_d^{(1)}(t_a)$. At the new stage the equation (2) solution



Figure 3. Evolution of impurities content in dislocation core for series of 12 transitions of initially "fresh" dislocation for lattice period at $c_0 = 0.1$, $t_a = 5\tau$.

will be the following

$$c_{d}^{(2)}(t) = \frac{(c_{d}^{(1)}(t_{a}) + c_{0})(1 - c_{0})\exp[(1 - c_{d}^{(1)}(t_{a}) - c_{0})t/\tau] - c_{d}^{(1)}(t_{a})}{(1 - c_{0})\exp[(1 - c_{d}^{(1)}(t_{a}) - c_{0})t/\tau] - c_{d}^{(1)}(t_{a})}.$$
(5)

This expression along with new initial conditions gives recurrent relation for description of co-evolution of dislocation and impurity subsystem.

When describing the dislocation movement as series of successive jumps we will neglect a statistical variability of transition time t_a , that to some degree is justified with regularity of barriers, created by periodic crystal relief. Evolution of kinetic dependencies of $c_d(t)$ for several successive stages, starting from "fresh" dislocation (i.e. without excessive number of impurities compared to their average concentration in crystal volume c_0), is illustrated in Fig. 3. As seen from the figure, there is a tendency of establishing some limited self-reproducing kinetic dependence $c_d^s(t)$.

In a time scale, larger compared to time t_a of elementary transition, the dislocation movement at reproducing kinetic dependence $c_d^s(t)$ is stationary (and will be called such further for the specified meaning). Impurities content at such stationary dislocation movement will be characterized with amplitude value $c_d^s(t)$ in interval $(0, t_a)$, that we designate as c_{da}^s . Amplitude value of impurity content in the core c_{da}^s , established at large number of dislocation transitions, can be derived from equation, resulting from (5) at $t = t_a$ and comparable $c_d^{(2)}(t_a)$ and $c_d^{(1)}(t_a)$,

$$t_a/\tau = \frac{1}{1 - c_0 - c_{da}^s} \ln \left[\frac{c_{da}^s (1 - c_{da}^s)}{c_0 (1 - c_0)} \right].$$
 (6)

Inverted expression (6) is an equivalent of formula (1) for the case of dislocations movement with defining impact of crystal relief. This expression allows to calculate the dependence of impurity content at dislocation on the specified speed of its movement $V = a/t_a$, average impurity concentration in volume c_0 , temperature T and other parameters. Another option of dislocation ageing kinetics is possible, particularly at the specified dislocation driving force (or, equivalently, stress). In this case the speed of dislocation movement through barriers should be expressed depending on the driving force, for instance, using the thermoactivation law

$$V = V_0 \exp\left[-\frac{E_{d0} - \gamma \sigma_{ef}(c_d)}{kT}\right].$$
 (7)

Here E_{d0} — energy of dislocation movement activation in impurity-free material at vanishingly small load, γ activation volume, σ_{ef} — effective stress, considering decelerating influence of impurities, segregated at dislocation. In various cases the activation energy can be expressed differently through impurities concentration in dislocation core. At low concentration the discreteness of impurities location and their individual interaction with dislocation should be considered separately, as it was done in [23,26,27]. This is the case, when the perturbations of dislocation configuration, introduced by one impurity, are not overlapped among themselves. Such perturbation length is close to kink size $d_k \sim a (G/\sigma_P)^{1/2}$ [26], in typical BCC metals greatly exceeding the atomic spacing. Here G shear module, σ_P — Peierls stress. In case, when the average distance between impurities c_d/a is less than d_k , it is possible to use the averaged description of interaction between impurities and dislocations and characterize it with some decelerating stress σ_i , proportional to the excessive impurity concentration: $\sigma_i = \beta(c_d - c_0)$, that will be performed further. Proportionality factor β can be considered as some phenomenological parameter. At the same time, the effective stress, included in activation energy in (7), is the following: $\sigma_{ef} = \sigma - \sigma_i = \sigma - \beta(c_d - c_0)$, where σ – external applied stress. It should be noted, that linearity of the effective stress by concentration is true, until the average distance between impurities a/c_d becomes equal to radius of their interaction along dislocation. At large concentrations the energy of dislocations hitching the impurity atmosphere is calculated similar to the Ising chain task [28,29], that will not be discussed in this work.

Since σ_{ef} depends on time, at large dislocation runs, compared to lattice period, the average speed should be calculated over the cycle from 0 to t_a

$$V_{av} = \frac{1}{t_a} V_0 \int_0^{t_a} dt \exp\left\{-\frac{E_{d0} - \gamma[\sigma - \beta c_d(t) + \beta c_0]}{kT}\right\}.$$
 (8)

The established dislocation movement will be examined. Using relation (3) it is possible to transit from time integration to concentration integration c_d

$$V_{av} = V_0 \exp\left\{-\frac{E_{d0} - \gamma(\sigma + \beta c_0)}{kT}\right\} \frac{\tau}{t_a} J(c_{da}^s) = \frac{a}{t_a}, \quad (9)$$

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Figure 4. Dependence of dislocations speed, normalized at $V_i = a/\tau$, on stress for three values of average impurities concentration (left figure). In the right figure the curve, corresponding to the volume concentration $c_0 = 0.001$, is presented in inverted coordinate axes. Parameters values: $E_i/E_0 = 0.5$, $\gamma\beta/kT = 3$, $a/V_{d0}\tau_0 = 1$.

where

$$J(c_{da}^{s}) = \int_{c_{0}}^{c_{da}^{s}} \frac{dc_{d}}{(1-c_{d})(-c_{d}+c_{ad}^{s}+c_{0})} \exp\left\{-\frac{\gamma\beta c_{d}}{kT}\right\}.$$

Equation, relating c_{da}^s with stress and temperature from relation (9), is

$$(\gamma/E_0)\sigma = 1 - E_i/E_0 - (kT/E_0)\ln[J(c_{da}^s)V_0\tau_0/a].$$
 (10)

It should be noted, that c_{da}^s depends on dislocations speed and, therefore, on stress, that, as a result, should be selfconsistently derived using relation (6). Let's re-write this relation as

$$V_{av} = \frac{a}{\tau} \frac{1 - c_{da}^s - c_0}{\ln\{(1 - c_{da}^s)c_{da}^s/[(1 - c_0)c_0]\}}.$$
 (11)

Equations (10) and (11) provide parametric representation of the force law (parameter c_{da}^{s}), expressing dependence of dislocation speed on stress at various values of impurity subsystem characteristics. This behavior is illustrated in Fig. 4, a. By exchanging the places of coordinate axes we get the force law, illustrating the existence of three modes of dislocations mobility, corresponding to the ones mentioned in the introduction: mode with strengthening impact of impurities at low dislocation speed, dragging their impurity atmospheres (A), mode with negative speed sensitivity at intermediate dislocation speeds, comparable to impurities mobility (B), and mode of relatively low individual impact of impurities at high dislocation speeds (C) (Fig. 4, b). It can be seen, that at high stress the impurities impact is low, but with reduction of stress due to impurities segregation in dislocation core the change of dislocations movement mode happens with sharp reduction of their speed. In some range of parameters one stress value corresponds to three solutions or three speed values, as illustrated in Fig. 4. In

this range there is a "negative speed sensitivity" for one of the solutions, when dislocation speed reduces with stress growth. Such behavior at macroscopic mechanical tests often results in instability of materials plastic flow, called as Portevin–Le Chatelier effect [7–11].

Figure 5 shows the boundaries of areas of dislocation mobility instability (boundaries between areas A-B and B-C in Fig. 4) at various average impurity concentrations in volume and temperature.

Dynamic ageing of dislocations also results in anomaly of temperature dependence of stress, applied to provide the desired speed of dislocations movement. This anomaly appears as stress growth with temperature in some temperature range, as illustrated in Fig. 6.



Figure 5. Boundaries of areas of negative speed sensitivity of dislocation mobility at parameters values of $\gamma \sigma/kT = 4$ (*I*), = 3 (2), = 2.3 (3), = 2 (4). Dashed line corresponds to merging of three branches into one with disappearance of dislocation movement instability areas.



Figure 6. Temperature dependence of the driving force, demonstrating the presence of anomalous positive behavior in some interval. Parameters values: $E_i/E_0 = 0.7$, $\gamma\beta/E_0 = 0.5$.

Rate sensitivity $d\sigma/dV$ is derived using equations (10), (11) as

$$\frac{d\sigma}{dV} = -\frac{kT}{\gamma J} \frac{dJ}{dc_{da}^{s}} \frac{dc_{da}^{s}}{dV} \\
= \frac{kT}{\gamma} \frac{dJ}{dc_{da}^{s}} \Big/ \left\{ \frac{\ln\{(1-c_{da}^{s})c_{da}/[(1-c_{0})c_{0}]\} + \\
+ (1-c_{da}^{s}-c_{0})(1-2c_{da}^{s})/[(1-c_{0})c_{0}]}{\ln^{2}\{(1-c_{da}^{s})c_{da}^{s}/[(1-c_{0})c_{0}]\}} \right\}, (12)$$

where

$$\frac{dJ}{dc_{da}^{s}} = \frac{1}{(1-c_{0})c_{da}^{s}} \exp\left(-\frac{\gamma\beta c_{0}}{kT}\right) - \frac{\gamma\beta}{kT} J(c_{da}^{s}) + \int_{c_{0}}^{c_{da}^{s}} \frac{dc_{d}}{(1-c_{d})^{2}(-c_{d}+c_{ad}^{s}+c_{0})} \exp\left\{-\frac{\gamma\beta c_{d}}{kT}\right\}.$$
(13)

4. Macroplasticity

Synergetics of dynamic dislocation and impurity subsystems appears in macroscopic processes of crystals plastic yield, available for observation. We will derive the rate of plastic flow $\dot{\varepsilon}$ using Orowan's law, $\dot{\varepsilon} = \rho bV$, where dislocations density ρ is approximately considered constant. Here b — value of dislocations Burgers vector. Expressing the dislocation speed through $\dot{\varepsilon}$, we transform the equation (11) to

$$\frac{\dot{\varepsilon}}{\rho b} = \frac{a}{\tau} \frac{1 - c_{da}^s - c_0}{\ln\{(1 - c_{da}^s)c_{da}^s / [(1 - c_0)c_0]\}}.$$
 (14)

This equation, along with equation (10), consists the system, from which the dependence of stress on strain rate is self-consistently derived.

Experimental activation volume is defined as

$$\gamma_{\rm exp} = \frac{kT}{d\sigma/d\ln\dot{\epsilon}}.$$
 (15)

where $d\sigma/d \ln \dot{\varepsilon} = V d\sigma/dV$ and $d\sigma/dV$ are derived from expression (12). Boundary of dislocation mobility instability area corresponds to rate sensitivity vanishing, thus resulting in peaks of effective activation volume, experimentally observed in diffuse form [3].

5. Discussion

Presence of impurities in the core due to dislocations hitching crystal lattice slows down dislocation movement. As a result, to get the same dislocation speed, for instance, at plastic straining, the increase in applied driving force is required, thus indicating the material hardening. Additional contribution to the driving force will reflect behavior of impurity content in the core at various parameters change. At slow movement of dislocations the impurities content in their cores is close to equilibrium and pinning force behavior is similar to the one, that is observed at static ageing of dislocations: pinning force reduces with temperature growth. Specifics of dynamic ageing of dislocations appear at their sufficiently fast movement and is caused by presence of a special initial stage in kinetics of impurities redistribution around dislocation core, as presented in this work. The predicted growth of impurities content causes anomalies of various type, which were repeatedly observed in experimental works in many materials: in metals with BCC structures of Mo, V, etc., in disordered solid solutions, at prismatic slip in metals with HCP structure of Ti, Zr, Be and intermetallics (see review in [3]).

It should be noted, that for these specifics the most important is not the sample-average concentration of impurities c_0 , but the excessive concentration in dislocation core c_d , which, depending on temperature, changes in wide ranges until saturation of $c_d \rightarrow 1$. Sufficiently large increase of impurities content in the cores can reduce the dislocations mobility below the observed limit, actually resulting in immobilization of dislocations [30] or to material embrittlement [23,24]. Therefore, the strong concentration growth, predicted by equation (11), can be the cause of such interesting phenomenon as "inverse brittle-ductile transition", when material loses its plasticity not with temperature lowering as usual, but, quite opposite, with its increase, as was observed in olivine [31], GaAs [32] or SrTiO₃ [33].

6. Conclusion

According to the results of the performed calculations, the proposed model has the sufficient potential to reveal the causes and describe the mechanism of anomalous behavior of crystal materials plastic yield. At the same time, it does not consider many processes, that can appear significantly at later stages, for instance, long-range diffusion of impurities or some specifics of certain materials. These processes are required for describing the recovery from anomalous mode, but they have small impact on this mode formation. Therefore, when describing the conditions of anomalies formation, we can stick to the developed simplified model, which advantage is its universality.

Let's specify the main results of the study.

1. The model of dynamic ageing of fast-moving dislocations in impurity materials with high crystal relief, when continuum description of impurity atmospheres can not be applied, is formulated.

2. Presence of the stage of dynamic ageing of dislocations with formation of significantly non-equilibrium impurity content near dislocation core is shown.

3. Kinetics of dynamic ageing of dislocations, reasonably distinct from the ones, arbitrary postulated in the classic theory, is calculated.

4. It is shown, that presence of the stage of initial fast growth of impurity content in dislocation core is a mechanism of anomalous negative rate sensitivity of materials plastic flow and positive temperature dependence of strain stress.

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Conflict of interest

The author declares that he has no conflict of interest.

References

- [1] G.A. Malygin. FTT 60, 6, 1232 (2018) (in Russian).
- [2] Zh. Fridel'. Dislokatsii. Mir, M. (1967). 643 p. (in Russian).
- [3] D. Caillard, J.L. Martin. Thermally Activated Mechanisms in Crystal Plastisity. Pergamon, Amsterdam–Boston–London–N.Y.–Oxford–Paris–San Diego–San Francisco–Singapore–Sidney–Tokyo (2003). 433 p.
- [4] U. Messerschmidt. Dislocation Dynamics During Plastic Deformation / Ed Hull R. Berlin. Heidelberg: Springer Series in Material Science (2010).
- [5] B.V. Petukhov. Dinamika dislokatsiy v kristallicheskom rel'efe. Dislokatsionnye kinki i plastichnost' kristallicheskikh materialov. Saarbrücken: Lambert Academic Publishing. (2016). 385 p.
- [6] B.V. Petukhov. J. Physics: Conf. Ser. 240, 012012 (2010).
- [7] A. Portevin, F. Le Chatelier. Trans. Am. Soc. St. Tr. 5, 457 (1924).
- [8] P.G. McCormick. Acta Met. 20, 3, 351 (1972).
- [9] A. van den Beukel. Phys. Status Solidi A **30**, *1*, 197 (1975).

- [10] G. Ananthakrishna. Phys. Rep. 440, 4-6, 113 (2007).
- [11] Y. Estrin, L.P. Kubin. In: Continuum Models for Materials with Microstructure / Ed. Mühlhaus H.B. Chichester. Wiley (1995). P. 395.
- [12] T.S. Gross, V.K. Mathews, R.J. De Angelis, K. Okazaki. MSE A117, 9, 75 (1989).
- [13] A.H. Cottrell, M.A. Jaswon. Proc. Roy. Soc. A. 199, 1056, 104 (1949).
- [14] H. Yoshinaga, S. Morozumi. Phil. Mag. 23, 186, 1351 (1971).
- [15] G.A. Malygin. Phys. Status Solidi A 72, 2, 493 (1982).
- [16] Y. Wang, D.J. Srolovitz, J.M. Rickman, R. Lesar. Acta Mater. 48, 9, 2163 (2000).
- [17] D. Maroudas, R.A. Brown. J. Mater. Res. 6, 11, 2337 (1991).
- [18] W.A. Curtin, D.L. Olmsted, L.G. Hector. Jr. Nature Mater. 5, 11, 875 (2006).
- [19] N. Louat. Scr. Met. 15, 11, 1167 (1981).
- [20] G. Hirt, I. Lote. Teoriya dislokatsiy. Atomizdat, M. (1972). 598 p. (in Russian).
- [21] B.V. Petukhov. Phys. Status Solidi 2, 6, 1864 (2005).
- [22] S.C. Park, L.P. Beckerman, R.E. Reed-Hill. Metallurg. Trans. A 14, 3, 463 (1983).
- [23] M. Itakura, H. Kaburaki, M. Yamaguchi, T. Okita. Acta Mater. 61, 18, 6857 (2013).
- [24] P. Gong, I.H. Katzarov, J. Nutter, A.T. Paxton, W.M. Rainforth. Sci. Rep. 10, 10209 (2020).
- [25] Y. Zhao, L. Dezerald, M. Pozuelo, X. Zhou1, J. Marian. Nature Commun. 11, 1227, 1 (2020).
- [26] B.V. Petukhov. Fiz. met. i metallovedenie 56, 6, 1177 (1983) (in Russian).
- [27] B.V. Petukhov. Mater. Sci Eng. A. 234-236, 177 (1997).
- [28] B. Petukhov. Electron. Proc. MRS Spring Meeting, 683E, BB3.3 (2001).
- [29] B. Lüthi, L. Ventelon, D. Rodney, F. Willaime. Comput. Mater. Sci. 148, *1*, 21 (2018).
- [30] I.E. Bondarenko, V.G. Eremenko, V.I. Nikitenko, E.B. Yakimov. Phys. Status Solidi A 60, 2, 341 (1980).
- [31] H.W. Green II, T.E. Young, D. Walker, C.H. Scholz. Nature 348, 12, 720 (1990).
- [32] T. Suzuki, T. Tokuoka, I. Yonenaga, H.O.K. Kirchner. Scripta Mater. 43, 7, 645 (2000).
- [33] P. Gumbsch, S. Taeri-Baghbadrani, D. Brunner, W. Sigle, M. Rühle. Phys. Rev. Lett. 87, 085505 (2001).