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NONEQUILIBRIUM KINETICS OF ELECTRON-PHONON SUBSYSTEM OF A CRYSTAL IN STRONG ELECTRIC AND MAGNETIC FIELD AS A BASE OF ELECTRO- AND MAGNETOPLASTIC EFFECTS

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The results of kinetic consideration of nonequilibrium dynamics of electron-phonon system of a crystal in a strong electric field based on a proposed method of numerical solution of a set of Boltzmann equations for electron and phonon distribution functions without expansion of electron distribution function in a series by phonon energy are presented. It has been shown that electromagnetic action excites electron subsystem which by transferring energy to the phonon subsystem creates large amount of short-wave phonons which effectively influence the lattice defects (point, linear, boundaries of different phases) that results in redistribution and decrease of lattice defects density, damage healing, decrease of local peak stress and decrease of construction materials properties degradation level.
KEYWORDS: kinetics, electron, phonon, electric and magnetic fields, lattice defects, peak stress, electroplastic and magnetoplastic effects.

НЕРІВНОВАЖНА КІНЕТИКА ЕЛЕКТРОН-ФОНОННОЇ ПІДСИСТЕМИ КРИСТАЛУ В СИЛЬНОМУ МАГНІТНОМУ ПОЛЯХ ЯК ОСНОВА ЕЛЕКТРО- ТА МАГНІТОПЛАСТИЧНОГО ЕФЕКТІВ

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Наведені результати кінетичного розгляду нерівноважної динаміки електрон-фононної системи кристалу в сильному електричному полі на основі запропонованого методу числового розв'язку системи кінетичних рівнянь Больцмана для електронної та фононної функцій розподілу без використання розкладення функції розподілу електронів в ряд по енергії фонону. Показано, що електромагнітна дія збуджує електронну підсистему, створює велику кількість короткохвильових фононів, які ефективно діють на дефекти (точкові, лінійні, межі розділу та виділення різних фаз) кристалічної решітки, що призводить до перерозподілу та зниження густини дефектів кристалічної решітки, заліковування пошкоджень, зменшення локальної пікової напруги та зниження рівня деградації властивостей конструкційних матеріалів.
КЛЮЧОВІ СЛОВА: кінетика, електрон, фонон, електричне та магнітне поля, дефекти решітки, критична напруга, електропластичний та магнітопластичний ефекти.

НЕРАВНОВЕСНАЯ КИНЕТИКА ЭЛЕКТРОН-ФОНОННОЙ ПОДСИСТЕМЫ КРИСТАЛЛА В СИЛЬНОМ ЭЛЕКТРИЧЕСКОМ И МАГНИТНОМ ПОЛЯХ КАК ОСНОВА ЭЛЕКТРО- И МАГНИТОПЛАСТИЧЕСКОГО ЭФФЕКТОВ

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Приведены результаты кинетического рассмотрения неравновесной динамики электрон-фононной системы кристалла в сильном электрическом поле на основе предложенного метода численного решения системы кинетических уравнений Больцмана для электронной и фононной функций распределения без использования разложения функции распределения

электронов в ряд по энергии фонона. Показано, что электромагнитное воздействие возбуждает электронную подсистему, которая, передавая энергию в фононную подсистему, создает большое количество коротковолновых фононов, эффективно воздействующих на дефекты (точечные, линейные, границы раздела и выделения различных фаз) кристаллической решетки, что приводит к перераспределению и снижению плотности дефектов кристаллической решетки, залечиванию повреждений, уменьшению локальных пиковых напряжений и снижению уровня деградации свойств конструкционных материалов.
КЛЮЧЕВЫЕ СЛОВА: кинетика, электрон, фонон, электрическое и магнитное поля, дефекты решетки, критическое напряжение, електропластический и магнитопластический эффекты.

In the sixtieth of the XX century a phenomenon of abrupt decrease of plastic deformation resistance of metals in case of excitation of their conductivity electron subsystem by irradiation or conduction of electron current of high density $j=10^8$-10^9A/m^2 was discovered. This phenomenon has been called electroplastic effect (EPE) [1]. This effect is already being applied in industry in the processes of drawing and rolling of metallic products.

Since then soviet and american scientists have carried out series of experiments on metal deformation under electric current influence and also at irradiation of samples by accelerated electrons. In that experiments the manifestation of EPE under different conditions has been studied and also has been ascertained the dependence of the phenomenon intensity on such parameters as:

- kind of the sample being deformed
- temperature
- current density amplitude
- current pulse frequency
- current pulse duration
- current direction
- dopant concentration in sample
- orientation of crystal samples being deformed
- deformation rate

Creation of ab initio theory of electroplastic effect is complicated by that fact that for explanation of the results of the experiments on crystal deformation under the influence of electric current it is necessary to take into account different mechanisms of current influence on the deformation processes. These mechanisms include:

- thermic influence of the current that results in thermal expansion of the sample and also in softening.
- skin effect.
- pinch effect i.e. influence of the pressure of the magnetic field created by current inside of the sample.
- electron-dislocation interaction which appears in momentum and energy transfer to the dislocations from both electrons directly and collective excitations such as plasmons.
- phonon mechanism i.e. electrons which gain energy from the electric field create phonons that excite the dislocation vibrations which can result in dislocation depinning from stoppers.
- magnetic field influence i.e. magnetoplastic effect.

Let us enumerate some experimental regularities of EPE.

In the most pure state EPE can be observed in monocrystals of Zn, Cd, Sn, Pb. If during the deformation one passes through the samples of that materials pulse electric current with density of $j=10^2$-10^3A/mm^2 or if the samples are irradiated by accelerated electrons (with the energy less than atomic knocking-out threshold from the lattice node) in the slip direction, than softening of the samples which exhibits itself in spasmodic drops of deforming stress is revealed [1].

For monocrystals a strongly expressed dependence of the effect magnitude on the orientation of the samples being deformed is observed. At such crystal orientations when the basal slip is complicated the magnitude of deforming stress drop if small and the stress from which plastic deformation begins is large. Maximum stress drop magnitude can be obtained for medium crystal orientations which are characterized by easy basal slip. In this case the stress of the drop start has its minimum [1].

The EPE magnitude dependence on the current density has threshold character, i.e. it starts to become apparent with particular value of the pulse current density. This value depends on the sort of crystals being deformed and also on the temperature and on the deformation rate. For zinc at T=77 K it is equal 400-500 A/mm^2 [1].

The temperature dependence is almost absent in a wide range of temperature. For zinc this interval is 77-300 K. For titan the threshold current density magnitude from which the effect begins with cooling from 300 down to 78 K increases by hundreds of A/cm^2 [1].

EPE is sensitive to external factors. The effect intensity is influenced by surface active media. For example specific crystallographic shift of amalgamated zinc monocrystals at the temperature of 300 K and under influence of current pulses with j=600-1000 A/mm^2, pulse repetition frequency of 0.1…0.5 Hz and pulse duration of $t_p=10^{-4}$ c increases by 50-60% [1].

The dopant presence also influence upon spasmodic metal deformation. As a result of doping the drop magnitude can grow by dozens of percents (up to 100%). Within the scope of relatively small substitutional impurity the magnitude of the effect grows linearly with concentration as it has been shown in the experiments with zinc, doped by cadmium from10^{-3} up to 10^{-1}at. % (other impurities content did not exceed $2\cdot10^{-3}$at. %). The brittle strength of zinc

crystals grows by 50-70% depending on dopant concentration. This fact can be connected with general increase of the critical shearing stress in the doped crystals [1].

The increase of the current pulse repetition frequency decreases the deforming stress threshold value but also decreases stress drop magnitude. Pulse duration growth at constant amplitude increases the depth of stress drops. This phenomenon was registered both in stress relaxation tests and in creep tests [1].

The main EPE regularities, revealed at monocrystal deformation can be observed in weaker form also in experiments with polycrystal materials. However the EPE magnitude decreases with structure refinement and even disappears in nanocrystal state [2]. Thus EPE is a structure-sensitive phenomenon.

Similar phenomena are observed at irradiation of the material by pulse packets of accelerated electrons. Plasticizing action enhances with the increase of electron energy up to atomic knockout threshold. At further energy increase the intensity of the effect decreases at the expense of radiation strengthening. The combination of current action and irradiation results in the intensification of the metal strength loss effect [1].

Mechanisms, connected with the action of electron wind on dislocations, pinch-effect and also thermal influence of the current on deformation processes are reviewed in detail in the work [1]. It is shown, that they are not sufficient for the quantitative explanation of the EPE.

In this work the phonon mechanism of the influence on dislocation is considered [3, 4].

The purpose of this work is to show that experimentally observed regularities of electroplastic effect can be explained quantitatively if one takes into account the influence of nonequilibrium phonons excited by electrons that gain energy from the electric field upon the dislocations.

ABOUT THE INFLUENCE OF PHONONS ON DISLOCATIONS

Plastic deformation of crystals under the action of external loads in most cases is accomplished by dislocation glide. The main equation describing the kinetics of the process of the plastic deformation – the Orovan modified equation (see for example [5]):

$$\dot{\varepsilon}_d = bl\rho_d \nu_d(\sigma^*), \quad \sigma^* = \sigma - \sigma_i, \tag{1}$$

where $\dot{\varepsilon}_d$ is the strain rate, b the Burger`s vector, l the mean distance between stoppers, ρ_d the mobile dislocations density, $\nu_d(\sigma^*)$ the frequency of the stoppers overcoming by dislocations, σ^* the effective shear stress, σ_i the internal shearing stress in the glide plane.

For the case of thermodynamic equilibrium the expression $\nu_d(\sigma^*, T)$ has the form of:

$$\nu_d(\sigma^*, T) = \nu_d^0 \exp\left(-\frac{H(\sigma^*)}{k_B T}\right). \tag{2}$$

The explicit form of the $H(\sigma^*)$ function depends on the potential barrier model. For the consideration of a more general case, i.e. when electron and phonon subsystems can be, generally speaking, not in the state of equilibrium the Landau-Hoffman model will be used [6].

The potential pit has parabolic form:

$$U(x) = \begin{cases} \zeta x^2, |x| \le x_{cr} \\ 0, |x| > x_{cr} \end{cases}, \zeta x_{cr}^2 = U_0. \tag{3}$$

The displacement of the dislocation segment of length L under the stress σ will be described in the approximation of the elastic string vibrations (Granato-Lücke model [6,7]:

$$M\frac{\partial^2 u}{\partial t^2} + B\frac{\partial u}{\partial t} - C\frac{\partial^2 u}{\partial y^2} = b\sigma + f(t). \tag{4}$$

Here $u(y,t)$ is the displacement of the dislocation line at the point y in the direction x, $M = \frac{\rho b^2}{2}$ is the effective mass of the length unit, ρ the material density, B the coefficient of the dynamic friction force per unit of length, $C = \frac{Gb^2}{2}$ the linear tension of the string, G the shear modulus, $f(t)$ the force of the random pushes that are exerted by crystal upon the unit of dislocation length.

Boundary conditions:

$$u'(0,t) = ku(0,t);\ -u'(L,t) = ku(L,t); k = \frac{2\zeta}{C}. \tag{5}$$

The equation is linear, so its solution can be written as a sum

$u(y,t) = u_{st}(y) + u_{osc}(y,t)$, where $u_{st}(y)$ is the static deflection, caused by external stress σ, and $u_{osc}(y,t)$ the oscillations under the action of a random force.

$$u_{st}(y) = \frac{by(L-y)}{2C} + \frac{bL\sigma}{2Ck};\quad u_{osc}(y,t) = \sum_{n=1}^{N} Q_n(t)\left(\sin(q_n y) + \frac{q_n}{k}\cos(q_n y)\right);\quad \mathrm{ctg}(q_n y) = \frac{q_n^2 - k^2}{2q_n k} \tag{6}$$

The quantity of $Q_n(t)$ satisfies the following equation:

$$M\ddot{Q}_n(t) + B\dot{Q}_n(t) + M\omega_n^2 Q_n(t) = f_n(t);\ \omega_n^2 = q_n^2\frac{C}{M} \tag{7}$$

Let us consider a "fixing point" at y=0. Let the segment lengths on both sides of it be equal to L. Then the total deflection at the "fixing point" is equal to:

$$\tilde{u}(0,t) = 2u_{st}(y) + 2u_{osc}(y,t) = \tilde{u}_{st}(y) + \tilde{u}_{osc}(y,t) \quad (8)$$

The case of a random force was considered in the work [8]. We shall now provide some of the calculations for the reference purpose. If at some time moment occurs a random event such that $\delta\tilde{u}(0,t) \geq \delta\tilde{u}_{cr}$ then the condition of obstacle overcoming in the direction on the loading action will be satisfied. Let $f_n(t)$ be a stationary Gauss process. Since the equation (7) is linear, $Q_n(t)$ and correspondingly $\tilde{u}(0,t)$ is also stationary Gauss process for which the mean number of exceeding a particular quantity $\delta\tilde{u}_{cr}$ per unit of time is equal to:

$$\nu = \frac{1}{2\pi}\sqrt{-\frac{\Psi''(0)}{\Psi(0)}}\exp\left\{-\frac{\delta\tilde{u}_{cr}^2}{2\Psi(0)}\right\}, \quad (9)$$

$$\Psi(\tau) = 2\sum_{n=1}^{\tilde{n}}\frac{q_n^2}{k^2}\overline{Q_n(t)Q_n(t+\tau)} \equiv 2\sum_{n=1}^{\tilde{n}}\frac{q_n^2}{k^2}\psi(\tau), \quad (10)$$

$$\delta\tilde{u}_{cr} = x_{cr} - \frac{bL\sigma}{Ck} = x_{cr}\left(1 - \frac{\sigma}{\sigma_{cr}}\right),\ \sigma_{cr} \equiv \frac{Ckx_{cr}}{bL}, \quad (11)$$

where $\Psi(\tau)$ is the random process $\delta\tilde{u}(0,t)$ correlation function expressed by means of random process $Q_n(t)$ correlation function $\psi(\tau)$; $\Psi''(0)$ is the second derivative with respect to τ at $\tau = 0$. For the Fourier components $(Q_n)_\omega$ of $Q_n(t)$ we can write:

$$\psi(\tau) = \int_{-\infty}^{\infty}(Q_n)_\omega^2 e^{-i\omega\tau}d\omega, \quad (12)$$

where the definition of the quantity $(Q_n)_\omega^2$ is given by the relation

$$\overline{(Q_n)_\omega(Q_n)_{\omega'}} = (Q_n)_\omega^2\delta(\omega + \omega') \quad (13)$$

Each harmonic can be formally considered as an independent vibrator with friction χ and frequency ω_n:

$$m\ddot{Q} + \chi\dot{Q} + m\omega_n^2 Q = F, \quad (14)$$

where m is the proportionality coefficient between the generalized momentum and velocity $\dot{Q}$, χ the friction coefficient, F the random force [9].

$$m = M\frac{L\xi_n}{2},\quad \chi = B\frac{L\xi_n}{2},\ F = f_n\frac{L\xi_n}{2},\quad \xi_n = 1 - \frac{2}{kL} + \frac{q_n^2}{k^2} \quad (15)$$

So for the Fourier component we obtain the following formula:

$$(Q_n)_\omega^2 = \frac{(F_\omega)^2}{m^2\left(\omega_n^2 - \omega^2\right)^2 + \chi^2\omega^2} \quad (16)$$

Random force spectral density can be found from the expression [8]:

$$(F_\omega)^2 = \frac{\chi}{\pi}\hbar\omega\left(\frac{1}{2} + N(\omega)\right). \quad (17)$$

Hence to estimate the force exerted by phonons upon dislocations one must first find the phonon distribution function $N(\omega)$.

KINETIC EQUATIONS

In some works on electron-phonon subsystem dynamics in metal films an assumption about Fermi form of isotropic part of the electron distribution function with time-dependent temperature was used [10]. In the given work we do not make that assumption and thus the distribution functions can be, generally speaking, not thermodynamically equilibrium. In such case the behavior of electrons and phonons is described by means of distribution functions.

For the description of the electron-phonon system nonequilibrium dynamics it is necessary to solve a set of kinetic Boltzmann equations for electron and phonon distribution functions correspondingly. For electron distribution function the Boltzmann equation has the form of:

$$\frac{\partial f}{\partial t} + \vec{v}\frac{\partial f}{\partial \vec{r}} + \frac{\partial f}{\partial \vec{p}}\frac{d\vec{p}}{dt} = I_{ee} + I_{ep} + I_{ed}, \quad (18)$$

$$\frac{d\vec{p}}{dt} = e\left\{\vec{E}(\vec{r},t) + \left[\vec{v},\vec{B}(\vec{r},t)\right]\right\}, \quad (19)$$

where $\vec{v}$ is the velocity, $\vec{p}$ the momentum, t the time, $\vec{r}$ the radius-vector, $\vec{E}$ the electric field strength, $\vec{B}$ the magnetic induction. Hereinafter we consider the magnetic field absent. The electric field and also electron distribution function we consider spatially uniform.

- I_{ee} is the electron-electron collision integral. In the general case of quantum mechanics it has the form of [11-13]:

$$I_{ee} = \frac{2}{(2\pi\hbar)^6}\int d\vec{p}_1 d\vec{p}_2 d\vec{p}_3 W(\vec{p},\vec{p}_1|\vec{p}_2,\vec{p}_3)\left[f(\vec{p}_2)f(\vec{p}_3)\left(1 - f(\vec{p}_1)\right)\left(1 - f(\vec{p})\right) - f(\vec{p})f(\vec{p}_1)\left(1 - f(\vec{p}_2)\right)\left(1 - \right.\right.$$
$$\left.\left. - f(\vec{p}_3)\right)\right]\delta(\varepsilon + \varepsilon_1 - \varepsilon_2 - \varepsilon_3)\delta(\vec{p} + \vec{p}_1 - \vec{p}_2 - \vec{p}_3), \quad (20)$$

where $f(\vec{p})$ are the occupation numbers, $W(\vec{p},\vec{p}_1|\vec{p}_2,\vec{p}_3)$ the matrix element that describes screened coulomb interaction.

$$W(\vec{p},\vec{p}_1|\vec{p}_2,\vec{p}_3) = (2\pi\hbar)^3 2e^4\left(|\vec{p}_1 - \vec{p}_3|^2 + a_1^2\right)^{-2} \quad (21)$$

where $W(\vec{p},\vec{p}_1|\vec{p}_2,\vec{p}_3)$ the transition probability for electrons with momenta $\vec{p}_2 and\ \vec{p}_3$ to the state with momenta $\vec{p}$ and $\vec{p}_1$ as a result of collision. For relatively small electric fields the contribution from electron-electron collisions is essentially less than the contribution from the electron-phonon interaction and thus hereinafter at small time intervals electron-electron collisions will not be taken into account.

I_{ep} is the electron-phonon collision integral [11-13]:

$$I_{ep} = \int d\vec{q}w(\vec{q})\{\delta(\varepsilon(\vec{p}+\vec{q})-\varepsilon(\vec{p})-\hbar\Omega(\vec{q}))[f(\vec{p}+\vec{q})(1-f(\vec{p}))(N(\vec{q})+1)-f(\vec{p})(1-f(\vec{p}+\vec{q}))N(\vec{q})]+$$
$$+\delta(\varepsilon(\vec{p}-\vec{q})-\varepsilon(\vec{p})+\hbar\Omega(\vec{q}))[f(\vec{p}-\vec{q})(1-f(\vec{p}))N(\vec{q})-f(\vec{p})(1-f(\vec{p}-\vec{q}))(N(\vec{q})+1)]\} \quad (22)$$

I_{ed} is the electron-impurity and electron-defect collision integral. It can be obtained by setting in I_{ep} $\hbar\Omega = 0$ and N=0.

$$I_{ed} = \int d\vec{\acute{p}}\, w_{ed}(\vec{\acute{p}}-\vec{p})\delta\left(\varepsilon(\vec{\acute{p}})-\varepsilon(\vec{p})\right)\{f(\vec{\acute{p}})-f(\vec{p})\} \quad (23)$$

Phonon distribution function also satisfies the kinetic equation:

$$\frac{\partial N(\vec{q})}{\partial t}+\vec{v}_q\frac{\partial N(\vec{q})}{\partial \vec{r}} = I_{pe}+I_{pp}+I_{pd}, \quad (24)$$

I_{pe} is the phonon-electron collision integral [11-13]:

$$I_{pe} = \int d\vec{p}w(\vec{q})\{\delta(\varepsilon(\vec{p}+\vec{q})-\varepsilon(\vec{p})-\hbar\Omega(\vec{q}))[f(\vec{p}+\vec{q})(1-f(\vec{p}))(N(\vec{q})+1)]-f(\vec{p})(1-f(\vec{p}+\vec{q}))N(\vec{q})\} \quad (25)$$

The phonon-phonon and phonon-defect collision integrals in τ-approximation have the following form:

I_{pp} is the phonon-phonon collision integral.

$$I_{pp} = -\nu_{pp}(\vec{q})[N(\vec{q})-N_T(\vec{q})], \quad \nu_{pp}(q)=\nu_{pp0}q^2; \quad \nu_{pp0}=\frac{T^3 s}{a_c T_D^4 M_c} \quad (26)$$

I_{pd} is the phonon-defect collision integral

$$I_{pd} = -\nu_{pd}(\vec{q})[N(\vec{q})-\overline{N(\vec{q})}] \quad (27)$$

where $N_T(\vec{q})=\left[\exp\left(\frac{\hbar\Omega}{T}\right)-1\right]^{-1}$ is the thermodynamically equilibrium phonon distribution function – Bose-Einstein function; $\overline{N}(q)=\frac{1}{4\pi}\int N(\vec{q})d\mathrm{O}$ is the phonon distribution function, averaged over the angles.

Since electron-impurity, electron-defect and electron-phonon collisions result in distribution function isotropization, we shall search it in the form of the sum of isotropic function and small anisotropic additive:

$$f(\vec{p},t)=f(\varepsilon(p),t)+\vec{f}_1(\varepsilon(p),t)\frac{\vec{p}}{p}, \quad (28)$$

$$w(q)=w_0 q; \ w_0=\frac{\varepsilon_{1A}^2}{2(2\pi\hbar)^2\hbar\rho s}; \quad \hbar\Omega(q)=sq. \quad (29)$$

After concretization we obtain:

$$I_{pp} = -\nu_{pd0}q[N(\vec{q})-N_T(\vec{q})], \quad (30)$$

$$I_{ed}\left\{\vec{f}_1(\varepsilon)\frac{\vec{p}}{p}\right\}=-\nu_{ed}\vec{f}_1(\varepsilon)\frac{\vec{p}}{p}, \quad (31)$$

where ν_{ed} =3·10^{13} s^{-1} is the electron-impurity collision frequency which in the given case (of low temperatures) determines the electron distribution function isotropization.

$$I_{ep}\left\{\vec{f}_1(\varepsilon)\frac{\vec{p}}{p}\right\}=-\nu(\varepsilon)\vec{f}_1(\varepsilon)\frac{\vec{p}}{p}; \quad \nu(\varepsilon)=\frac{\pi w_0}{\sqrt{m\varepsilon^3}}\int_0^{\sqrt{8m\varepsilon}}dqq^3\left[N(q)+\frac{1}{2}\right]. \quad (32)$$

For anisotropic additive we have the equation:

$$\frac{\partial\vec{f}_1}{\partial t}\frac{\vec{p}}{p}-e\vec{E}v\frac{\partial f_0}{\partial\varepsilon}\frac{\vec{p}}{p}=-\nu_{ed}\vec{f}(\varepsilon)\frac{\vec{p}}{p}, \quad (33)$$

Collisions with defects and impurities occur very often, i.e. at a time scale that is small compared to characteristic time of interaction of phonons with electrons, therefore the anisotropic additive can be considered stationary and also spatially uniform.

As a result we obtain the final set of two equations for isotropic electron and acoustic phonon distribution functions [3,4,14] which has to be solved without electron distribution function Tailor expansion:

$$\frac{\partial f}{\partial\tilde{t}}-4\Delta\tilde{\varepsilon}\frac{1}{\tilde{\varepsilon}^{1/2}}\frac{\partial}{\partial\tilde{\varepsilon}}\left[\tilde{\varepsilon}^2\frac{\partial f}{\partial\tilde{\varepsilon}}\right]=\frac{1}{8}\alpha^{-\frac{5}{2}}\left\{\frac{1}{\sqrt{\tilde{\varepsilon}}}\int_0^{\varepsilon_-}d\tilde{\varepsilon}_{ph}\tilde{\varepsilon}_{ph}{}^2\left[f(\tilde{\varepsilon}-\tilde{\varepsilon}_{ph})N(\tilde{\varepsilon}_{ph})+f(\tilde{\varepsilon})(f(\tilde{\varepsilon}-\tilde{\varepsilon}_{ph})-N(\tilde{\varepsilon}_{ph})-1)\right]+\right.$$
$$\left.\frac{1}{\sqrt{\tilde{\varepsilon}}}\int_0^{\varepsilon_+}d\tilde{\varepsilon}_{ph}\tilde{\varepsilon}_{ph}{}^2\left[f(\tilde{\varepsilon}+\tilde{\varepsilon}_{ph})[N(\tilde{\varepsilon}_{ph})+1]-f(\tilde{\varepsilon})\left(f(\tilde{\varepsilon}+\tilde{\varepsilon}_{ph})+N(\tilde{\varepsilon}_{ph})\right)\right]\right\}, \quad (34)$$

$$\frac{\partial N(q)}{\partial\tilde{t}}=\frac{1}{2\alpha}\int_{\varepsilon_0}^{\infty}d\tilde{\varepsilon}\left[\left(f(\tilde{\varepsilon}+\tilde{\varepsilon}_{ph})-f(\tilde{\varepsilon})\right)N(\tilde{\varepsilon}_{ph})+f(\tilde{\varepsilon}+\tilde{\varepsilon}_{ph})(1-f(\tilde{\varepsilon}))\right]. \quad (35)$$

Here the following designations are used:

$$\alpha=\frac{ms^2}{2k_BT_e}; \ \Delta\tilde{\varepsilon}=\frac{e^2E^2\tau_{ep0}}{6m\nu_{ed}k_BT_e}; \ \tilde{\varepsilon}=\frac{\varepsilon}{k_BT_e}; \ \tilde{\varepsilon}_{ph}=\frac{\varepsilon_{ph}}{k_BT_e}; \ \tilde{t}=\frac{t}{\tau_{ep0}}; \ \tau_{ep0}=\frac{(2\pi\hbar)^3\hbar\rho}{\pi m^3 s\varepsilon_{1A}^2}=3.446\cdot10^{-7}s.$$

Integration limits which are obtained with respect to the energy conservation law are correspondingly equal:

$$\varepsilon_- = \min\left[4\left(\sqrt{\tilde{\varepsilon}\alpha}-\alpha\right), \tilde{\varepsilon}_{ph_D}\right], \varepsilon_+ = \min\left[4\left(\sqrt{\tilde{\varepsilon}\alpha}+\alpha\right), \tilde{\varepsilon}_{ph_D}\right], \varepsilon_0 = \frac{\tilde{\varepsilon}_{ph}{}^2}{16\alpha} - \frac{\tilde{\varepsilon}_{ph}}{2} + \alpha \quad (36)$$

Distribution functions of electrons $f(\varepsilon)$ and phonons $N(q)$ are dimensionless quantities that satisfy the following normalizing conditions:

$$\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \int_0^\infty \varepsilon^{\frac{1}{2}} f(\varepsilon) d\varepsilon = n, \quad (37)$$

where n is the electron density in the valence band (for metals also conductivity band as it is only partially filled).

$$\frac{1}{2\pi^2}\left(\frac{1}{\hbar^3}\right) \int_0^{q_D} q^2 N(q) dq < \infty, \quad (38)$$

where q_D is the Debye phonon momentum which is determined by the equality:

$$q_D = \frac{\pi\hbar}{a}. \quad (39)$$

All quantities are taken for nickel: s=2.96·10^5 cm/s is the transverse sound velocity, n=2.5·10^{22} cm^{-3} the conductivity electron concentration, a=3.5·10^{-8} cm the lattice constant, $\rho_s^{-1} = 0.333 \cdot 10^6$ Sm/cm.

Thermodynamically equilibrium electron energy distribution function is the Fermi-Dirac function:

$$f_0(\varepsilon) = \left[\exp\left(\frac{\varepsilon-\varepsilon_F}{k_b T_e}\right) + 1\right]^{-1}. \quad (40)$$

For nickel ε_F=5·10^{-19} J.

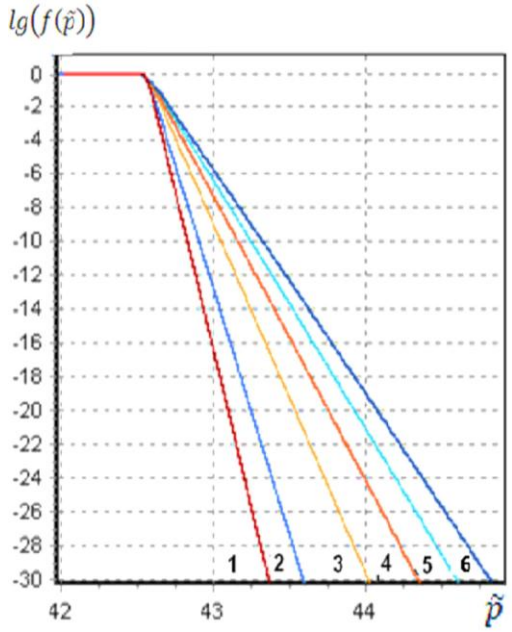

Fig. 1. Dependence of the electron distribution function decimal logarithm on dimensionless electron momentum $\tilde{p}$ at E=1.68 V/cm for different time moments t=0; 1; 5; 10; 15; 20. The curves correspond to these time moments in such order: 1, 2, 3, 4, 5, 6.

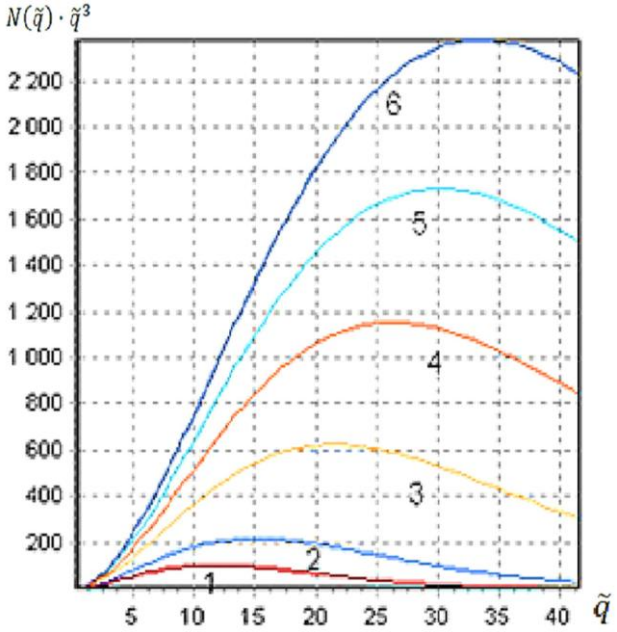

Fig. 2. Dependence of the phonon distribution function multiplied by dimensionless phonon momentum $\tilde{q}$ cubed on dimensionless phonon momentum at E=1.68 V/cm for different time moments t=0; 1; 5; 10; 15; 20. The curves correspond to these time moments in such order: 1, 2, 3, 4, 5, 6.

NUMERICAL SOLUTION OF THE KINETIC EQUATIONS SET FOR ELECTRON AND PHONON DISTRIBUTION FUNCTIONS AND DISCUSSION OF THE RESULTS

For the numerical solution of the equation set (34-35) the finite difference method of the first order approximation over time and second order over space coordinates was used. The system (34-35) was presented by the following set of difference equations [15]:

$$\frac{f_i^{\nu+1}-f_i^{\nu}}{\tilde{\tau}} = 6\Delta\tilde{\varepsilon}\frac{f_{i+1}^{\nu+1}-f_{i-1}^{\nu+1}}{2h_{\tilde{\varepsilon}}} + 4\tilde{\varepsilon}_i\Delta\tilde{\varepsilon}\frac{f_{i+1}^{\nu+1}-2f_i^{\nu+1}+f_{i-1}^{\nu+1}}{h_{\tilde{\varepsilon}}{}^2} + J_i, \quad (41)$$

$$J_i = \frac{1}{8\sqrt{\tilde{\varepsilon}_i\alpha^5}}\frac{1}{2}\Big\{\sum_{j=0} h_{\tilde{\varepsilon}_{ph}}\tilde{\varepsilon}_{ph_j}{}^2\left[f_k^{\nu}N_j + f_i^{\nu}\left(f_k^{\nu} - N_j - 1\right)\right] + \sum_{j=0} h_{\tilde{\varepsilon}_{ph}}\tilde{\varepsilon}_{ph_j}{}^2\left[f_l^{\nu}\left(N_j+1\right) - f_i^{\nu}\left(f_l^{\nu} + N_j\right)\right] +$$
$$\sum_{j=0} h_{\tilde{\varepsilon}_{ph}}\tilde{\varepsilon}_{ph_{j+1}}{}^2\left[f_{k-1}^{\nu}N_{j+1} + f_i^{\nu}\left(f_{k-1}^{\nu} - N_{j+1} - 1\right)\right] + \sum_{j=0} h_{\tilde{\varepsilon}_{ph}}\tilde{\varepsilon}_{ph_{j+1}}{}^2\left[f_{l+1}^{\nu}\left(N_{j+1}+1\right) - f_i^{\nu}\left(f_{l+1}^{\nu} + N_{j+1}\right)\right]\Big\}, \quad (42)$$

$$\frac{N_j^{\nu+1}-N_j^{\nu}}{\tilde{\tau}} = \frac{1}{2\alpha}\frac{1}{2}\sum_i \; h_{\tilde{\varepsilon}}\left[(f_k^{\nu}-f_i^{\nu})N_j^{\nu} + f_k^{\nu}(1-f_i^{\nu}) + (f_{k+1}^{\nu}-f_{i+1}^{\nu})N_j^{\nu} + f_{k+1}^{\nu}(1-f_{i+1}^{\nu})\right], \tag{43}$$

$$f_k^{\nu} = f\left(\tilde{\varepsilon}_i - \tilde{\varepsilon}_{ph_j}\right), \;\; f_l^{\nu} = f\left(\tilde{\varepsilon}_i + \tilde{\varepsilon}_{ph_j}\right). \tag{44}$$

The summation limits are determined from (26). Grid steps were chosen in such way that:

$$\tilde{\varepsilon}_i - \tilde{\varepsilon}_{ph_j} = \tilde{\varepsilon}_k, \;\; \tilde{\varepsilon}_i + \tilde{\varepsilon}_{ph_j} = \tilde{\varepsilon}_l \tag{45}$$

Here *k* and *l* are natural numbers. As a result of calculations electron and phonon distribution functions have been found.

On the Fig. 1 and Fig. 3 is presented the dependence of the electron distribution function decimal logarithm on dimensionless electron momentum for different time moments and two values of the electric field strength: 1.68 V/cm and 33.6 V/cm. On the Fig. 2 and 4 is presented the dependence of the phonon distribution function multiplied by dimensionless phonon momentum cubed on the dimensionless momentum. The curves illustrate uninterrupted growth of the number of high-energy electrons and phonons with time. The curves for the time t=0 correspond to equilibrium distribution functions. In particular, phonon distribution function multiplied by dimensionless phonon momentum cubed for the electric field strength of 33.6 V/cm at the time moment (*t*=1.0) of an order less than for the field of 1.68 V/cm (*t*=10) is more than 66 times greater. For the same values of *t* and electric field strengths the values of the electron momentum at which the electron distribution function equals to 10^{-30} differ in 1.23 times.

For clearness on Fig. 5 is presented a dependence of the phonon distribution function on the dimensionless momentum at electric field strength *E*=16.8 V/cm for different time moments: *t*=0;0.25;0.5;0.75;1;1.25.

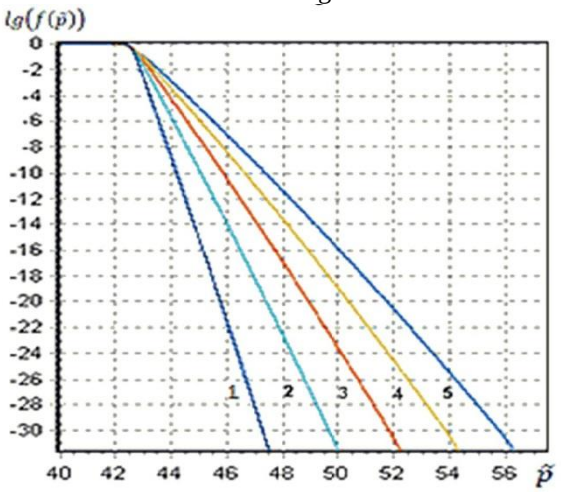

Fig. 3. Dependence of the electron distribution function decimal logarithm on dimensionless electron momentum at *E*=33.6 V/cm for different time moments: *t*=0; 0.25; 0.5; 0.75; 1; 1.25. The curves correspond to these time moments in such order: 1, 2, 3, 4, 5.

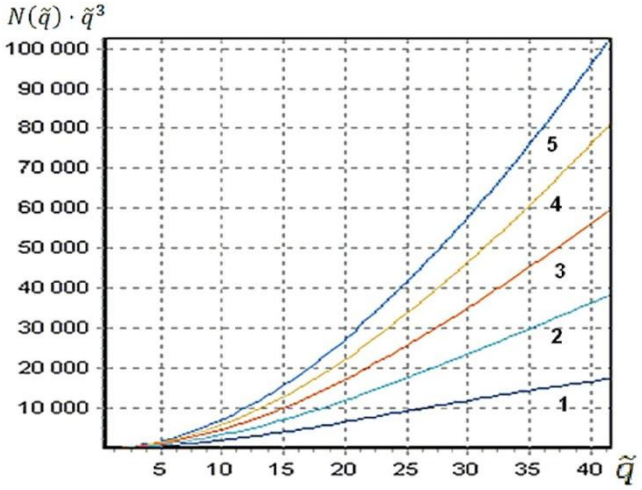

Fig. 4. Dependence of the phonon distribution function multiplied by dimensionless phonon momentum cubed on dimensionless phonon momentum at *E*=33.6 V/cm for different time moments: *t*=0; 0.25; 0.5; 0.75; 1; 1.25. The curves correspond to these time moments in such order: 1, 2, 3, 4, 5.

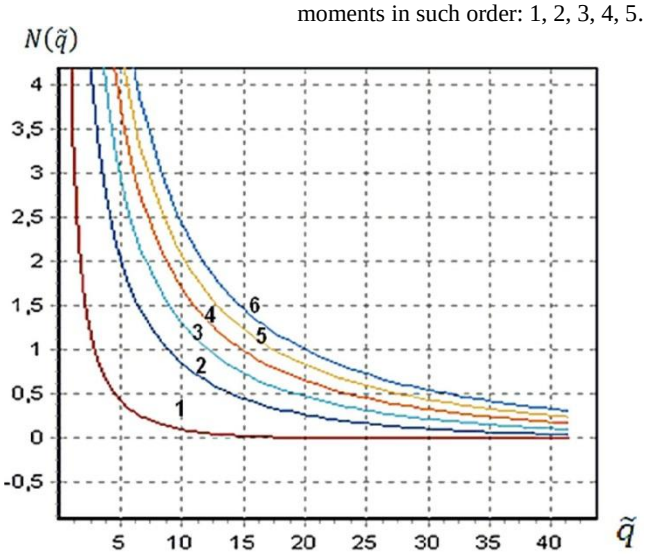

Fig. 5. Dependence of the phonon distribution function on the dimensionless phonon momentum.
E = 16.8 V/cm for different time moments: *t*=0; 0.25; 0.5; 0.75; 1; 1.25.
The curves correspond to these time moments in such order: 1, 2, 3, 4, 5, 6.

For estimation of the influence on the plastic deformation, let us plot the dependence:

$$\frac{\left(F_{\tilde{q}}\right)^2}{\left(F_{\tilde{q}_0}\right)^2} = \frac{\left(\frac{1}{2}+N(\tilde{q})\right)}{\left(\frac{1}{2}+N_0(\tilde{q})\right)} \tag{46}$$

where $N_0(\tilde{q})$ is the Bose-Einstein function for the temperature of 32K, i.e. 12K more than the initial temperature. In the most part of the experiments [1] the heating did not exceed 0.5-3K. $N(\tilde{q})$ is the phonon distribution function found as a result of numerical calculations.

From Fig. 6 and Fig. 7 one can see that the force exerted by phonons upon dislocation is greater than in case of simple heating and it has trend to grow with time.

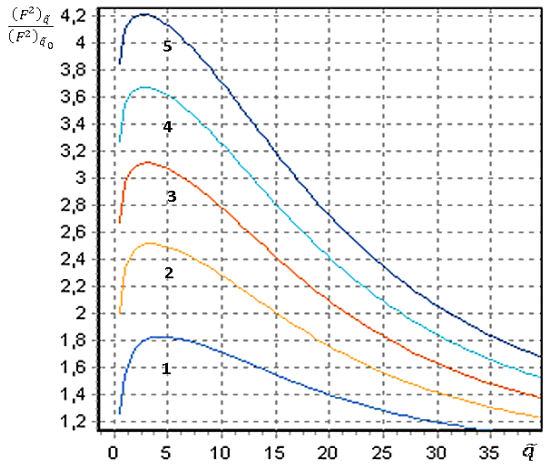

Fig. 6. Dependence of the ratio $\frac{\left(F_{\tilde{q}}\right)^2}{\left(F_{\tilde{q}_0}\right)^2}$ on the dimensionless phonon momentum for different time moments: t=0.25; 0.5; 0.75; 1; 1.25 at E=16.8 V/cm. The curves correspond to these time moments in such order: 1, 2, 3, 4, 5.

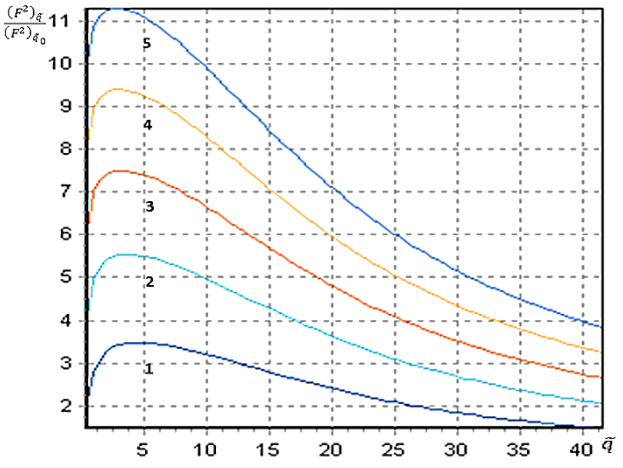

Fig. 7. Dependence of the ratio $\frac{\left(F_{\tilde{q}}\right)^2}{\left(F_{\tilde{q}_0}\right)^2}$ on the dimensionless phonon momentum for different time moments: t=0.25; 0.5; 0.75; 1; 1.25 at E=33.6 V/cm. The curves correspond to these time moments in such order: 1, 2, 3, 4, 5.

COMPARISON WITH THE EXPERIMENTAL RESULTS

Fig. 8 presents the dependence in double logarithmic scale of the phonon distribution function multiplied by dimensionless phonon momentum cubed on dimensionless momentum for different situations:

- thermodynamic equilibrium phonon distribution functions at 20K (curve 1) and 32K (curve 2), correspondingly;
- the nonequilibrium phonon distribution function which was obtained as a result of numerical calculations at the electric field strength E=16.8 V/cm for the time moment of t=2.5 (curve 3).

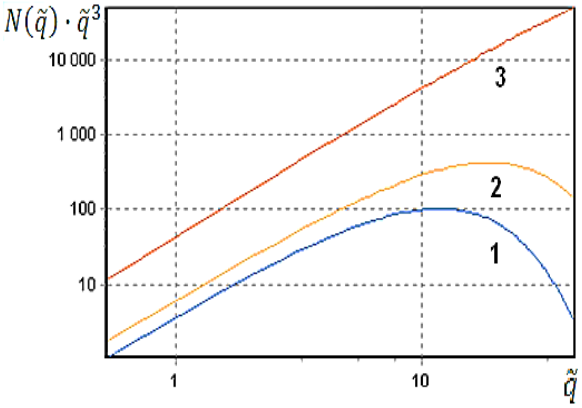

Fig. 8. Dependence of the phonon distribution function multiplied by dimensionless phonon momentum cubed on dimensionless electron momentum. The curve 1 and curve 2 refer to the equilibrium state at 20K and 32K correspondingly. Curve 3 is for the phonon distribution function obtained as a result of numerical calculations the electric field of E=16V/cm at the time moment of t=2.5.

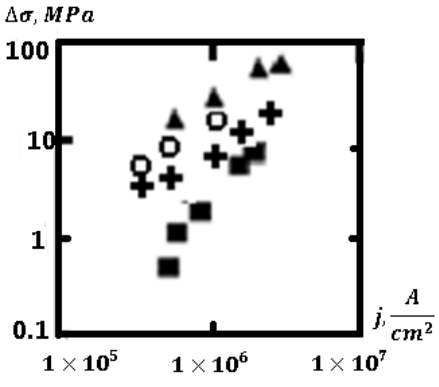

Fig. 9. Dependence of the loading drop [MPa] on the current density [A/cm^2]. Squares are the experimental data provided by Troitsky [1]. Triangles correspond to the experiments of Lebedev [16]. Crosses correspond to our results obtained on the base of Granato-Lücke and Landau-Hoffman model with phonon distribution function at time moment t=2.5μs for electric field strength of 1.6;2;4;8;16;V/cm, empty circles – results for time moment t=15μs for electric field strength of 1.6;2;4 V/cm.

The value of the loading drop has been found in the following order. First of all we substituted the obtained values of phonon distribution function into the formula (17) and found the random force spectral density. Then we have put this result into (16) and found $(Q_n)^2_\omega$.

$$(Q_n)^2_\omega = \frac{\frac{\chi}{\pi}\hbar\omega\left(\frac{1}{2}+N(\omega)\right)}{m^2\left(\omega_n^2-\omega^2\right)^2+\chi^2\omega^2}, \tag{47}$$

Knowing $(Q_n)^2_\omega$ we calculated the correlation function $\psi(0)$ and it's second derivative using the formula (12).

$$\psi\big(0,\mathrm{N}(\omega)\big) = \lim_{\tau\to 0}\int_{-\infty}^{\infty}\frac{\frac{\chi}{\pi}\hbar\omega\left(\frac{1}{2}+N(\omega)\right)}{m^2\left(\omega_n^2-\omega^2\right)^2+\chi^2\omega^2}e^{-i\omega\tau}d\omega,\ \psi''\big(0,\mathrm{N}(\omega)\big) = -\lim_{\tau\to 0}\int_{-\infty}^{\infty}\frac{\frac{\chi}{\pi}\hbar\omega^3\left(\frac{1}{2}+N(\omega)\right)}{m^2\left(\omega_n^2-\omega^2\right)^2+\chi^2\omega^2}e^{-i\omega\tau}d\omega, \tag{48}$$

After that we found $\Psi(\tau)$ and $\Psi''(0)$ using (10).

$$\Psi\big(0,\mathrm{N}(\omega)\big) = 2\sum_{n=1}^{\tilde{n}}\frac{q_n^2}{k^2}\psi\big(0,\mathrm{N}(\omega)\big), \tag{49}$$

$$\Psi''\big(0,\mathrm{N}(\omega)\big) = 2\sum_{n=1}^{\tilde{n}}\frac{q_n^2}{k^2}\psi''\big(0,\mathrm{N}(\omega)\big), \tag{50}$$

After substituting (9) into (1) we have the following relation which allows us to find $\delta\tilde{u}_{cr}^2$ when all other quantities are known:

$$\dot{\varepsilon}_d = bl\rho_d\frac{1}{2\pi}\sqrt{-\frac{\Psi''(0,\mathrm{N}(\omega))}{\Psi(0,\mathrm{N}(\omega))}}\exp\left\{-\frac{\delta\tilde{u}_{cr}^2}{2\Psi(0,\mathrm{N}(\omega))}\right\}, \tag{51}$$

$$\delta\tilde{u}_{cr}\big(\mathrm{N}(\omega)\big) = \sqrt{2\Psi\big(0,\mathrm{N}(\omega)\big)\ln\left(\frac{bl\rho_d}{2\pi\dot{\varepsilon}_d}\sqrt{-\frac{\Psi''(0,\mathrm{N}(\omega))}{\Psi(0,\mathrm{N}(\omega))}}\right)} \tag{52}$$

Finally we find σ from (11):

$$\sigma = \sigma_{cr}\left(1-\frac{\delta\tilde{u}_{cr}\big(\mathrm{N}(\omega)\big)}{x_{cr}}\right), \tag{53}$$

$$\Delta\sigma\big(N(\omega)\big) = \sigma_{ext} - \sigma\big(N(\omega)\big) \tag{54}$$

The comparison between the calculation results and experimental data was made for nickel at following values of experimental parameters: the applied external stress $\sigma_{ext} = 68.885$ MPa, $\dot{\varepsilon}_d = 1.19\cdot 10^{-4}\ \mathrm{s}^{-1}$, $b = 3.52\cdot 10^{-8}$ cm, and the product of $l\rho_d = 435\ \mathrm{cm}^{-1}$, U_0=3.34·10^{-19} J, $x_{cr} = 0.2b$, $L = 3.5\cdot 10^{-5}$cm, $B = 2\cdot 10^{-10}\ \mathrm{N\cdot s\cdot cm^{-2}}$.

The Fig. 9 clearly demonstrates that our approach gives results that are of the same order with experimental data. The expected loading drop in case of heating under the conditions of thermodynamic equilibrium is several orders less that the loading drop observed in experiments. That is why we don't even put it on our figure. The loading drop that was calculated using the obtained data must be considered as lower estimate because the time moments at which the calculation was finished are several times less than the current pulse duration in the experiments.

CONCLUSIONS

In the given work a kinetic consideration of nonequilibrium dynamics of the electron-phonon system of a crystal in a strong electric field has been carried out.

A method of numerical solution of kinetic Boltzmann equations system for electron and phonon distribution function without expansion of the electron distribution function in a series by phonon energy has been proposed.

It has been shown that under the influence of a strong electric field the electron distribution function becomes nonequilibrium in the vicinity of Fermi energy and the influence of electron-phonon collisions becomes commensurable with the influence of the field. Phonon distribution function gets "heated" while remaining nonequilibrium in the region of long-wave phonons.

Basing on the Granato-Lücke and Landau-Hoffman model and using the calculated phonon distribution function it has been shown that the force of the action of the phonons on the dislocations is greater than it would be in case of thermodynamic equilibrium at heating by 12K.

More early results were defined more precisely. The conditions of applicability of the Tailor expansion of the electron distribution function by the phonon energy depending on temperature have been obtained.

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