NONEQUILIBRIUM KINETICS OF ELECTRON-PHONON SUBSYSTEM OF A CRYSTAL IN STRONG ELECTRIC FIELD

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Abstract. 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 can effectively influence on the lattice defects.

1. Introduction

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 by conduction of electric current of high density $j=10^8$-$10^9 A/m^2$ was discovered. This phenomenon has been called electroplastic effect (EPE) [1]. For creation of ab initio theory of electroplastic effect we proposed and preliminary studied [2-4] the mechanism in the framework of the model of stoppers overcoming by a dislocation string as a result of its excitation by phonons, which obtain energy due to nonequilibrium kinetics of the electron-phonon subsystem of crystal in strong electric field, i.e. the phonon mechanism – electrons that get energy from the electric field create phonons that can move dislocations from stoppers. In this work we consider the nonequlibrium kinetics of electron-phonon subsystem in electric field.

2. 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 [7]. In the given work we do not make that assumption and thus

the distribution functions can be, generally speaking, nonequilibrium. For the description of the electron-phonon system nonequilibrium dynamics it is necessary to solve a set of kinetic Boltzmann equations for electron *f* and phonon *N* distribution functions correspondingly. For electron distribution function the Boltzmann equation has the form of:

$$\frac{\partial f}{\partial t} + \vec{v}\frac{\partial f}{\partial \vec{r}} + \frac{\partial f}{\partial \vec{p}}\frac{d\vec{p}}{dt} = I_{ee} + I_{ep} + I_{ed}, \quad (1)$$

$$\frac{d\vec{p}}{dt} = e\{\vec{E}(\vec{r},t) + [\vec{v},\vec{B}(\vec{r},t)]\}. \quad (2)$$

where $\vec{v}$is the velocity, $\vec{p}$ the momentum, t the time, $\vec{r}$ the radius-vector, $\vec{E}$ the electric field, $\vec{B}$ 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. 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 [5,6]:

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

$$w(q) = w_0 q;\ \ w_0 = \frac{\varepsilon_{1A}^2}{2(2\pi\hbar)^2\hbar\rho s};\ \ \hbar\Omega(q) = sq, \quad (3)$$

where $f(\vec{p}_i)$ are the occupation numbers, $\vec{q}$ is the phonon momentum, 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.

$$I_{ed} = \int d\vec{\acute{p}}\, w_{ed}(\vec{\acute{p}} - \vec{p})\delta\left(\varepsilon(\vec{\acute{p}}) - \varepsilon(\vec{p})\right)\{f(\vec{\acute{p}}) - f(\vec{p})\}. \quad (4)$$

Phonon distribution function also obeys the kinetic equation:

$$\frac{\partial N(\vec{q})}{\partial t} + \vec{v}_q\frac{\partial N(\vec{q})}{\partial \vec{r}} = I_{pe} + I_{pp} + I_{pd}, \quad (5)$$

I_{pe} is the phonon-electron collision integral [5,6]:

$$I_{pe} = \int d\vec{p}w(\vec{q})\{\delta(\varepsilon(\vec{p}+\vec{q}) - \varepsilon(\vec{p}) - \hbar\Omega(\vec{q}))[f(\vec{p}+\vec{q})(1 - f(\vec{p}))(N(\vec{q})+1)] - f(\vec{p})(1-f(\vec{p}+\vec{q}))N(\vec{q})\}. \quad (6)$$

The phonon-phonon I_{pp} and phonon-defect I_{pd} collision integrals in τ-approximation have the following forms:

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

$I_{pd} = -\nu_{pd}(\vec{q})\left[N(\vec{q}) - \overline{N(\vec{q})}\right]$, 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; $\overline{N}(q) = \frac{1}{4\pi}\int N(\vec{q})dO$ is the phonon distribution function, averaged over the angles. Collisions with defects and impurities occur very often ν_{ed} = $3{\cdot}10^{13}$c^{-1}, 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 that has to be solved.

$$\frac{\partial f}{\partial \tilde{t}} - 4\Delta\tilde{\varepsilon}\frac{1}{\tilde{\varepsilon}^{1/2}}\frac{\partial}{\partial\tilde{\varepsilon}}\left[\tilde{\varepsilon}^{\frac{3}{2}}\frac{\partial f}{\partial\tilde{\varepsilon}}\right] = \alpha^{-\frac{5}{2}}\left\{\frac{1}{\sqrt{\tilde{\varepsilon}}}\int_0^{\varepsilon_-} d\tilde{\varepsilon}_{ph}\tilde{\varepsilon}_{ph}{}^2\left[f\left(\tilde{\varepsilon}-\tilde{\varepsilon}_{ph}\right)N\left(\tilde{\varepsilon}_{ph}\right) + \right.\right.$$
$$+f(\tilde{\varepsilon})\left(f\left(\tilde{\varepsilon}-\tilde{\varepsilon}_{ph}\right) - N\left(\tilde{\varepsilon}_{ph}\right) - 1\right)\Big] + \frac{1}{\sqrt{\tilde{\varepsilon}}}\int_0^{\varepsilon_+} d\tilde{\varepsilon}_{ph}\tilde{\varepsilon}_{ph}{}^2\left[f\left(\tilde{\varepsilon}+\tilde{\varepsilon}_{ph}\right)\cdot\right.$$
$$\left.\left.\left[N\left(\tilde{\varepsilon}_{ph}\right)+1\right] - f(\tilde{\varepsilon})\left(f\left(\tilde{\varepsilon}+\tilde{\varepsilon}_{ph}\right) + N\left(\tilde{\varepsilon}_{ph}\right)\right)\right]\right\}, \quad (7)$$

$$\frac{\partial N(q)}{\partial\tilde{t}} = \frac{1}{2\alpha}\int_{\varepsilon_0}^{\infty} d\tilde{\varepsilon}\left[\left(f\left(\tilde{\varepsilon}+\tilde{\varepsilon}_{ph}\right) - f(\tilde{\varepsilon})\right)N\left(\tilde{\varepsilon}_{ph}\right) + f\left(\tilde{\varepsilon}+\tilde{\varepsilon}_{ph}\right)\times\right.$$
$$\left.\left(1 - f(\tilde{\varepsilon})\right)\right]. \quad (8)$$

Here the following designations are used:

$$\alpha = \frac{ms^2}{2k_BT_e};\ \Delta\tilde{\varepsilon} = \frac{e^2E^2\tau_{ep0}}{6m\nu_{ed}k_BT_e};\ \tilde{\varepsilon} = \frac{\varepsilon}{k_BT_e};\ \tilde{\varepsilon}_{ph} = \frac{\varepsilon_{ph}}{k_BT_e};$$
$$\tilde{t} = \frac{t}{\tau_{ep0}};\ \tau_{ep0} = \frac{(2\pi\hbar)^3\hbar\rho}{\pi m^3 s\varepsilon_{1A}^2} = 3.125{\cdot}10^{-7}\ \text{s}.$$

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

$$\varepsilon_- = min\left[4\left(\sqrt{\tilde{\varepsilon}\alpha} - \alpha\right), \tilde{\varepsilon}_{ph_D}\right], \varepsilon_+ = min\left[4\left(\sqrt{\tilde{\varepsilon}\alpha} + \alpha\right), \tilde{\varepsilon}_{ph_D}\right],$$
$$\varepsilon_0 = \frac{\sqrt{\tilde{\varepsilon}_{ph}}}{16\alpha} - \frac{\tilde{\varepsilon}_{ph}}{2} + \alpha. \quad (9)$$

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

$$\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^{\infty}\varepsilon^{\frac{1}{2}}f(\varepsilon)d\varepsilon = n, \quad (10)$$

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

$$\frac{1}{2\pi^2}\left(\frac{1}{\hbar^3}\right)\int_0^{q_D} q^2N(q)dq < \infty, \quad (11)$$

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

$$q_D = \frac{\pi\hbar}{a}, \tag{12}$$

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

$$f_0(\varepsilon) = \left[exp\left(\frac{\varepsilon-\varepsilon_F}{k_b T_e}\right) + 1\right]^{-1}. \tag{13}$$

All quantities are taken for nickel: s= $2.96\cdot10^5$cm/s is the longitudinal sound velocity, n = $2.5\cdot10^{22}$cm^{-3} the conductivity electron concentration, a = $3.5\cdot10^{-8}$cm the lattice constant, $\varepsilon_F = 5\cdot10^{-19}$J.

3. Numerical solution of the kinetic equations set for electron and phonon distribution functions and discussion of the results

The system (17-18) was presented by the following set of difference equations:

$$\frac{f_i^{\nu+1}-f_i^{\nu}}{\tilde{\tau}} = 6\Delta\tilde{\varepsilon}\frac{f_{i+1}^{\nu+1}-f_{i-1}^{\nu+1}}{2h_{\tilde{\varepsilon}}} + 4\tilde{\varepsilon}_i\Delta\tilde{\varepsilon}\frac{f_{i+1}^{\nu+1}-2f_i^{\nu+1}+f_{i-1}^{\nu+1}}{{h_{\tilde{\varepsilon}}}^2} + \frac{1}{\sqrt{\tilde{\varepsilon}_i\alpha^5}}J_i, \tag{14}$$

$$J_i = \frac{1}{\sqrt{\tilde{\varepsilon}_i\alpha^5}}\Big\{\sum_{j=0} h_{\tilde{\varepsilon}_{ph}}{\tilde{\varepsilon}_{ph}}_j{}^2\left[f_k^{\nu}N_j + f_i^{\nu}\left(f_k^{\nu} - N_j - 1\right)\right] +$$

$$+\sum_{j=0} h_{\tilde{\varepsilon}_{ph}}{\tilde{\varepsilon}_{ph}}_j{}^2\left[f_l^{\nu}\left(N_j + 1\right) - f_i^{\nu}\left(f_l^{\nu} + N_j\right)\right]\Big\}, \tag{15}$$

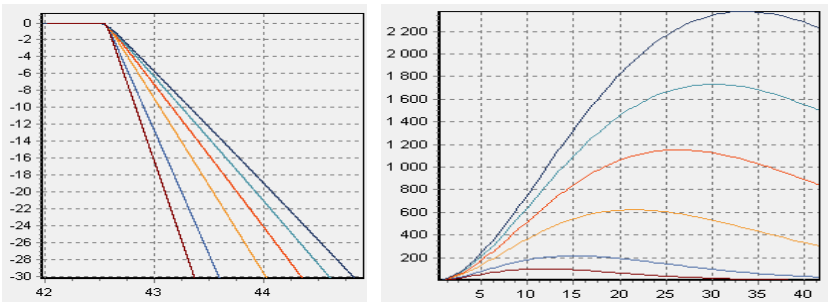
$$\frac{N_j^{\nu+1}-N_j^{\nu}}{\tilde{\tau}} = \frac{1}{2\alpha}\sum_i h_{\tilde{\varepsilon}}\left[(f_k^{\nu} - f_i^{\nu})N_j^{\nu} + f_k^{\nu}(1 - f_i^{\nu})\right], \tag{16}$$

$$f_k^{\nu} = f\left(\tilde{\varepsilon}_i - {\tilde{\varepsilon}_{ph}}_j\right), \quad f_l^{\nu} = f\left(\tilde{\varepsilon}_i + {\tilde{\varepsilon}_{ph}}_j\right). \tag{17}$$

The upper summation limit is determined from (9). Grid steps were chosen in such way that:

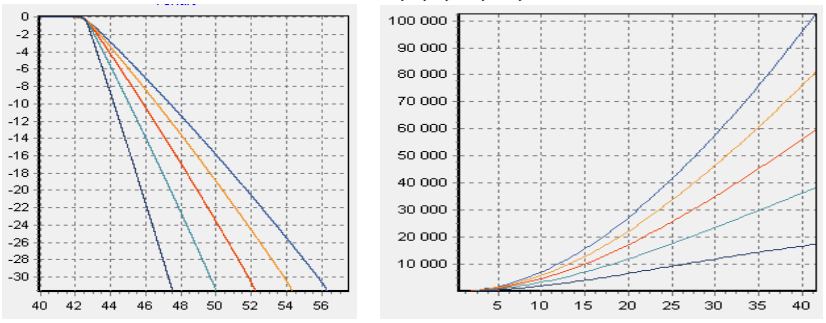
$\tilde{\varepsilon}_i - {\tilde{\varepsilon}_{ph}}_j = \tilde{\varepsilon}_k$, $\tilde{\varepsilon}_i + {\tilde{\varepsilon}_{ph}}_j = \tilde{\varepsilon}_l$, where k and l are natural numbers.

As a result of calculations electron and phonon distribution functions have been found. On the fig. 1a and 2a is presented the dependence in the logarithmic scale of the electron distribution function on dimensionless electron momentum for different time moments. On the fig. 1b and 2b is presented the dependence in the logarithmic scale of the phonon distribution function multiplied by dimensionless phonon momentum cubed on the dimensionless momentum.



a b

Fig. 1. Dependence in the logarithmic scale of the electron distribution function (a), the phonon distribution function multiplied by dimensionless phonon momentum cubed (b) on dimensionless electron momentum for different time: t=0,1,5,10,15,20 at E=1.68 V/cm.



a b

Fig. 2. Dependence in the logarithmic scale of the electron distribution function (a), the phonon distribution function multiplied by dimensionless phonon momentum cubed (b) on dimensionless electron momentum for different time: t=0.25;0.5;0.75;1;1.25 at E=33.6 V/cm.

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.

4.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. 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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