Simulation of Interaction of the Ultra-Short Pulses of Power Electron and Laser Radiation with Metals[1]

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Abstract – The physical mechanisms of energy absorption of the power ultra-short pulses of laser and electronic radiation in metals are discussed. The dynamic equations for describing physical processes in metal at influence of the ultra-short laser or electronic radiation are obtained and discussed.

1. Introduction

Influence of high-intensity streams of energy on the condensed substance is widely used, both in the scientific, and technological purposes. Last achievements in creation of electronic accelerators with pico- and sub-picosecond duration of a beam [1], and also – in obtaining power laser radiation with femto- and sub-picosecond duration [2] have allowed to find out the new physical phenomena, in particular, generation of fast particles and soft x-ray radiation [3]. Interaction of ultra-short electronic and laser radiation with the condensed substance is nonlinear. As duration of a pulse may be much less time of the electron and phonon relaxation on momentums, and also of the electron-phonon relaxation, the nonequilibrium system of the electrons and phonons has a time and, probably, spatial memory. The aim of our work is: (i) discussion of the mechanisms determining absorption of energy of power ultra-short pulses of electronic and laser radiation in irradiated metals; (ii) construction of mathematical model of the physical processes occurring in irradiated targets, and also their computer simulation.

2. Physical mechanisms of absorption of the power sub-picosecond laser and sub-nano-second electron radiation in metals

Let's discuss physical mechanisms of absorption of energy of powerful ultra-short laser and electronic radiation in metals. As a rule, in experiments with subpico- and femtosecond lasers are applied Nd: YAG lasers with generation of radiation on 2, 3 or 4 harmonic. We shall make some estimations for a substantiation of a choice of the description of interaction of radiation with metal. As basic units we shall choose atomic units of measurements: lengths a_H=0.5917·10^{-10}m, velocity v_a=1.1877·10^{6} m/s, time $t_a=a_H/v_a$=2.4189·10^{-17} s, energy $\varepsilon_a=e^2/a_H$=27.229 eV, temperature T_a=3.1578·10^5 K, an electric field strength $E_a=ea_H^{-2}$=5.1455·10^{11} V/m, laser radiation intensity – $I_a=cE_a^2/(8\pi)$=2.245011·10^{20} W/m^2, a magnetic induction B_a=4.33232·10^5 T and "relativistic" intensity of laser radiation $I_{rel}=m^2\omega^2c^3/(2\pi e^2)\sim 10^{23}$ W/m^2. Wavelengths of the first four harmonics of the Nd: YAG laser are equal to, accordingly: $\lambda_1=1.06\ \mu$m; $\lambda_2=0.5321\ \mu$m; $\lambda_3=0.3547\ \mu$m; $\lambda_4=0.266\ \mu$m. The period and frequency of the first and fourth harmonics are equal to, accordingly: T_1=3.536·10^{-15} s=146.176t_a ω_1=5.634·10^{14} Hz=0.041ω_p; T_4=8.873·10^{-16} s=36.68t_a; ω_4=1.127·10^{15} Hz=0.0814ω_p. (For estimations aluminum is taken, plasma frequency in which is equal to ω_p=1.384·10^{16}Hz.) The average interatomic distance in Al is equal to $r_s=(3/4\pi n)^{1/3}=1.5\cdot 10^{-10}$ m. Its comparison with wavelength of the fourth harmonic shows, that $\lambda_4 \gg r_s = 28.364a_H$. The length of absorption of laser radiation in aluminum in result of the back bremsstrahlung effect is equal to $d=\alpha^{-1}\sim 10$ nm [4]. Time of an establishment of local thermodynamic equilibrium in electron and phonon subsystems is equal to $\tau_e\sim\tau_{ph}=\tau_r=1.5\cdot 10^{-14}$ s; time of electron-phonon relaxation on energy is $k_BT_{ph}\tau_r(2mC_{s0}{}^2)^{-1}=1.465\cdot 10^{-12}\ \text{s}<\tau_\varepsilon<m_i\tau_r(2m)^{-1}=$ $=3.781\cdot 10^{-10}$ s. (The bottom estimation is obtained on the basis [5].) Thus, $\tau_\varepsilon>>\tau_y>>t_a$. The made estimations allow to draw conclusions: 1) dynamics of electrons and phonons at influence subpico- and femtosecond laser radiation on metals, and also an electromagnetic field can be described in quasiclassical approximation (this conclusion is valid as well for influence of a subnano- and picosecond electron beam on metal); 2) at influence of the subpico- and femtosecond laser radiation in metal the "hot" electrons are generated at practically cold lattice.

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At influence of ultra-short laser radiation on metal the quasi-neutrality is not broken practically, even at absorption due to multiphoton ionization of electrons from internal levels of the ion skeletons. The "delta-like" electrons originating as a result of multiphoton ionization, and conduction electrons warmed up in laser field excite in "free" electronic gas the Lengmuir fluctuations. The Langmuir turbulence, as is known from plasma physics [6], is the basic channel of energy absorption of laser radiation. The "hot" electrons with a free path length more than r_s deform a lattice, exciting in it the nonequilibrium phonons and defects.

In case of influence of an ultra-short electron beam on metal the situation is a little different: the non-compensated negative charge of an electron beam excites not only the Langmuir fluctuations, but also directly deforms a lattice, promoting generation of the nonequilibrium phonons and defects.

A vivid example of influence power subpicosecond laser radiation on metal, which result cannot be explained absorption due to normal back bremsstrahlung effect [4], is experiments of Milchberg with coworkers [7]. Authors [7], measuring intensity falling on an aluminum target and the power laser radiation reflected from it with the fixed duration of a pulse τ_p=400 fs, have established, that the factor of reflection is decreased with laser radiation intensity growth. According to spectral estimations the electron temperature T_e is changed in [7] from room temperature up to 100 eV. With the help of solving an inverse problem in [7] dependence of specific resistance of aluminum plasma from laser radiation intensity was established. The maximal value of specific resistance in experiments [7] is equal to 200μΩ-cmat $I\approx 10^{14}$ W/cm^2. At radiation intensity $I\leq 10^{12}$ W/cm^2 the specific resistance of an aluminum target practically does not vary, i.e. radiation practically is not absorbed due to back bremsstrahlung effect.

It agrees with the estimations given above, in conditions of experiments of authors [7] the "hot" electrons are formed with the free path length more than r_s. In this case, the small-scale kinetic instabilities [6] is responsible for growth of specific resistance of the aluminum target at its heating of femtosecond laser radiation.

In the work of one of us (VNB) [8] results of these experiments are explained, in the assumption that specific resistance of aluminum plasma in experiments of authors [7] is determined by scattering on the density fluctuations excited by ion-acoustic fluctuations. It has shown, that the maximal value of specific resistance $200\,\mu\Omega$-cm is achieved at electron temperature $T_e = 10$ eV and a cold lattice. To this value T_e an average charge of an ion (an average electron number per atom) $Z_i \approx 3.5-4$ and value of the nonideality parameter of ion components $\Gamma_i = e^2 Z_i^2 n^{1/3}/(k_B T_i) \approx 5\cdot 10^3$ are coincident. Thus, down to $T_e = 2$ eV an average charge of ions, and also number free electrons remain practically constants. At $T_e = 100$ eV, corresponding to the maximal intensity of laser radiation $\sim 10^{16}$ W/cm^2 Z_i is more than 8. The character of dependence of the non-ideality parameter of ion components of unisothermal aluminum plasma of solid-state density from electronic temperature Γ_i is similar to character of dependence of an average ion charge, i.e. in conditions of experiments of authors [7] Γ_i is completely determined by electron concentration.

These results show that in analyzing the mechanisms for the absorption of intense ultra-short laser radiation it is necessary to take into account nonlinear collective processes, in particular, Langmuir and ion-acoustic turbulence.

3. Dynamics equations for metals irradiated with power ultra-short pulses of laser or electronic radiation

In agrees with analysis made above the influence of power sub nanosecond electron beams, and also of pico- and femtosecond laser radiation on metals is possible to consider in quasiclassical approximation. As the free path length of electrons may essentially exceed interatomic distance, it is necessary to consider the dynamics of conduction electrons with the help of the kinetic equation. As dispersive lows for the conduction electrons and beam electrons, and also their energy are various, it is necessary to use two kinetic equations. One of them describes dynamics and a loss of the beam electrons; another does dynamics of the conduction electrons. As they make the contribution to a change of an atom momentum of a target we shall describe the metal dynamics in continuum approximation taking into account a space-time evolution of the integer coordinates N^α of the atoms measured in units of the periodicity vectors of a lattice $\mathbf{a}_\alpha\,(\alpha = 1,2,3)$ similarly to [9]. The physically infinitesimal differential of coordinates $d\mathbf{r}$ is connected with integer coordinates at each moment of time by the relation $d\mathbf{r} = \mathbf{a}_\alpha dN^\alpha + \mathbf{u}dt$ [9], where $\mathbf{u} = \dot{\mathbf{r}}$ is a mass velocity.

The local reciprocal lattice vectors, which determine the energy and the quasimomentum of conduction electrons, are introduced according to the relations $\mathbf{a}_\alpha \cdot \mathbf{a}^\beta = \delta_\alpha^\beta, a_{\alpha i} a_k^\alpha = \delta_{ik}$. The invariant metrical tensors of a direct and reciprocal lattice, and also a deformation tensor become: $g_{\alpha\beta} = \mathbf{a}_\alpha \mathbf{a}_\beta$, $g^{\alpha\beta} = \mathbf{a}^\alpha \mathbf{a}^\beta$, $w_{\alpha\beta} = (g_{\alpha\beta} - \hat{g}_{\alpha\beta})/2$ with $\hat{g}_{\alpha\beta}$ being the metrical tensor of an undeformable lattice. The deformation tensor w_{ik} is expressed trough $w_{\alpha\beta}$ according to the relation

$w_{ik} = w_{\alpha\beta} a_i^\alpha a_k^\beta$ [9]. The space-time evolution of the local vectors of a direct and reciprocal lattice is determined by the following equations [9]:

$$\frac{\partial \mathbf{a}_\alpha}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{a}_\alpha - (\mathbf{a}_\alpha\cdot\nabla)\mathbf{u} = 0, \qquad (1)$$

$$\frac{\partial \mathbf{a}^\alpha}{\partial t} + \nabla(\mathbf{a}^\alpha \mathbf{u}) = 0. \qquad (2)$$

The lattice density ρ_l is expressed trough $g = \det g_{\alpha\beta}$ according to the relation $\rho_l = m_i/\sqrt{g}$ with m_i being an ion mass. The Hamiltonian and conduction electron energy in a deformed lattice are determined by the following expressions [9]:

$$H = \varepsilon(k_\alpha, g^{\alpha\beta}) + k_\alpha \mathbf{a}^\alpha\cdot\mathbf{u} + mu^2/2, \qquad (3)$$

$$\varepsilon = \varepsilon(k_\alpha, g^{\alpha\beta}) = \varepsilon(\mathbf{k}\cdot\mathbf{a}_\alpha, g^{\alpha\beta}) = \varepsilon(\mathbf{a}_\alpha\cdot(\mathbf{p}-m\mathbf{u}), g^{\alpha\beta}) \qquad (4)$$

with k_α being the invariant quasimomentum of a conduction electron. The kinetic equation for conduction electrons in a defect-less deformable lattice looks like:

$$\frac{\partial f_e}{\partial t} + \tilde{\mathbf{V}}(\nabla f_e)_{\mathbf{k}} - \mathbf{a}_\alpha \frac{\partial f_e}{\partial k_\alpha}\left\{ \begin{aligned} &\left(\nabla(\varepsilon + m\mathbf{u}^2/2)\right)_{\mathbf{k}} + \frac{e}{c}\tilde{\mathbf{V}}\times\tilde{\mathbf{B}} + \\ &+ e\mathbf{E} + m\frac{\partial \mathbf{u}}{\partial t} \end{aligned} \right\} = \frac{\delta f_e}{\delta t}, \qquad (5)$$

with $\tilde{\mathbf{V}} = \mathbf{u} + \mathbf{a}_\alpha \partial\varepsilon/\partial k_\alpha$, $\tilde{\mathbf{B}} = \mathbf{B} - (mc/e)\nabla\times\mathbf{u}$.

The kinetic equation for phonons follows from (5) if we shall put a quasiparticle weight equal to zero. The kinetic equation for the beam electrons in the deformable lattice may be written as:

$$\frac{\partial f_b}{\partial t} + \tilde{\mathbf{V}}_b \nabla f_b - \frac{\partial f_b}{\partial \mathbf{v}_b}\left\{ \begin{aligned} &\nabla\left(\frac{\mathbf{v}_b^2}{2} + (\mathbf{v}_b\cdot\mathbf{u}) - \frac{\mathbf{u}^2}{2}\right) + \\ &+ \frac{e}{m}\left(\mathbf{E} + \frac{1}{c}\tilde{\mathbf{V}}_b\times\mathbf{B}\right) \end{aligned} \right\} = \frac{\delta f_b}{\delta t}, \qquad (6)$$

where $\tilde{\mathbf{V}}_b = \mathbf{v}_b + \mathbf{u}$. In case of a laser radiation influence the kinetic equation (5) for fast electrons is absent. The operators of collisions in the equations both (4) and (5) take into account elastic and inelastic collisions with the lattice defects, phonons and electrons, and also the Langmuir plasmons.

The electromagnetic field in (5) and (6) is the result of the self-consistent response of an electron-phonon system of metal on influence of an electron beam or laser radiation. An electromagnetic field outside of and inside medium will be coordinated to the help of boundary conditions known from the electrodynamics of moving media.

The Maxwell equations for the nonmagnetic and non-polar medium in laboratory coordinate system have a usual form:

$$\nabla\times\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{H}}{\partial t},\ \nabla\times\mathbf{H} = \frac{4\pi}{c}\mathbf{j}_e + \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t}, \qquad (7)$$

$$\nabla\cdot\mathbf{E} = 4\pi q,\ \nabla\cdot\mathbf{H} = 0. \qquad (8)$$

The time evolution of a lattice charge $q_l = Z_i e/\sqrt{g}$ is determined by the following equation:

$$\frac{\partial Z_i}{\partial t} + (\mathbf{u}\nabla)Z_i = \frac{\delta Z_i}{\delta t}. \qquad (9)$$

The electrical current density in the laboratory and co-moving coordinate systems is determined by the expression

$$\begin{aligned} \mathbf{j}_e &= q_l\mathbf{u} - e\mathbf{a}_\alpha\left\langle \frac{\partial\varepsilon}{\partial k_\alpha} f_e \right\rangle - e\langle f_e\rangle\mathbf{u} - \\ &- e\langle \mathbf{v} f_b\rangle - e\langle f_b\rangle\mathbf{u} = q\mathbf{u} + \mathbf{j}'_e. \end{aligned} \qquad (10)$$

With accuracy to $|\mathbf{u}|/c$ the vectors of an electromagnetic field in co-moving frame take the form as in [9]:

$$\mathbf{E}' = \mathbf{E} + \frac{1}{c}\mathbf{u}\times\mathbf{H},\ \mathbf{H}' = \mathbf{H} - \frac{1}{c}\mathbf{u}\times\mathbf{E}. \qquad (11)$$

Let us write the balance equation of the momentum of continuum medium with quasiparticles, an electron beam and an electromagnetic field as

$$\frac{\partial(\rho u_i)}{\partial t} = -\frac{\partial}{\partial x_k}(\Pi_{ik} + T'_{ik}) + \frac{m}{e}\frac{\partial j'_{ei}}{\partial t} - \frac{\partial g_i}{\partial t}, \qquad (12)$$

Where $\Pi_{ik} = L_{ik} + P_{ik}$; $L_{ik} = -(\sigma_{ik} + E_l\delta_{ik}) + \rho_l u_i u_k$;

$\sigma_{ik} = 2(\partial E_l/\partial g^{\alpha\beta}) a_i^\alpha a_k^\beta$; $P_{ik} = \sigma_{ik}^{(e)} + \sigma_{ik}^{(p)} +$
$= m a_i^\alpha \langle f_e \partial\varepsilon/\partial k_\alpha\rangle u_j + m u_i a_j^\beta \langle f_e\partial\varepsilon/\partial k_\beta\rangle$;

$T'_{ik} = (E'_i E'_k + H'_i H'_k)/4\pi$; $\mathbf{g} = \mathbf{E}\times\mathbf{H}/(4\pi c)$;

$\sigma_{ik}^{(e)} = 2\langle f_e \partial\varepsilon/g^{\alpha\beta}\rangle a_i^\alpha a_k^\beta$;

$\sigma_{ik}^{(p)} = 2\langle \sum_s f_s \partial\varepsilon_p/g^{\alpha\beta}\rangle a_i^\alpha a_k^\beta$.

To the equation (12) it is necessary to add the equations of balance of energy in system "a deformable crystal – quasiparticles – a field" and also the balance equations for energy of the conduction electrons, phonons, and beam electrons.

At a certain level of excitation the dynamics of a metal electron-phonon system together with an electromagnetic field may result in generation of continuity microbreaks (microdestructions) of a crystal, growth of its vulnerability to damage and, finally, its destruction.

By virtue of limited size of pulse duration of the electron beam or laser radiation the system of the dynamic equations for a crystal may be simplified for solving the specific problems.

4. Conclusion

Thus, in the present work it has shown that at influence of the ultra-short power pulses of electronic and laser radiation on nonmagnetic metal targets it is necessary to take into account excitation of the small-scale kinetic instabilities as one of the main mechanisms of they energy absorption. The dynamic equations for the description of the "plasma-like medium – quasiparticles – an electron beam or laser radiation – the self-consistent electromagnetic field" system have been obtained. The further specification of the formulated mathematical model will be directed on construction of physical and mathematical model of formation of the continuity micro breaks and micro destructions of a crystal structure during its relaxation after the ending of the electronic or laser radiation pulse.

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