

Numerical modelling of physical processes and structural changes in metals under intensive irradiation with use of CRS code: dislocations, twinning, evaporation and stress waves

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Abstract. CRS computer program is presented, which calculates the dynamical deformation of metals under irradiation by high-current electron and powerful ion beams. The incorporated mathematical models allow one to calculate stresses, deformations and structural changes induced by the irradiation. The CRS code numerically solves the equations system, which consists of continua mechanics equations, supplemented by equations of dynamics and kinetics of structural defects: dislocations, grain boundaries, twins, micro-cracks and vapour bubbles. The dislocation plasticity model, the grain boundary sliding model, the mechanical twinning model, the spall fracture model and the non-equilibrium evaporation model are incorporated in the code. The energy release function for electron beam can be calculated within the code, while it can be exported from over programs for ion beam. The CRS code can be a useful tool in theoretical estimation and interpretation of experiments in the field of materials modification by intensive energy fluxes. Restricted rate of plastic deformation provides high values of shear stresses and action of several competitive plasticity mechanisms. Non-equilibrium evaporation of metal in the energy release zone leads to a metastable state of overheated melt, which results in formation of tensile wave following the stress wave in the solid part of the irradiated metal.

1. Introduction

Numerical simulation is an important instrument to reveal conditions and physical processes in the irradiated material, to analyse the obtained experimental data and even to predict possible results of the electron-beam and ion-beam treatment. The BETAIN computer code [1] was developed by A. P. Yalovets especially for the problem of intensive irradiation of metal targets by the beams of accelerated charged particles. It combines numerical solution of the continuum mechanics equations and the transport of fast particles. This code was used for evaluation of stress fields inside the irradiated material [2] and thermodynamic conditions on its surface [3]. In spite of universality and embedded solution of transport problem, the simplest model of perfectly plastic body is used for shear stresses in the BETAIN code, as well as equilibrium approximation for the liquid-vapour transition.

The presented here CRS computer program incorporates more complex plasticity model, which allows one to calculate stresses and deformations in the material of irradiated target together with the



structural changes induced by the stresses. The dislocation plasticity model [4], the grain boundary sliding model [5] and the mechanical twinning model [6] are used for determination of shear stresses and density of lattice defects. Various combinations of these three plasticity mechanisms can reveal themselves depending on the material and the irradiation conditions. Thus, the possibility of accounting of all these mechanisms widens the domain of applicability of CRS. The spall fracture model [7] and the nonequilibrium evaporation model [8] describe the metal fracture near the irradiated [8] and back [9] surfaces. Accounting the non-equilibrium evaporation and the possible metastable state of expanded (overheated) liquid in the energy release zone makes the calculations of stresses more precise in comparison with the approximation of equilibrium liquid-vapour transition [1]. In addition, the non-equilibrium evaporation model allows one to estimate the size of melt drops in the ablated material. The fracture model [7] is necessary for prediction of the spall fracture in the solid material near the back free surface of target.

All mentioned features make the considered program more adequate for simulation of the material behaviour under intensive irradiation in spite of the corresponding complication of underlying models in comparison with [1]. The incorporated models had been previously verified by comparison with experimental results on high-speed impact, for example; and now they are applied to the problems of high-current electron and intensive ion irradiation of metal targets. The CRS makes calculations in 1D approximation, which is sufficient for the most of the problems concerning the metal irradiation.

2. Mathematical model

In general case there are three phases in the irradiated metal: solid, liquid and vapour. Solid and liquid are treated as a single condensed phase for simplicity; meanwhile, shear stresses are accounted for solid and not accounted for liquid. Liquid and solid states can be distinguished most accurately by a wide-range equation of state with explicit tracking of phase boundaries [10]; in the case of simpler equation of state [11] the controlling of temperature can be used. Accounting of separate vapour phase (voids) allows one to describe the dynamic fracture and non-equilibrium evaporation.

2.1. Substance dynamics

The irradiated metal is treated as a two-phase mixture of the carrying agent and the disperse phase. Condensed phase initially is the carrying agent, while pores and cracks form the disperse phase in those parts of metals where they appear. If the voids grow a lot and coalescence, the complete fracture occurs, the carrying agent and the disperse phase change over. The multiphase flow approach [12,13] is used, which is applicable if the characteristic size of phase heterogeneities is much smaller than the scale of flow. The one-velocity approximation is also used: both phases move with the same velocity, which is determined by stresses in the carrying agent [12]:

$$\rho \frac{dv}{dt} = -\frac{\partial P_c}{\partial z} + \frac{\partial S_{zz}}{\partial z}, \quad (1)$$

where v is the substance velocity; z is the coordinate; P_c is the pressure in the carrying agent; S_{zz} and similar are the stress deviators, which are accounted only in the solid carrying agent; ρ is the average density of mixture. Subscript “c” identifies the carrying agent, while “d” identifies the disperse phase. Volume fractions of the carrying agent α_c and the disperse phase α_d :

$$\frac{d\alpha_c}{dt} = \alpha_d \frac{\partial v}{\partial z} - W, \quad \frac{d\alpha_d}{dt} = -\alpha_d \frac{\partial v}{\partial z} + W, \quad (2)$$

where W is the growth rate of the dispersed phase volume per unit volume of mixture. True densities of phases:

$$\frac{d\rho_c}{dt} = \frac{\rho_c}{\alpha_c} \left(-\frac{\partial v}{\partial z} + W \right) - \frac{J}{\alpha_c}, \quad \frac{d\rho_d}{dt} = -\frac{\rho_d}{\alpha_d} W + \frac{J}{\alpha_d}, \quad (3)$$

where J is the growth rate of the dispersed phase mass per unit volume of mixture. The average density in equation (1) is calculated as $\rho = \alpha_c \cdot \rho_c + \alpha_d \cdot \rho_d$. Equations for internal energies:

$$\alpha_c \rho_c \frac{dU_c}{dt} = -P_c \cdot \left(\frac{\partial v}{\partial z} - W \right) - Q + \rho_c \alpha_c \cdot D - J \cdot (U_{tr} - U_c) + \frac{\partial}{\partial z} \left(\kappa \frac{\partial T_c}{\partial z} \right) + Q_{pl},$$

$$\alpha_d \rho_d \frac{dU_d}{dt} = -P_c \cdot W + Q + \rho_d \alpha_d \cdot D + J \cdot (U_{tr} - U_d), \quad (4)$$

where Q is the power of heat exchange between phases per unit volume of mixture; T is the temperature; subscript “tr” identifies the phase which mass is increasing; Q_{pl} is additional heating rate due to the plastic deformation. The energy release function D for fast electrons is calculated by CRS with use of the method [14] for electron transport; for ions this function is exported from BETAIN [1]. Equations (2)–(4) follows from the conservation of volume, mass and energy in a mixture element; functions W , J and Q express the exchange rates between phases, including phase transition.

2.2. Dynamic fracture in liquid and solid states

Liquid is unstable against the phase transition into vapour at pressure lower than the saturation vapour pressure, particularly, at any negative pressure. It is typical for expanding heated layer of metal near the irradiated surface. In these conditions the cavitation occurs consisting in nucleation and growth of vapour cavities, it finally results in ablation of metal from the irradiated surface. Nucleation of cavities demands the work against the surface tension; therefore, the melt can exist in a metastable state of expanded liquid (at negative pressure) during some time [15]. Nucleation of cavities due to the thermal fluctuations is dominant at high strain rates especially for the intensive irradiation. Spherical shape of cavities is preferable due to the surface tension; their growth is described by the Rayleigh-Plesset equation [16]. Equations for nucleation and growth of cavities [8] and the mass exchange due to the phase transition allow us to determine the exchange rates W , J and Q in this case.

A similar situation takes place in the expanded solid at the shock wave reflection from the back target surface. From the one hand, fracture in solid state is more complex because of complicated shape of voids (from spherical one to narrow cracks) and influence of shear stresses. From another hand, the mass and heat exchange rates, J and Q , can be supposed to be zero with high accuracy because the cavities are almost empty. The fracture model [7] is used in CRS, which considers nucleation (due to thermal fluctuations) and growth of cracks, it allows us to determine W ; the model had been tested for wide range of strain rates—from 10^4 s^{-1} to 10^9 s^{-1} .

2.3. Plasticity

Total plastic strain of polycrystalline metal can be represented as a result of the combined action of three competing processes: i) the dislocation motion, ii) the mechanical twinning and iii) the sliding along the grain boundaries. According to this viewpoint, the plastic deformation tensor w_{ik} is represented by the following sum of three tensors: $w_{ik} = w_{ik}^D + w_{ik}^{tw} + w_{ik}^{gb}$, where w_{ik}^D is the part of plastic deformation caused by the dislocation motion, w_{ik}^{tw} is caused by the mechanical twinning and w_{ik}^{gb} is caused by the grain boundary sliding. Then the Hooke law [17] with accounting of the plastic strain w_{ik} is used for determination of the stress deviators:

$$S_{ik} = 2G \left[\left(\frac{2}{3} \right) u_{zz} \delta_{iz} \delta_{kz} - w_{ik} \right], \quad (5)$$

where G is the shear modulus; δ_{iz} is the bivalent mixed tensor; indexes i and k range over x , y and z . The geometrical deformation u_{zz} is induced by the macroscopic motion of substance:

$$\frac{du_{zz}}{dt} = \frac{\partial u}{\partial z}. \quad (6)$$

It should be noted that all components of the plastic strain and stress deviator tensors can be nonzero even in the case of considered 1D motion of substance [4].

2.3.1. Dislocation plasticity. Dislocations are characterized by scalar densities of mobile ρ_D^β and immobilized dislocations ρ_I^β and velocity of mobile dislocations V_D^β relative to substance; these quantities are determined for all possible slip systems. The slip system of dislocations is determined by the Burgers vector b_i^β and by the normal n_i^β and numerated by superscript β . The plastic strain w_{ik}^D produced by the dislocation plasticity can be found from the generalized Orowan equation [18]:

$$\frac{dw_{ik}^D}{dt} = \sum_{\beta} \frac{1}{2} (b_i^\beta n_k^\beta + b_k^\beta n_i^\beta) V_D^\beta \rho_D^\beta. \quad (7)$$

The equation of dislocations motion is following:

$$m_0 \xi_\beta^3 \frac{dV_D^\beta}{dt} = \left[\sum_i \sum_k S_{ik} b_i^\beta n_k^\beta \mp \frac{1}{2} bY \right] - B \xi_\beta^3 V_D^\beta, \quad (8)$$

where $\xi_\beta = 1/\sqrt{1 - (V_D^\beta/c_t)^2}$ is the quasi-relativistic factor, which accounts that $|V_D^\beta| < c_t$; $c_t = \sqrt{G/\rho}$ is the transverse sound speed in the material; m_0 is the rest mass of dislocations; Y is the static yield strength; B is the phonon drag coefficient. Dislocations move only if the force of the shear stresses is higher than the resistance force $bY/2$; the sign “ \mp ” means that the resistance is always directed opposite to the dislocation motion. Kinetics equations for dislocation densities are described in [7] and reflect the balance between the generation of new dislocations, immobilization and annihilation of the existing one. Generation rate is determined through the energy dissipation rate at the plastic deformation—approximately 0.1 part of the dissipated energy is spent on formation of new defects [19].

2.3.2. Twinning. Twinning becomes an alternative plasticity mechanism at low temperatures and high strain rates [20,21]. Twins are supposed to be cylindrical and characterized by concentrations of mobile N_{TW}^γ and immobilized N_{IM}^γ twins (with fixed boundaries), their radii, R_{TW}^γ and R_{IM}^γ , and thicknesses, h_{TW}^γ and h_{IM}^γ ; possible crystallographic orientations of twins are numerated by γ . The plastic strain caused by twinning is expressed through its volume fraction α^γ :

$$\frac{dw_{ik}^{TW}}{dt} = \sum_{\gamma} \frac{d\alpha^\gamma}{dt} (\tau_i^\gamma n_k^\gamma + \tau_k^\gamma n_i^\gamma) \varepsilon_{TW}, \quad (9)$$

where ε_{TW} is the deformation of twinned material, which is $\varepsilon_{TW} = 1/\sqrt{2}$ in fcc metals [20]; unit vectors τ_i^γ and n_i^γ describe the crystallographic orientation of twins. The volume fraction is calculated from the concentration and size of twins, which are determined in accordance with [6].

2.3.3. Grain boundary sliding. Submodel of the grain boundary sliding [5] includes the equation for the plastic strain w_{ik}^{gb} based on the Maxwell model of highly viscous liquid [17]:

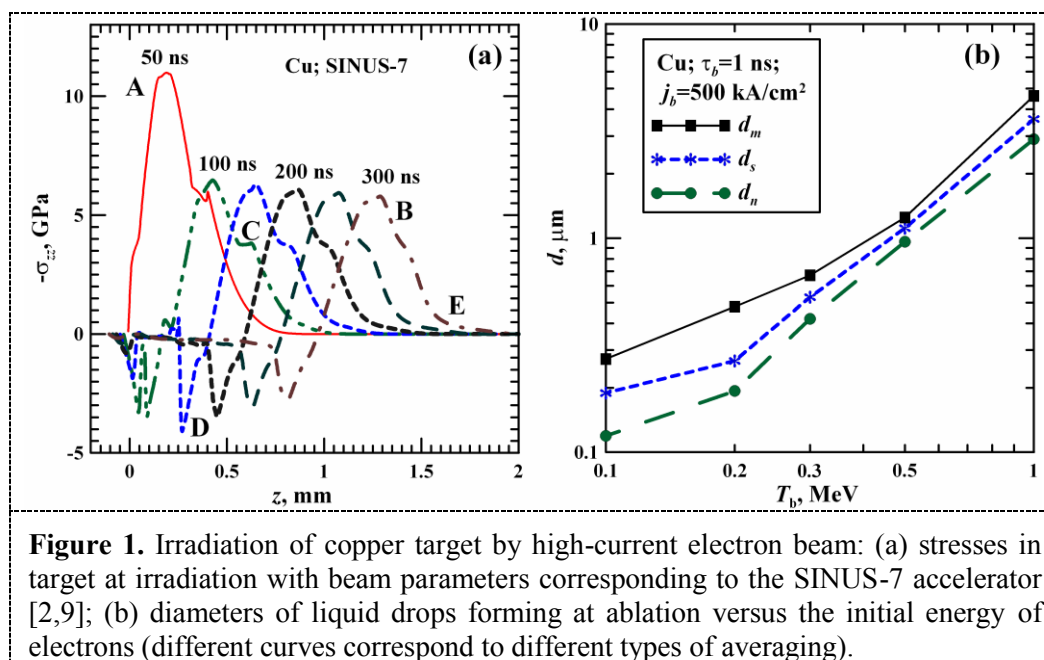
$$\frac{dw_{zz}^{gb}}{dt} = \frac{S_{zz} \mp y_b}{GT}, \quad (10)$$

where T is the relaxation time, which is proportional to the grain diameter [5]. A simple expression was obtained in [5] for the barrier resistance stress y_b —it is proportional to G .

3. Numerical implementation

The described above mathematical model is numerically realized in the CRS computer program written on FORTRAN. This program is designed to simulate the intensive actions on metals: the high-speed impact, intensive electron and ion irradiation. It is supplied by handy data output including the dynamic visualization. Various equations of state can be attached, including the interpolation one [11] and the tabulated one [10]. The bank of plasticity model constants includes aluminium, copper, nickel, iron and stainless steel at this point in time.

Method of separation by physical processes is used at the numerical solution. The substance dynamics is calculated by modification of the numerical method [22]; modification consists in eliminating of the artificial viscosity and accounting of the physical viscosity instead and allows one to obtain the stable solution by using of a fine enough computational grid [23]. Equation (8) for the dislocation velocity is solved with use of the approximate analytical solution. Other equations are solved by Euler method with varied time step. All the described in previous section physical processes can be accounted simultaneously in CRS, or part of them can be excluded for simplicity of analysis.



4. Calculation results

Figure 1 shows the calculation results for irradiation of copper target by high-current electron beam. Figure 1(a) demonstrates the evolution of compression wave generated by irradiation (by the fast energy release): “A” is the high-pressure area in the energy release zone; “B” is the propagating compression wave evolving to the steady shock wave; “E” is the elastic precursor; “D” is the tensile wave, which amplitude is restricted by cavitation (non-equilibrium evaporation); “C” marks the melting boundary between the energy release zone and the main part of the target. Accounting of the non-equilibrium evaporation and the metastable state of expanded liquid in the energy release zone makes possible existence of negative pressures in the tensile wave, while in the frames of equilibrium approximation for the liquid-vapour transition [1] the pressure is limited below by the zero value.

Figure 1(b) presents the size of liquid drops forming at ablation of the surface layer versus the initial energy T_b of fast electrons; the average drops size grows from about 100 nm up to several micrometers with the increase of the fast electrons range in substance together with T_b .

Figure 2 shows the non-equilibrium nature of plastic deformations at the strain rates typical for the intensive irradiation problems. The amplitude of elastic precursor of the shock wave in iron is plotted versus the target thickness: experimental data [24-26] in comparison with our simulations. One can see that the elastic precursor can be very high—up to the amplitude of compression pulse itself (about 10 GPa in the considered case)—in thin targets, therefore, the elastoplastic properties is of high importance in this case. The dislocation plasticity model incorporated in the CRS can describe the experimentally observed evolution of the elastic precursor. Reduction of the target thickness and the thickness of the energy release zone increases the strain rates realized in the target material. High values of shear stresses near the loaded or irradiated surface are explained by restricted density of defects (dislocations)—the concentration of defects is not enough to provide an effective plastic relaxation of shear stresses at high strain rates. It can provoke activation of competitive plasticity mechanisms, such as twinning or the grain boundary sliding.

Figure 3 demonstrates the calculation results for volume fraction of twins and scalar density of dislocations in copper after the high-current electron irradiation (electrons energy is 1.5 MeV, current density is 100 kA/cm², and the pulse duration is 50 ns). The stress wave generated by irradiation initiates the structural changes in the target material—increasing of dislocations density and formation of twins. The twinning becomes an important only at very high intensities of irradiation for materials with low stacking fault energy. Comprehensive numerical investigation of the dislocation density change in metals in the result of intensive electron and ion irradiation are presented in [4,27], while investigation of twinning is a new result.

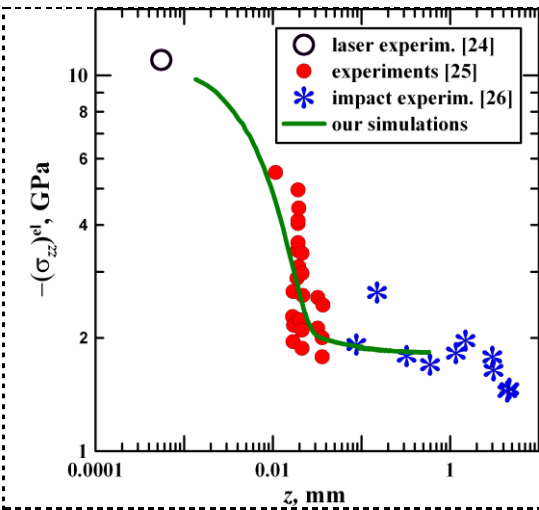


Figure 2. Attenuation of elastic precursor in iron: experimental data [24-26] versus our simulations with us of CRS program.

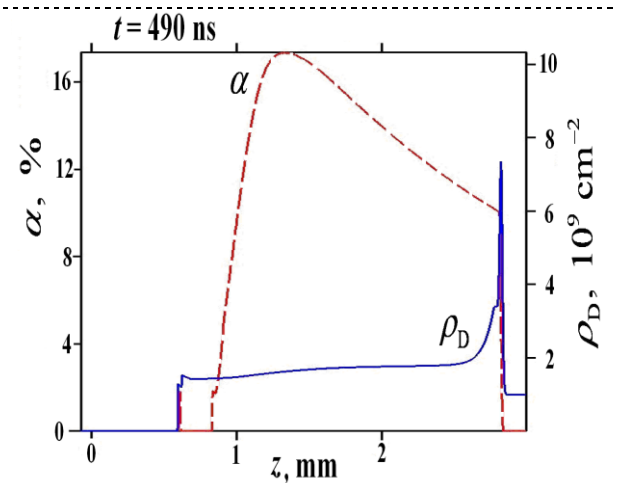


Figure 3. Spatial distributions of the volume fraction of twins α and scalar density of dislocations ρ_D in copper target after irradiation.

5. Conclusions

The mathematical model underlying the CRS computer code is briefly described. It allows one to account non-equilibrium nature of the plastic deformation, evaporation in the energy release zone and spall fracture near the back surface. In addition it determines characteristics of the material microstructure during and after the beam action, including the size of ablated drops, density of dislocations etc. It makes the CRS code a useful tool for analyzes of the metal irradiation by intensive electron and ion beams. Some calculation results are presented and discussed. For example, restricted

rate of plastic deformation provides high values of shear stresses near the irradiated surface and action of several competitive plasticity mechanisms in general case.

Acknowledgments

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