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Numerical investigation of the change of dislocation density and microhardness in surface layer of iron targets under the high power ion- and electron-beam treatment

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ABSTRACT

The effect of the Low Energy High Current Pulsed Electron Beam (LEHCPEB) and High Power Pulsed Ion Beam (HPPIB) surface treatment on the dislocation density in iron target has been numerically investigated. At typical technological irradiation parameters the major factors for modification of dislocation density are the thermo-stresses in the heat affected zone. Irradiation regimes, within the process of which there is no melting, generate one maximum of dislocation density, at the same time the regimes resulting in melting produce two maximums of dislocation density: one of them is localized inside the layer which has crystallized from melt, and the other one at the melt–solid interface. The increase of enclosed energy density and the reduction of pulse duration make the excited stress wave even more significant for the dislocation modification. This wave causes hardening of the material in deeper layers which may eventually result in the influence on the whole volume of the target.

1. Introduction

Nowadays methods of surface modification based on the application of intensive charged particle beams are widely used for the improvement of target surface performance characteristics in medical, aircraft, automobile and reactor construction spheres. One of these techniques is an irradiation by Low Energy High Current Pulsed Electron Beam (LEHCPEB) [1–9]; another one is a High Power Pulsed Ion Beam (HPPIB) treatment of metals and alloys [10–13]. Typically used for processing of metals LEHCPEB and HPPIB have the following parameters: the power density lying in the range 10^7–10^8 W/cm^2, the enclosed energy density — 1–100 J/cm^2, the characteristic electron energy for LEHCPEB — 10–50 keV and the characteristic particle energy for HPPIB — 0.3–1.5 MeV. The well-known results of beam treatment are increase of target hardness and increase of wear and corrosion resistance [2,3,6–8,10,11,13].

The main effect produced by LEHCPEB and HPPIB consists of the fast non-uniform heating of the target substance which consequently leads to the formation of stress fields and shock waves of various intensities. The modified layer usually has three regions located on the different depths within the material: 1) an energy release zone, where beam fast particles lose their energy, the range of LEHCPEB electrons and HPPIB ions in metals makes an order of several micrometers, typically this layer is melted; 2) a heat affected zone with temperature of about 1000 K and more is determined by the heat conductivity and constitutes about tens of micrometers; and 3) a stress affected zone, which thickness can reach hundreds of micrometers.

Intensive plastic deformation accompanied by an increase of dislocation density and by the formation of various dislocation structures is one of the principal causes that leads to the improvement of the substance properties during the LEHCPEB and HPPIB processing; as shown in [14,15] the hardness of pure iron irradiated by electron beam depends on the dislocation density. At the same time such effects as grain size refinement, formation of metastable phases, generation of microcraters, change of chemical composition and others can contribute much in the material hardness modification in the irradiated layer. Moreover, there were reports by some authors who told about the decrease of surface layer hardness as a consequence of tensile stresses forming together with target solidification after the electron beam action produced in the regimes with melting [6,16–18]. However, in this work we are focused only on the consideration of plastic deformation and its accompanying evolution of dislocation ensemble and their importance for the irradiated target property improvement.

The thermo-stresses and propagating stress wave excited by irradiation in the heat affected zone are two fundamental factors of a dislocation structure evolution in the conditions of intensive irradiation [19–23]. The problem of contributing these two factors in the dislocation ensemble evolution is of great importance. The thermo-stresses are enough for

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effective dislocation generation but they have the effect only near the irradiated surface of the target [19–23]. The amplitude of the propagating stress wave may essentially vary. As shown in [24] it is in the diapason from 0.1 to 0.5 GPa at the electron and ion irradiation with parameters usually used in the engineering design [7,11]. Numerical analysis in [20] reports about motion of stress wave with amplitude of about 3 GPa at electron irradiation (particle energy 27 keV, enclosed energy density 27 J/cm^2, duration 1 μs). In the first case amplitude of the wave is not enough for considerable structural transformations in the target material as far as essential increase of dislocation density is observed at passage of shock wave with amplitude greater than several GPa [25], but in the second case the material is exposed to severe plastic deformation in the deep target layers. Theoretical analysis [26] suggests complementary mechanism of the long-range target hardening under ion implantation; the authors demonstrate that dislocations accelerated by stresses in the ion affected zone penetrate into the target with a distance of the order of 20–30 μm.

The rather typical pattern observed with an increase of enclosed energy is the change in the dislocation distribution on depth from the monotone distribution with a maximum located near the target surface to the two-hump one [2,27].

In this paper we numerically investigate the electron and ion beam actions on iron with the help of the continuum mechanics model directly considering plastic deformations of the material by solving the dynamic and kinetic equations for dislocations. As it is presented in the paper, dislocation generation occurs in the heat affected zone under the influence of thermo-stresses at the irradiation of typical technological modes. The dislocation density in the surface layer of the target depends on the input energy density non-monotonically. The process of forming two dislocation density maximums is connected with the dislocation annealing in the zone subjected to melting. The generated shock wave becomes essential only when the enclosed energy exceeds some threshold value depending on the particle energy, pulse duration and properties of the material.

2. Model description

Substance deformation and stress generation under the irradiation are modeled at continual level by equations of continuum mechanics. Plastic deformation of target material is described with the help of a plasticity model formulated in [28] which contains the equations of dynamics and kinetics for dislocations. A beam influence on the target is reduced to the non-uniform heat release. In order to find the spatial distribution of energy released in the target material we solve a kinetic equation for fast particles of the beam by the method described in [29]. The process of modeling is carried out in one-dimensional statement.

Let us formulate the constitutive equations supposing that deformations of medium occur along a direction of the z-axis. The continuity equation and equation of motion are the next form

$$\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\frac{\partial v}{\partial z}, \tag{1}$$

$$\rho\frac{\mathrm{d}v}{\mathrm{d}t} = \frac{\partial \sigma_{zz}}{\partial z}, \tag{2}$$

here ρ is the mass density, v is the substance velocity, σ_{zz} is the full stress decomposed to spherical part, which is pressure P, and to deviatoric part S_{zz}

$$\sigma_{zz} = -P(\rho, U) + S_{zz}. \tag{3}$$

The energy conservation law, in case when both elastic and plastic deformations are taken together with beam action, is given below

$$\rho\frac{\mathrm{d}U}{\mathrm{d}t} = -P\frac{\partial v}{\partial z} + S_{ik}\frac{\mathrm{d}w_{ik}}{\mathrm{d}t} + \frac{\partial}{\partial z}\left(\kappa\frac{\partial T}{\partial z}\right) + \rho\cdot D. \tag{4}$$

U and T are the specific internal energy and the thermodynamic temperature respectively, κ is the heat-conduction coefficient. The electron beam influence on the target has been calculated in Eq. (4) through the function D, which is a rate of energy deposition per unit mass of the substance under the influence of the charged particle beam. The second term describes the change of the internal energy rate due to the dissipation of elastic energy together with plastic deformation of medium, w_{ik} is the plastic distortion tensor, changes in which are provided by the dislocation movement by the relation [30]

$$\frac{\mathrm{d}w_{ik}}{\mathrm{d}t} = -\sum_{\beta}\zeta^{\beta}_{ik}V^{\beta}_{D}\rho^{\beta}_{D}, \tag{5}$$

index β runs all the possible slip systems for a specific type of crystal lattice [28,31], coefficients ζ^{β}_{ik} allow for the orientations of dislocation and slip plane β, V^{β}_{D},ρ^{β}_{D} indicate velocity and density of dislocations in the fixed slip plane β. In this work we study only the connection between dynamics and evolution in dislocation ensemble and the properties of iron target, therefore we use the data on stable dislocations and slip systems for BCC lattice [31]. Dislocations are characterized by the slip plane with a normal vector $\vec{n}$, and by the Burgers vector $\vec{b}$, which lays in the slip plane, so the relation $\left(\vec{n},\vec{b}\right) = 0$ is satisfied. The direction of dislocation motion in the slip plane is defined by the unit vector $\vec{\chi}$, in case of the edge dislocation $\vec{\chi} = \pm\vec{b}/b$ and $\vec{\chi} = \pm\left[\vec{b},\vec{n}\right]/b$ for the screw dislocation, here $b = \left|\vec{b}\right|$ is module of Burgers vector. Signs «+» and «−» in these expressions correspond to "positive" and "negative" dislocations moving in the opposite sides at the same acting stresses. The quantity of possible combinations of $\vec{n}$ and $\vec{b}$ in the monocrystal is finite [31] and index β numbers all such combinations taking into account the edge or screw dislocation type and the sign of dislocation. Coefficients ζ^{β}_{ik} are connected with vectors $\vec{n}$ and $\vec{b}$ through the relation

$$\zeta^{\beta}_{ik} = -b^{\beta}_{i}n^{\beta}_{k}. \tag{6}$$

For BCC lattice physically realized systems of dislocation slip are $\{110\}\langle111\rangle$ and $\{112\}\langle111\rangle$, here Burgers vector is an equivalent for direction 1/2[111]. The module of Burgers vector is supposed to be equal to an average interatomic distance

$$b = \sqrt[3]{\mu/(N_A\cdot\rho)} \tag{7}$$

here μ is the molar mass of the substance, and N_A is the Avogadro number. For BCC lattice 22 slip planes are realized [31].

The plastic deformation of crystal leads to a deviation from Hook's law and, therefore, we use the modified equations for the deviatoric part of stresses

$$\begin{aligned}
&\frac{\mathrm{d}S_{zz}}{\mathrm{d}t} = \frac{4G}{3}\frac{\partial v}{\partial z} - 2G\frac{\mathrm{d}w_{zz}}{\mathrm{d}t},\\
&\frac{\mathrm{d}S_{xx}}{\mathrm{d}t} = -\frac{2G}{3}\frac{\partial v}{\partial z} - 2G\frac{\mathrm{d}w_{xx}}{\mathrm{d}t},\ \frac{\mathrm{d}S_{yy}}{\mathrm{d}t} = -\frac{2G}{3}\frac{\partial v}{\partial z} - 2G\frac{\mathrm{d}w_{yy}}{\mathrm{d}t},\\
&\frac{\mathrm{d}S_{ik}}{\mathrm{d}t} = G\left(\frac{\mathrm{d}w_{ik}}{\mathrm{d}t} + \frac{\mathrm{d}w_{ki}}{\mathrm{d}t}\right),\ \text{at}\ i\neq k
\end{aligned} \tag{8}$$

here G is the shear modulus. Motion of dislocations in crystals leads to the occurrence of S_{xz} and S_{yz} components even at the uniaxial deformations,

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