Propagation of shock waves and fracture in the Al–Cu composite: Numerical simulation

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Abstract. We investigate regularities of the shock wave propagation and fracture in the Al–Cu composite under high-current electron irradiation. A model of multiphase medium mechanics is used, which takes into account the finite rate of stress relaxation between phases, the heat transfer, and the relative motion and friction between components. The multiphase medium model is supplemented by the models of plasticity and fracture. The presence of inclusions in the matrix significantly influences the generation and propagation of stress waves in the irradiated target. In addition, molecular dynamics calculations of tensile strength are performed, which show that the presence of copper inclusions reduces the strength of the material. The reason for softening is the stress concentration near the inclusion, rather than the weak adhesion between copper and aluminum.

1. Introduction
A lot of structural and functional materials have a complex, heterogeneous structure and can be treated as multiphase media, which are the aggregations of volume elements occupied by different phases of one or different substances. In spite of the long history of research [1], the problem of computational description of the multiphase medium dynamics remains relevant up to date [2–5], which is first connected with a large variety of possible systems. The approach of multispeed interpenetrating continuums [1, 2, 4] is one of the developing methods in this field. Here we use this approach to study numerically the deformation and fracture of a composite material (aluminum with copper inclusions) under the action of high-current electron irradiation. In addition, molecular dynamics simulations are used to calculate the tensile strength of the aluminum matrix with copper inclusions.

2. Model of composite
We consider two levels of description of the heterogeneous material: mesolevel and macrolevel. At the mesolevel, at each point of space there is only one defined phase with a defined velocity and thermodynamic state. Each phase of the multiphase (heterogeneous) medium occupies its own volume; there are distinct interfaces between different phases, and material dynamics is described by ordinary (single-phase) continuum mechanics. The macrolevel is an averaging of the mesolevel; different phases are considered as embedded (interpenetrating) continuums at this level of description. Conservation laws, that is, continuity equations, motion equations and internal energy equations for each component, have universal forms for an arbitrary heterogeneous medium, but they do not constitute a closed system of equations. Additional
Equations are necessary for closing, which describe relaxation of phases to the equilibrium—the process of pressure, temperature and velocity equalizing. These equations of interaction between phases depend on the particular structure of the heterogeneous medium, and they are formulated in the mesoscopic framework. The mathematical model we use for heterogeneous medium dynamics is described in detail in [4]. Constitutive equations of this model are extended by the dislocation plasticity [6] and fracture [7] models.

Action of a high-current electron beam is taken into account as an external energy release in the corresponding layer of the substance. The electron transport problem is solved by the method [8]; the heterogeneous material is treated as a homogeneous one with a complex chemical composition at this step. Therefore, the energy release power per unit mass is the same for all phases, while the energy release per unit volume is different.

3. Dynamics of shock waves in irradiated composites

Here we present calculation results for a metal-matrix composite, which is an aluminum matrix with spherical copper inclusions, with a varied volume fraction and size of inclusions. High-current electronic irradiation is simulated with the beam parameters corresponding to the SINUS-7 facility [9]: maximum energy of fast electrons is 1.3 MeV, maximum current density is 8 kA/cm², and pulse duration on half-height is 45 ns. Figure 1a shows the energy release functions (spatial distributions of the deposited power), while figure 1b shows distributions of temperature in both phases. The increase in the volume fractions of inclusions leads to the increase in the mean density and, as a result, to the narrowing of the energy absorption zone (figure 1a). Therefore, a more narrow area with higher compressive stresses is formed in the case of the composite in comparison with pure aluminum. Copper inclusions are heated by the beam to a higher temperature in comparison with the aluminum matrix (figure 1b) due to the higher specific heat capacity of aluminum. Heat exchange between the phases is efficient enough for inclusions of 1 \( \mu \text{m} \) in size, and the temperatures of both phases rapidly become equal in this case (figure 1b). For inclusions of 10 \( \mu \text{m} \) in size the typical time of equalizing is about microseconds and the temperatures of the phases remain substantially different.

Figure 2 shows the distribution of mechanical stresses in the composite at the times of 100 and 500 ns from calculations with two different sizes of inclusions. Heating of the substance by the electron beam leads to the formation of a high-pressure area. The subsequent release of the heated substance forms a shock wave propagating into the bulk of the composite. In the case of small inclusions (1 \( \mu \text{m} \)), there is additional heating of the aluminum matrix from copper inclusions due to more effective heat exchange, which leads to the growth of stresses in the energy absorption zone and formation of a more intensive shock wave (figure 2a). In the course of time, the difference between stresses in pure aluminum and in the composites grows (figures 2b and 2c), first of all, due to the difference in the speeds of shock waves.

Figure 3a shows distributions of melting (0—solid, 1—completely melted) and fracture (0—undamaged, 0.5—completely fractured) indicators of the substance state for the aluminum matrix and copper inclusions. Fracture is calculated on the basis of the model [7]. In the energy absorption zone near the irradiated surface, the matrix and inclusions are subjected to melting. At the same time, there is a region \( 0.5 \text{ mm} \leq z \leq 1 \text{ mm} \), in which the aluminum matrix is melted, while the copper inclusions remain solid; in this region the temperature of the material is between the melting temperatures of aluminum and copper. The damage in the solid part of the aluminum matrix grows and is particularly intensive near the back surface of the target and near the interface with the melt. This damage leading to fracture is the result of action of tension waves, which are the shock waves, reflected from corresponding interfaces. In the case under consideration, the fracture of the composite goes through the fracture of the matrix.

Figure 3b shows distributions of the scalar density of dislocations in both matrix and
Figure 1. (a) Energy release function in pure aluminum and in the composite with various volume fractions of copper inclusions; (b) temperature distributions in the matrix (curves 1 and 3) and inclusions (markers 2 and 4) at the time of 100 ns after the beginning of irradiation; the diameters of inclusions are 1 µm (curves 1 and 2) and 10 µm (curves 3 and 4); the volume fraction of inclusions is 0.1.

Figure 2. (a) Stresses (with negative sign) in the composites with different sizes of inclusions, calculations with the volume fraction of inclusions of 0.1; (b, c) stresses in pure aluminum and in the composites with various volume fractions of inclusions.

inclusions calculated by the model [6]. Initial dislocation density is $10^8$ cm$^{-2}$. The mechanical stresses induced by high current electron irradiation increase by an order of magnitude the dislocations density in the solid part of the target and in the fragments of spalled material.

4. Molecular dynamic simulations
It is well known that fracture can start from the interface between components, because the interface has a lower energy of void formation. As a result, the presence of interfaces can reduce the tensile strength of the composite in comparison with the strength of the weakest component. In order to estimate this reduction, we performed a molecular dynamics calculation of tensile strength of pure aluminum and the composite (aluminum with spherical copper inclusions) using LAMMPS [10] with interatomic potential [11]. The results were used to improve the model. The
calculations were carried out for a system of about half a million atoms (size of $50 \times 50 \times 50$ lattice periods); periodic boundary conditions were used. The radius of the copper inclusions was chosen to be 10 lattice periods. Initial structure of copper and surrounding aluminum corresponded to pure single crystal; deviations from the regular structure were only near the interface. The system was equalized and after that tensioned at a constant stain rate and constant temperature.

Figure 3. (a) Target areas with molten and fractured aluminum matrix and copper inclusions; (b) spatial distributions of scalar density of dislocations in the matrix (Al) and in the inclusions (Cu). The volume fraction of inclusions is 0.1, the size of inclusions is 1 $\mu$m.

Figure 4. Pressure in pure aluminum and in the composite versus time at different temperatures. The strain rate is $10^9$ s$^{-1}$. 
At the initial stage, the elastic deformation of the material takes place while the order of the arrangement of atoms remains unchanged. This stage corresponds to a monotonic growth of the pressure modulus with time (see figure 4). Formation of dislocations is observed at the interface between the components when the tensile stress reaches a value in the range of 3.5 to 6 GPa (the precise value depends on temperature and strain rate). At this moment, the total stress begins to decrease due to the shear stress relaxation. Further tension leads to the formation of a cavity and a sharp drop of the total stress shown in figure 4. The presence of copper inclusions in the aluminum matrix reduces the tensile strength of the material in comparison with pure aluminum. Increased temperature also reduces the tensile strength.

Figure 5. Distribution of the centrosymmetry parameter at the time 101 ps. The strain rate is $10^9$ s$^{-1}$, the temperature is 300 K.

Figure 5 shows the distribution of the centrosymmetry parameter, which illustrates the distortion of the crystal structure in the system. Software package OVITO [12] is used for visualization. Void nucleation occurs near the interface but considerably inside the aluminum matrix. Several atomic layers (from 2 to 5) of aluminum remain on the copper inclusion. This fact shows good adhesion properties of such a system. The inclusion acts as a stress concentrator in this case. The formation of a void leads to a sharp drop in tensile stresses. Subsequent deformation of the material is reduced to the growth of voids.

5. Conclusions

Here we have investigated the initiation, propagation and influence of a shock wave on the material structure and integrity for the case of high-current electron irradiation of a metal-matrix composite. The model of multispeed interpenetrating continuums is used in these investigations with accounting of finite rates of exchange between phases (components). The conservation laws are formulated at the macroscopic level, while the laws of interaction between the phases are derived from the mesoscopic consideration. The presence of inclusions has a substantial impact on the generation and propagation of stress waves in the metal under irradiation. The dislocation plasticity and fracture models are incorporated as parts of constitutive equations of components. In the case under consideration, the fracture of the composite goes through the
fracture of the matrix. In addition, molecular dynamic simulations are used to determine the adhesion strength between aluminum and copper.

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