High-velocity impact of micro- and nanoparticles with metal surface: continuous and atomistic modelling

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ABSTRACT

We present results of continuous and atomistic modelling of the high-velocity impact of microscopic and nanoscale metallic particles with metal surface. Attention is focused on the plastic deformation in the surface layer of the treated metal, change of the defect structure in this layer, and, in the case of atomistic simulation, attachment of material of the particle to the surface. Practical importance of the presented research is connected with development of surface treatment technologies.

Continuous modelling is based on the dislocation plasticity model [1,2] and the mechanical twinning model [3,4], which are used as a part of constitutive relations together with a wide-range equation of state for pressure. These models use explicit description of ensembles of dislocations and twins in the framework of the crystal plasticity approach–with separation of different slipping system of dislocations and twinning systems. The explicit introduction of dislocations and twins allows one to take into account inertness of the plastic deformation, which is important for dynamical problems, and to estimate the change of the defect structure and the mechanical properties as a result of deformation. The equations of model are numerically solved in 2D axis-symmetric case with application of numerical method without artificial viscosity that is substantial for plastic deformation in thin layers and small areas.

Atomistic simulations in the form of classical molecular dynamics are performed with the use of LAMMPS code [5] with various embedded atom potentials.

Plastic flow in the impacted surface layer takes place in the area comparable with the particle size. Transition from the moving and multiplication of pre-existing defects (dislocations) to the homogeneous nucleation of defects takes place at the decrease of the particle size from micrometers to nanometers. Precise value of the threshold depends on the concentration of defects in the initial material, scalar density of dislocations, for instance.

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