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Dynamic methods of nanoparticle assembly: high-velocity impact and shock-wave compaction

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In the frames of additive manufacturing, assembly of metal particles into an object is traditionally performed by sintering or melting under the action of laser irradiation [1-3]. Here we consider another approach to the assembly, which is connected with attachment of nanoparticle by means of severe plastic deformation induced by a high-speed collision or a shock wave action. This deformation improves the contacts, increases the contact areas and allows the particles to be attached by interatomic forces. We refer the considered methods as dynamic methods of nanoparticle assembly and investigate here the corresponding elementary processes by means of molecular dynamics (MD).

Normal collision of single Cu nanoparticle with Al surface, resulting plastic deformation and adhesion have been previously investigated by part of us [4]. Now we investigate inclined collision, interaction with surface roughness (see Fig. 1) and multiple collisions. LAMMPS [5] is used for MD simulations and OVITO [6] is used for visualization and analysis. The inclined collision leads to decrease in the part of kinetic energy, which is spent on mutual plastic deformation of the nanoparticle and substrate. As a result, adhesion and imperfection decrease simultaneously together with the increase in the incidence angle. Interaction with surface roughness (Fig. 1) leads to more pronounced surface deformation, but decreases the generated dislocation length inside the substrate. Multiple collisions form porous structure with strong bonds between particles. Adhesion, nanohardness of the formed layers, as well as acceptable range of collision parameters are analyzed.

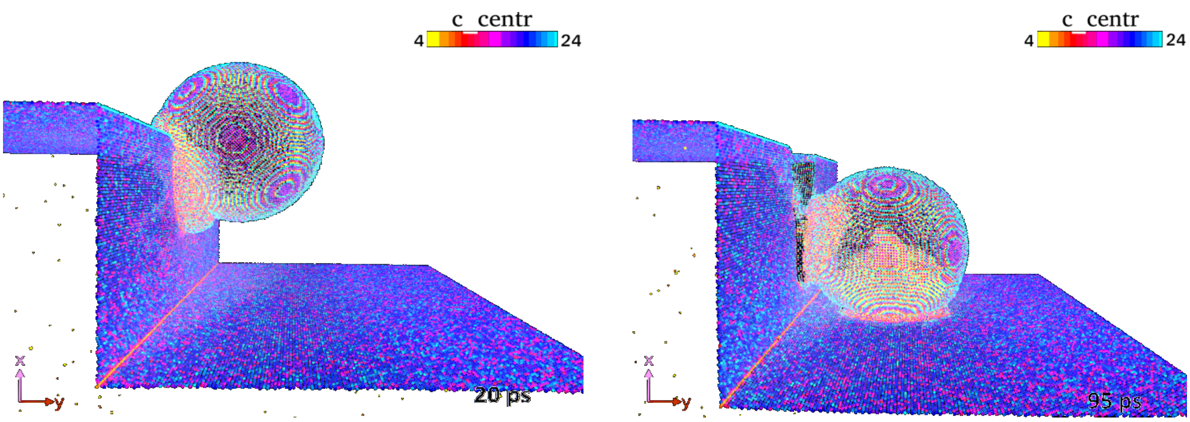

Figure 1. Collision of Cu nanoparticle d = 16 nm in diameter with a step-like protrusion on Al surface: the height of protrusion is equal to d, the overlap is equal to d/4; collision velocity is 500 m/s. MD simulations with about 10 million atoms: two time moments are shown.

Our previous MD investigations [7] have shown that entering of a shock wave on a free surface with nanorelief provokes a severe plastic deformation of the nanorelief elements. Here we analyze prospects of using this effect for consolidation of nanoparticles into solid layer (see Figure 2). Initial layer of nanoparticles can be deposited by the previously considered high-speed collision or, alternatively, by any soft deposition method. MD simulation show that shock compression pulses with nanosecond duration and amplitude about 10 GPa can be an efficient tool for nanoparticle compaction. Using of multiple pulses allows one to compact a layer of arbitrary thickness. Such compression pulses can be initiated by picosecond pulses of laser irradiation of the opposite surface or plate impact with an impactor of nanometer thickness.

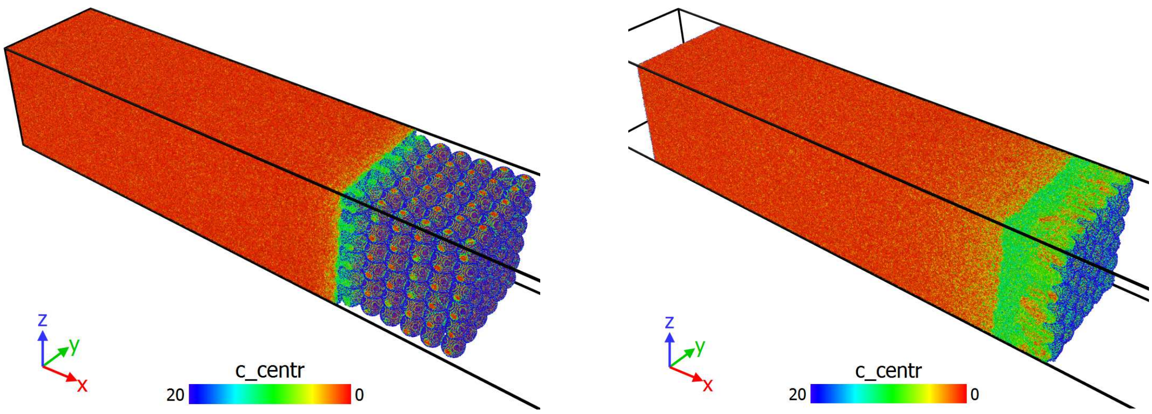

Figure 2. Shock-wave compaction of aluminum nanoparticles on aluminum substrate. Substrate thickness is 85 nm; nanoparticle diameter is 6 nm. Plane shock wave is induced by a high-velocity impact of a plate impactor with thickness of 40 nm and velocity of 800 m/s on opposite surface. MD simulations with 13.3 million atoms: initial (left picture) and final (right picture) states.

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