ATOMISTIC SIMULATION OF SHOCK-WAVE COMPACTION OF METALS NANOPARTICLES

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Shock wave compaction of particles [1,2] is one of the methods for producing nanostructured materials. A molecular-dynamic simulation of the compaction of metal nanoparticles under the action of a shock pulse of picosecond duration is considered. Such a compression pulse can occur when metals are irradiated with powerful femtosecond laser pulses. The layers of nanoparticles are placed in a container or placed freely on the surface of the sample and retained by adhesion forces [3,4]. The pressure pulse on the surface of the system was set by means of an additional external force acting on a thin layer of atoms. The external force acts during the pulse duration, after which the surface becomes free. A shock pulse is formed in the substrate, which is a shock wave and the following discharge wave. Under the action of the shock wave, compaction occurs due to strong plastic deformation of the nanoparticles. Calculations were carried out for aluminum and copper nanoparticles based on the embedded atom method (EAM). An analysis of structural defects was carried out using a centrally symmetric parameter. For the case of nanoparticles in a container, we studied the production of a compact, depending on the amplitude and duration of the shock compression pulse.Depending on the parameters of the action, either elastic compression of nanoparticles or their plastic deformation resulting in compaction was observed.It is shown that the impact of high impact pressures leads to an increase in the number of structural defects and to the danger of a sample breaking due to the rapid process of unloading behind the front of the shock wave. The parameters of the compression pulse are determined to obtain a compact. The impact of successive pulses of shock compression on the opposite surface of the substrate with a layer of nanoparticles adhered to by adhesion also leads to a gradual compaction of the layer into the nanostructured coating. The absence of ejection of nanoparticles is associated with a particularly high value of the adhesion force, which allows nanoparticles to adhere to each other and to the substrate when they are compacted by a shock compression pulse. Molecular-dynamic simulation shows that a rather wide range of parameters (amplitude, duration and number of compression pulses) can be obtained, leading to the compaction of nanoparticles without disrupting the integrity of the sample. The considered method can be generalized for the formation of nanostructured coatings of various compositions. The thickness of the nanocrystalline coating can be locally changed and controlled by the number of active pulses. The work is supported by the Ministry of Science and Higher Education of the Russian Federation, state task No. 3.2510.2017/PP.

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