NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2011, 2 (2), P. 98–101

UDC 538.91

SIMULATION OF STRUCTURAL TRANSFORMATIONS IN COPPER NANOPARTICLES UNDER COLLISION

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PACS 46.25.Cc, 68.35.Rh

The copper nano-sized particles collision under various loading condition was studied in the paper. The special attention was paid to changes in structure of the particles. The numerical investigations were performed by molecular dynamics method. The inter-atomic interaction was described within the embedded atom method. The initial particles were of ideal crystal structure, spherical shape, radius of 6–15 nm. The velocity of collision was varied from 200 up to 1000 m/s, rotation of the particles with the speed up to $1.5 \cdot 10^{13}$ s^{-1} was applied in some calculations. It was shown that specific changes in initial ideal crystal structure of the particles took place under interaction, and the shape of the final particle was not symmetric one. The changes in potential energy of the particles, structural transformation from one type of the crystal lattice to another one as well as quasi-amorphous regions formation were studied in detail.

Keywords: structural transformation, nanoparticles, collision, molecular dynamics.

Simulation of nanoparticles collision is an actual problem having many practical applications such as surface treatment, new materials manufacturing, etc. Here it is important to consider the structural transformation in material of the particles. In particular, for the powder coating on the substrate it is required to increase the degree of mechanical activity of both the particles and the substrate. In addition, the collision process of powders in high cumulative flows is one of the most promising techniques for the synthesis of nanoparticles of complex composition, as well as nanoparticles with a block structure having novel properties [1, 2].

3D case of nano-particles collision was studied using molecular dynamics method [3, 4]. Inter-atomic interaction was described within the embedded atom method (Mishin's potential) and corresponded to copper. This approach allows to describe elastic properties, energy of structural defects, surface energy, melting temperature and other properties with high level of accuracy [5–7].

In [5] calculations were performed for a wide range of collision velocities of copper clusters with a diameter 1 and 2 nm. It was shown that depending on the size and velocity of nanoclusters the two modes of repulsion or association were possible. The conditions of bound state formation and the parameters characterizing the interaction were established. In particular, it was shown that in such nano-objects kinetic temperature in the contact area under collision did not reache melting point and the resulting relationship is determined exclusively by the interaction potential.

In this paper the particle size was much large and varied from 6 up to 15 nm. At that the velocity of each particle varied from 100 up to 1000 m/s. The initial particles had almost spherical

shape and ideal crystal structure under zero temperature. The changes in potential energy and crystal structure of the particles, also as transformation from one type of crystal structure to another one and formation of quasi amorphous region was analyzed.

At the first step central collision of particles was investigated. Calculations showed that the final shape of the particles formed under collision varied from dumbbell to the disk-like depending on the velocity and the size of the initial nanoparticles. In collisions of nanoparticles with velocities ranging from 500 m/s and higher their initial ideal structure undergoes irreversible changes (Fig. 1,c). Nevertheless, after "annealing" at finite temperatures fragments of crystal structure appeared in the resulting nanoparticle. In Fig. 1,d small dots show the atoms not forming any srystal structure, and large gray spheres show atoms, forming a face-centered cubic (fcc) structure.

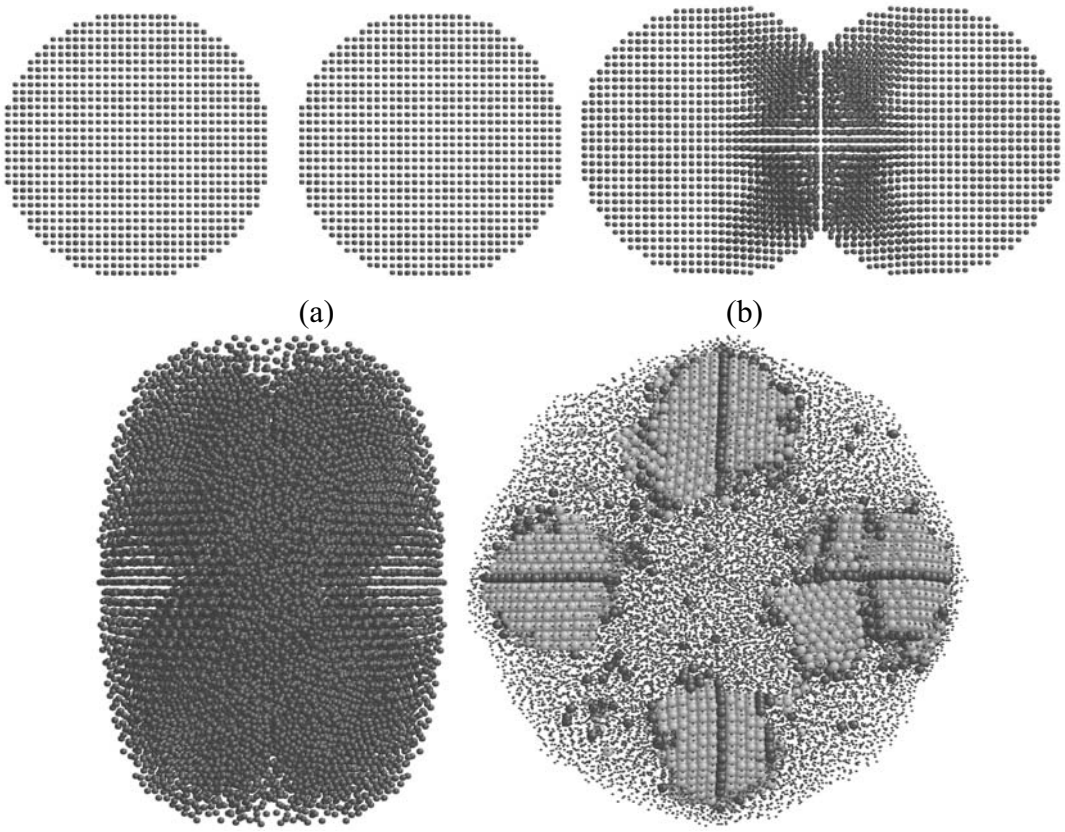

Fig. 1. Nanoparticle structure at different times of collision: a) t=0; b) t=1.1 ps; c) t=3.4 ps; and after "annealing" at 100°K and relaxation to $T = 0$°K (d)

It should be noted that because of their crystalline structure the original simulated nanoparticles, strictly speaking, had not perfect spherical shape but regular polyhedra. Therefore, the thresholds velocities at which the nanoparticles are deformed irreversibly, depend on how they touch under collision (by faces, edges, vertices, etc.).

The resulting nanoparticle fragmented after relaxation was rather stable and deffered from initial nanoprticles by redundant potential energy (Fig. 2).

At the second step of the study special attention was paid to the influence of particles rotation on the change in their structure during the impact. Linear velocity of the collision of the particles varied in the range from 200 to 1000 m/s, and their angular velocity from 0 to $1.5{\cdot}10^{13}$ c^{-1}.

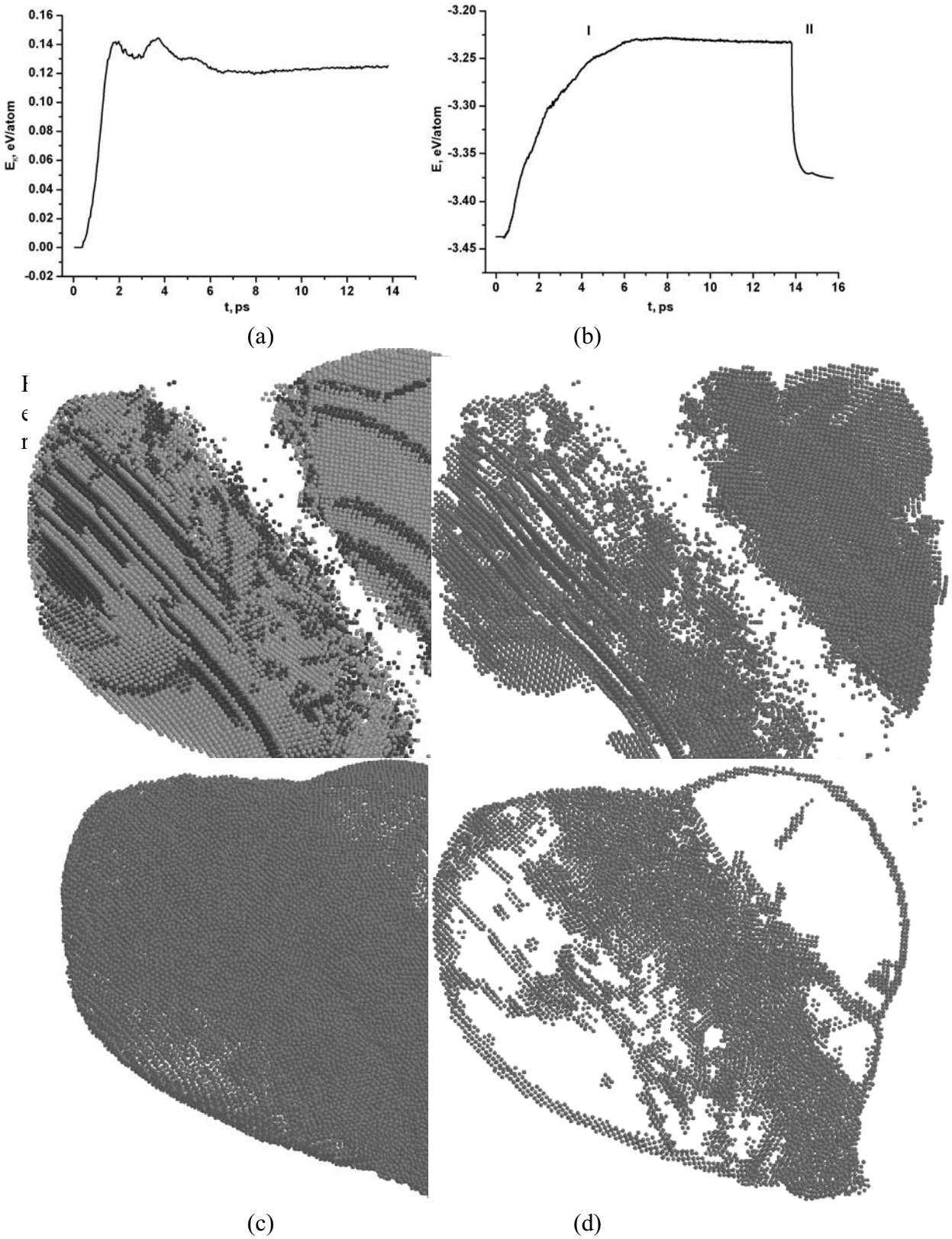

Fig. 3. Atomic structure after collision of two particles. Only atoms forming certain structures are shown: (a) fcc and hcp, (b) fcc, (c) quasi-amorphous structure, (d) section of quasi-amorphous structure by YZ-plane.

Fig. 3 shows the calculation results of two particles collision when one (right) is moving steadily with a velocity of $1000\,\text{m/s}$, and the second rotates with angular velocity $1.5{\cdot}10^{13}\,\text{c}^{-1}$. One can see that after the collision structure of nanoparticles degenerates from an ideal fcc crystal structure into a "mixture" of the fcc, hexagonal close-packed (hcp) and quasi-amorphous structure. Moreover, the atoms forming the hcp structure, are located in parallel planes, dispersed in space relatively to each other. The maximum concentration of a quasi-amorphous structure is attained in the zone of direct interaction between the nanoparticles.

Calculations showed that the shape of final nanoparticle can vary significantly depending on the angular and linear velocities of the collision. Obviously, that due to rotation of one of the particles the final shape of the resulting nanoparticle is not symmetric (Fig. 3) in contrast from the collision without rotation (Fig. 1).

Based on calculations conducted, one can conclude that as a result of collisions of copper nanoparticles of 6–$15\,\text{nm}$ in diameter at velocity above $500\,\text{m/s}$, their structure undergoes irreversible changes. The original crystal structure of nanoparticles is completely destroyed, subsequent relaxation leads to formation of fragmented crystal structure. The resulting nanoparticles after the relaxation processes have redundant potential energy, whose value depends on several factors, such as the geometric dimensions of the initial nanoparticles, the velocity of their collision, the relaxation and annealing temperature. The presence of rotation can play a very important role. For example, such collisions produce a larger part of the amorphous structure, which has a high degree of mechanical activity. In particular, this effect may be useful in the deposition, production of activated powders, etc.

Thus we have shown that as a result of high-velocity collision it is possible to arrange the synthesis of nanoparticles with a blocked crystalline structure having new properties, the production of which by conventional methods is difficult or impossible. The use of such nanoparticles is promising in various directions of high technology, particularly in the chemical processes (e.g. catalysis), and the development of new structural and functional materials with special physical properties (e.g., magnetic). As a further development of the above studies it is interesting to consider the interaction of particles of different material and particles with various defects such as vacancies and interstitial atoms.

Acknowledgements

This work was supported by the interdisciplinary integration project No. 32 of SB RAS for 2009–2011. The authors thank S. Yu. Korostelev and D. S. Kryzhevich for assistance in the calculations.

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