MODELLING OF STATIC AND DYNAMIC PROCESSES OF NANOPARTICLES INTERACTION

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Summary. The problem of dynamic and static of the nanoparticles interaction is considered. Object of research are singl nanoparticles and nanoparticles systems, making composites. By the method of molecular dynamics are investigated the fundamental mechanisms of dynamic and static of the nanoparticles interaction.

INTRODUCTION

. The problem of dynamic and static of the nanoparticles (NP) interaction is urgent for the number of nanotechnology tasks. For example, interaction NP with a surface of materials at the using NP both as modifying agents of a surface of materials and during treating materials, interaction between the NP at forming processes of nanocomposites, interaction NP with environment at the use of nanocomposites, and so on. It will be noted that the investigation of these processes by experimental methods requires substantial material resources and time. Hence the application of mathematical modeling methods allowing carrying out prior investigations of NP interaction save time and economize resources while developing new technologies is quite necessary. The task of modelling of the processes clusters and clusters structures forming was formulated by the author elsewhere [1-4]. The purpose of this work was to develop researches of the author in the field of the analysis of processes of formation and application of powder nanocomposites.

TASK FORMULATION

Problems of a statics NP include two basic tasks: definition of structure of an isolated particle in a quiet, static condition; calculation of parameters NP at its static interaction with an environment and others NP during static formation nanomaterials. Subject of NP dynamics is wider class of problems: formation NP, movement NP in gas and liquid environments,dynamic interaction NP among themselves and with external power (force) fields; division NP on parts and their association, etc. For the problem of modeling of the static and dynamic of NP interaction is present paper the method of molecular dynamics are used. The variant of a method based on use of concept of a power surface of the Bohr – Oppenheimer, being is used by the multivariate space describing energy of system as function of position of atoms nucleus forming it. Numerical integration of the equations of movement of NP atoms was carried out under Verlet method.

NUMERICAL RESULTS

For example, some results of the numerical investigation interaction between nanoparticles are shown in Fig.1-4. Change of a kind of connection cooperating nanoparticles (merging or coupling in larger particles) depending on the its sizes, it is possible to explain on the basis of the analysis of the graph of energy change of connection nanoparticles (fig. 1). From fig 1. follows, that, though with increase in the size of a particle energy of connection E_{np} grows also , its size in comparison with superficial energy of a particle E_S sharply increases at reduction of the sizes nanoparticles. Hence, for fineer particles energy of connection can appear sufficient for destruction of their configuration under action of a mutual attraction and merging in larger particle.

Spatial distribution of particles influences on rate of the forces holding nanostructures, formed from several nanoparticles, also. On fig.2 the chain nanoparticles, formed is resulted at coupling of three nanoparticles (from 512 atoms everyone), located in the initial moment on one line. Calculations have shown, that in this case nanoparticles form a stable chain. Thus particles practically do not change the form and cooperate on « small platforms ». In the same figure the result of connection of three NP, located in the initial moment on a circle and consisting of 256 atoms everyone is submitted. In this case particles incorporate among themselves "densely", contacting on a significant part of the external surface. Distance between particles at which they are in balance it is much less for the particles collected in group: $L^0_{3np} < L^0_{2np}$. It confirms also the graph of forces from which it is visible, that the maximal force of an attraction (F_{3np}) between particles in this case (is designated by a continuous line) in some times more, than at an arrangement of particles in a chain (dashed line) (F_{2np}).

In fig.3 is shown the dependence of strength of a composite on the nanoparticles sizes. It is visible, that at reduction of the sizes of structural elements of a composite (diameter of a nanoparticle) strength of a composite grows.

In fig.4 is shown the interactions of two particles are moving towards each other with different speed. At small speed of moving is formed steady agglomerate (fig.4 right). In a fig. 4(left) is submitted interaction of two particles moving towards each other with the large speed. It is visible, that steady formation in this case is not formed and the particles collapse.

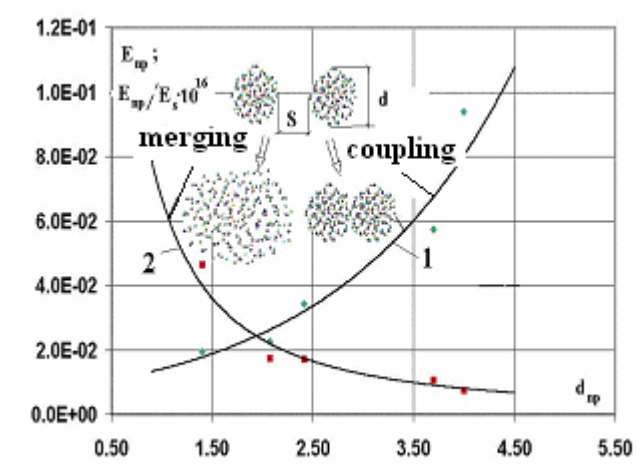

Fig.1

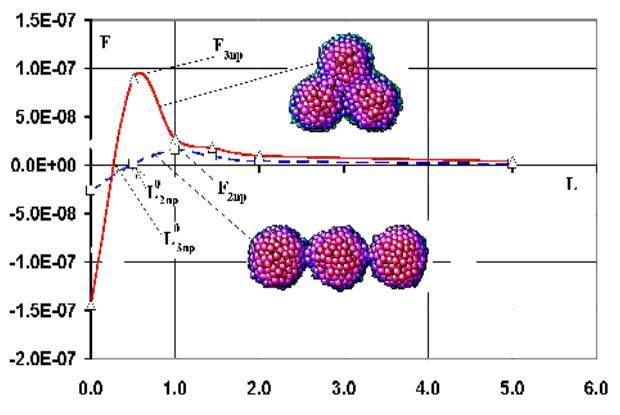

Fig.2

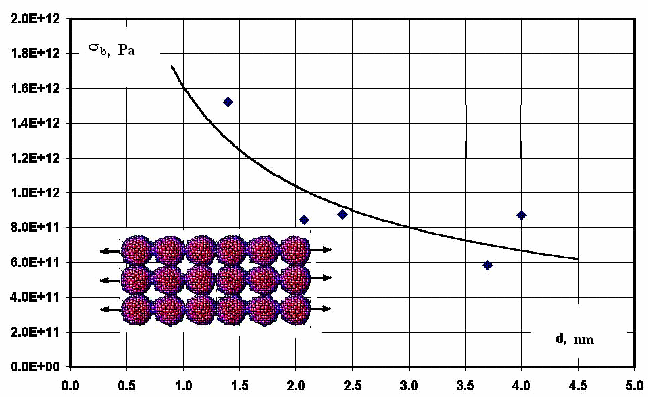

Fig.3

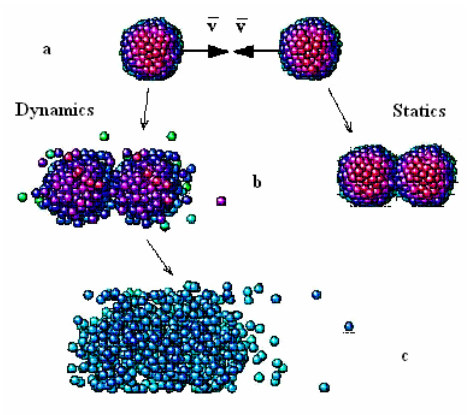

Fig.4

Fig. 1. Kinds of interaction of two nanoparticles and change of energy of their connection (1) and its attitudes to superficial energy (2) depending on nanoparticles diameter. Points designate the calculated values. Continuous lines – approximation

Fig. 2. Change of force of 3 nanoparticles interaction, consisting of 512 atoms everyone, and connected among themselves on a line and on the beams missing under a corner of 120 degrees, accordingly, depending on distance between them

Fig. 3 Dependence of strength of a composite on the nanoparticles sizes

Fig. 4 Pictures of dynamic interaction of two nanoparticles: à) an initial configuration nanoparticles, b) nanoparticles at dynamic interaction, c) the "cloud" of atoms formed as a result of dynamic destruction two nanoparticles

CONCLUSIONS

Thus, the numerical investigation allowed to cover the fundamental mechanisms of NP interaction and to ascertain the basic parameters, defining the conditions of stability NP. In particular, at NP-surface interaction processes nanoparticles can be shattered or dive inside of a material, depending on its drop energy of move, temperature and proportion between ultimate strengths of a material and particle. Depending on thickness of a material nanoparticle can as remain inside a material or pass it through. At low-level energy of move the particle is simple adheres to a surface of a material. At shock of particle at bevel way to a surface it can pull out a slice of a material of a surface, which one can fly away. At interaction nanoparticles among themselves the processes of agglomerate formation, formation of larger particles at merge of particles of the smaller size, absorption by large particles of the smaller ones, dispersion of particles on separate atoms are observed.

References

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