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MOLECULAR DYNAMICS INVESTIGATION OF DEFORMATION RESPONSE OF THIN-FILM METALLIC NANOSTRUCTURES UNDER HEATING

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Molecular dynamics simulation of nanostructure behavior under impulse heating is carried out. These structures are formed by self-rolling of nano-thickness bilayer crystal films. The interatomic interactions are described by potentials obtained by the embedded atom method. The calculation data are shown that simulated nanostructures can transform the supplied thermal energy into the mechanical oscillations of its free edges. The influence of heating rate and its duration, medium viscosity properties on kinematical characteristics of simulated nanostructures is investigated. The influence of mass and size of oscillating free edges of nanostructures on their behavior under heating is studied. The efficiency estimation of thermal energy transformation, supplied to nanostructures, into mechanical oscillations of their free edges versus nanostructure configuration, chemical composition and rate of impulse heating is carried out. The atomic mechanisms responsible for the peculiarities of local atomic structure transformations in bilayer nanofilm under its detaching from the substrate as well as mechanism of thermal energy conversion into mechanical one by nanostructures are investigated.

Keywords: heterogeneous nanostructures, kinematical properties, computer simulation, molecular dynamics, multiparticle potentials.

Introduction

At present, much attention is paid to the investigation of different properties of nanostructures and its use in nanodevices of different functionalities [1]. Nevertheless, the questions connected with atomic mechanisms responsible for nanostructure formation processes are still urgent. The methods of control over nanostructure motions are not sufficiently investigated as well as over capability of these structures to transform supplied energy. The study of the given subjects is the key stone in solution of many fundamental problems. It is of great importance for the practical use of nano-sized structures, for instance, in nanomachines and when designing the nanorobots and nanodevices.

1. Formulation of the problem

The given paper is aimed at studying the atomic mechanisms of structural changes, determining the behavior of non-closed nanostructures formed of bilayer metallic films during the formation process and under thermal loading.

All the calculations in the given paper were made under the molecular dynamics method [2], using the multiparticle interatomic potentials calculated by the embedded atom method [3].

2. Results of numerical simulation

The subject of the given research is the non-closed nano-sized structures formed on the basis of bilayer metallic films with crystalline structure. The simulation of nano-sized structure formation process composed of inclusions with regular internal structure is described in detail [4]. Each inclusion is composed of atoms of a kind; in particular, one type of inclusions was composed of aluminum atoms, another one - of copper atoms. The final shape of simulated non-closed nanostructures was determined by initial parameters of initial nano-sized films. When varying the geometric sizes of copper inclusions and their mutual arrangement in the initial aluminum film, one can obtain the non-closed nanostructures of different shape. In order to accelerate the rolling process of nanostructures, the etching processes of "victim layer" were neglected in papers [4-8]. It was assumed that initial nano-sized film under stress condition is already separated from substrate. Figure 1 presents the simulation results of non-closed nanostructures, composed of aluminum and copper inclusions.

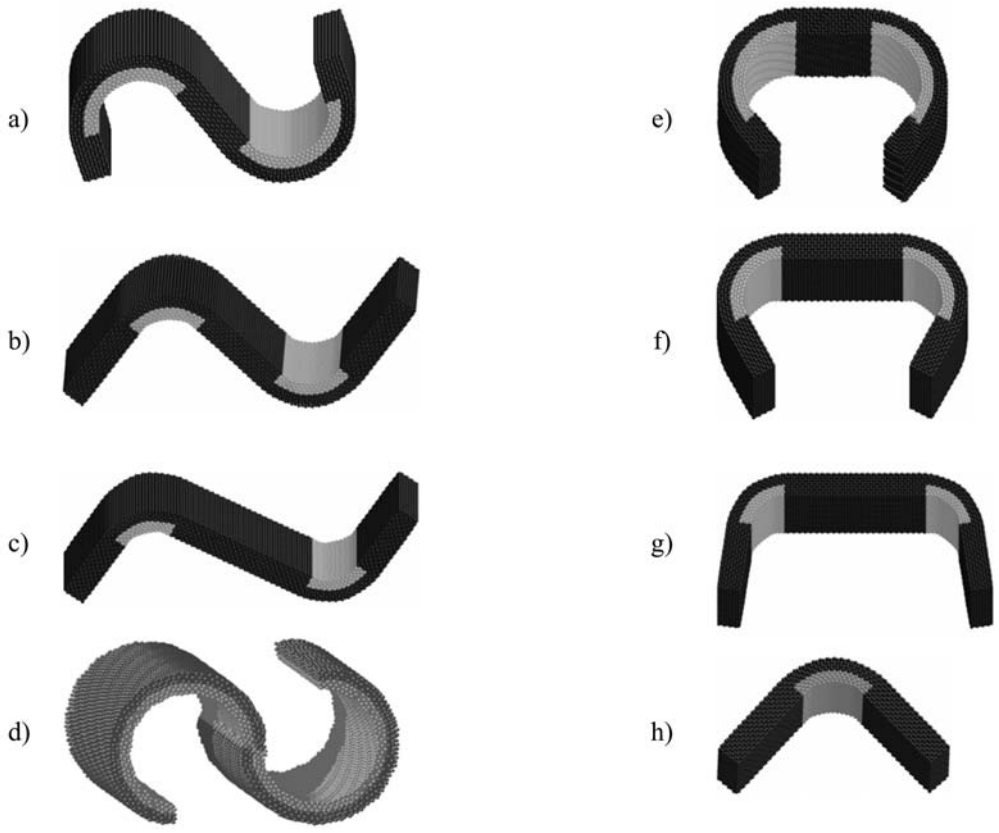

Fig. 1. Shapes of non-closed nanostructures. Copper inclusions of different length are found: a-d– on opposite sides of aluminum film; e-g– on one side of aluminum film; h– is the nanostructure with one inclusion. The copper atoms are shown by light grey color; the aluminum atoms are shown by dark-grey color

The behavior of non-closed nanostructures, presented in Fig. 1, was investigated under heating over the temperature interval from 50 to 500 K. The edges of these structures start oscillating under heating as far as the thermal-expansion coefficients of layers and their temperature dependence differ considerably. The edge oscillation frequencies of simulated nanostructures are essentially independent of heat intensity. At the same time, the length of copper inclusions and their mutual arrangement in the aluminum film affect on frequency and oscillation amplitude.

Increase of inclusion length can lead both to the oscillation frequency increase of non-closed nanostructures (inclusions are found on one side of the film (Fig. 1,e-g)), and to the oscillation frequency decrease (inclusions are found on opposite sides of the film (Fig. 1,a-c)).

The calculation results have shown that oscillation amplitude of edges is increased due to the increase in heating temperature and decreased when cooling the non-closed nanostructure. It points to the fact that a part of supplied thermal energy is transformed into the mechanical oscillation energy of free edges. The oscillation frequencies are found in the gigahertz interval for simulated nanostructures. Thus, when varying the arrangement geometry and copper inclusion sizes in films, one can change a response of the simulated non-closed nanostructure under thermal action.

The investigation of questions on supplied thermal energy transformation by the non-closed nanostructures, is not only of scientific interest, but also is very important from the point of view of design and production of nanoengines and energy converters. For this purpose, the simulation of thermal energy transformation into mechanical one by the example of the nanostructure presented in Fig. 1,f.

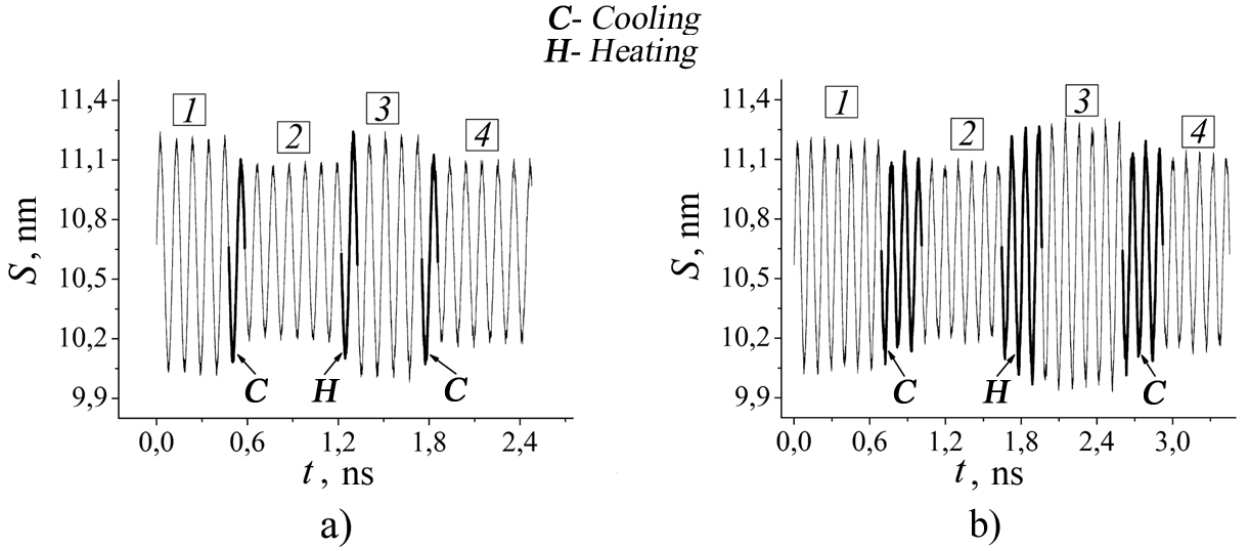

Fig. 2. Dependences of distance *S* between oscillating free edges of the simulated non-closed nanostructure on time. The duration of heating (cooling) made: a – is the one oscillation period; b – is the three oscillation periods

The temperature interval of performed calculations varied over the range of 130 to 230 K. In the model under investigation, the viscosity forces of the medium surrounding the nanostructure was not taken into account, and energy dissipation of mechanical motion (as well as thermal energy supply) was carried out due to the gradual decrease (increase) in nanostructure kinetic temperature by 100 K. Fig. 2,a,b presents the dependences of free edge displacement of the simulated structure on time. The curve sections numbered 1 and 3 correspond to the nanostructure condition with a kinetic temperature of 230 K while the fields numbered 2 and 4, correspond to the nanostructure condition with a kinetic temperature of 130 K. Thus, when varying the temperature of studied nanostructure, it is possible to change the oscillation amplitude of its edges. The influence of heat duration (cooling) for simulated system on the oscillatory motion behavior was also investigated. Heat (cooling) duration varied from one to three periods of nanostructure oscillation. The calculation results have shown that oscillation frequency of the nanostructure edges poorly depends on thermal action duration over the indicated temperature interval (Fig. 2,a,b).

It should be noted that the viscosity forces affecting the oscillatory edges should be accounted under heating for the more realistic behavior of non-closed nano-sized structures.

In order to take into account the viscosity characteristics of the medium, wherein the simulated nanostructure is arranged, the viscosity force was applied to the surface atoms of oscillatory edges (shown by light grey color in Fig. 3,a). The viscosity force affecting the surface atoms, was determined by the formula: $\overrightarrow{F} = -k\overrightarrow{V}$. Where $\overrightarrow{V}$ is the atom velocity; k is the proportionality coefficient.

For test determination of k in this expression, the oscillation damping behavior of nanostructure was investigated for different viscosity values (k varied over the interval from 0 to $6 \cdot 10^{-11}$ $\frac{N \cdot s}{m}$). The calculation results are presented in Fig. 3, b.

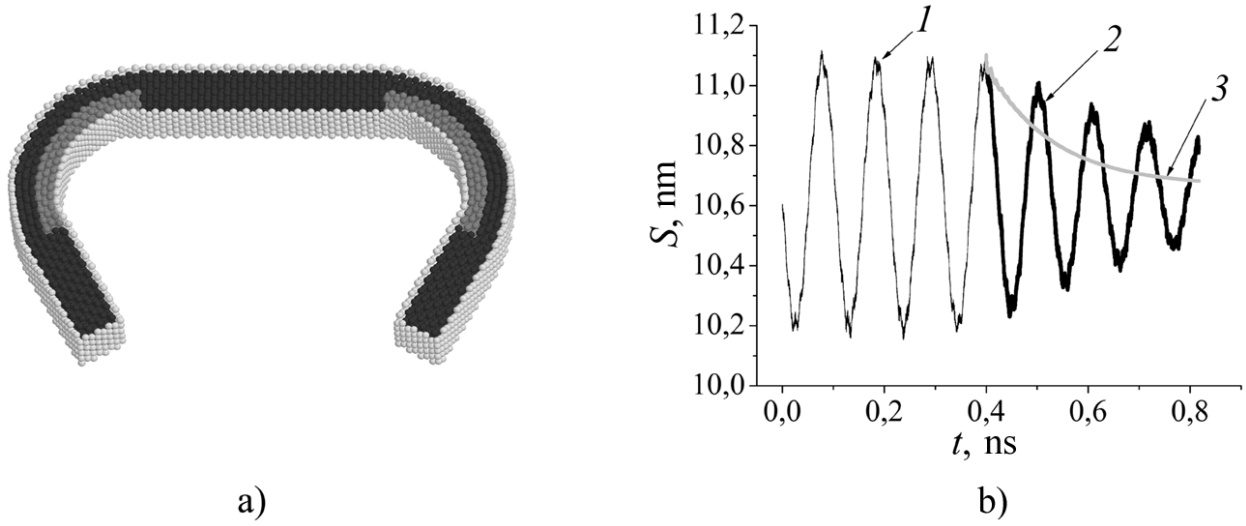

Fig. 3. Shape of nanostructure used for studying its behavior in the viscous medium. The aluminum atoms are shown by black color, copper atoms are shown by dark grey color; the surface atoms of nanostructure affected by viscous force are shown by light grey color (a); Dependences of distance S between oscillating free edges of the simulated non-closed nanostructure on time in mediums with different viscosity characteristics. The proportionality coefficient value of viscous force (k) made: *1*– $k = 0$ $\frac{N \cdot s}{m}$ (nanostructure oscillates without viscosity forces); *2*– $k = 26 \cdot 10^{-14}$ $\frac{N \cdot s}{m}$; *3*– $k = 26 \cdot 10^{-12}$ $\frac{N \cdot s}{m}$ (b).

For test calculations on studying the simulated structure response on pulse heating k is set to $k = 26 \cdot 10^{-14}$ $\frac{N \cdot s}{m}$. The test calculations were made in order to investigate the principle possibility of initial amplitude recovery for nanostructure oscillations (see Fig. 4) in the viscous medium by means of periodical pulsed heating. For this purpose in a certain time interval (here in about three oscillation periods) the simulated structure was heated up for one period. Note that, use of pico- or nanosecond lasers can be one of the methods for pulsed heating of the nanostructures in practice. The initial temperature of simulated nanostructure made 140 K. The oscillation amplitude of edges decreased approximately by 50 % over three periods, and kinetic temperature of the whole nanostructure decreased down to 90 K due to the viscous forces. Then due to the uniform artificial heating, the temperature increased up to 400 K. Under this heating, the oscillation amplitude of edges increased approximately by 40 % relative to its value at the previous section (Fig. 4).

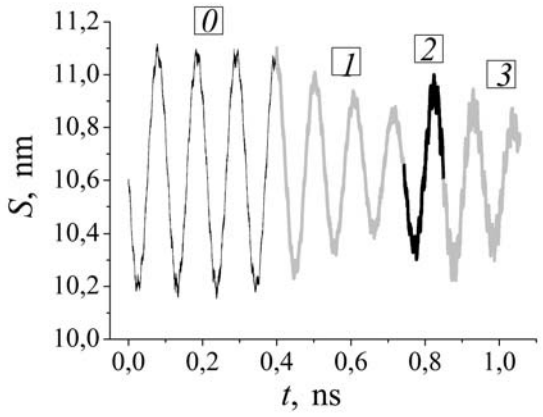

Fig. 4. Variation of nanostructural oscillation amplitude in the viscous medium under pulsed heating: *0*– is the nanostructure oscillations disregard of the viscous force; *1*– is the nanostructure oscillations in the viscous medium ($k = 26 \cdot 10^{-14}$ $\frac{N \cdot s}{m}$); *2*– is the pulsed heating of the nanostructure for one oscillation period; *3*– is the nanostructure oscillations in the viscous medium ($k = 26 \cdot 10^{-14}$ $\frac{N \cdot s}{m}$)

Analysis of using these systems as nanoengines of different functionality is one of the most important aspects of non-closed nanostructure simulation under thermal action. The atomic mechanisms of structural changes in the simulated nanostructures should be investigated, starting from the initial moment of its rolling and finishing with oscillations of the already formed nanostructures. The peculiarities of the atomic system behavior were studied as applied to the Cu-Ni films.

The atomic mechanisms responsible for peculiarities of local atomic structure transformations in bilayer nanofilm under its detaching from the substrate as well as mechanism of thermal energy conversion into mechanical one by nanostructures are reviled. The nanofilms of different thickness are investigated (from 10 to 30 atomic planes). The peculiarities of structural changes of atomic system are studied by analyzing the atomic displacement fields in different points in time for different areas of modeled films. The analysis of the of the atomic displacement fields show that immediately after separation of the film from the substrate, the atomic layers in the film are compressed in direction normal to the free surfaces. The self-rolling of nanofilm involves elastic atomic displacements as vortex collective atomic motion (Fig. 5). The elastic atomic displacements originate at the film edges and are symmetric about the film center. This vortex collective atomic motion is due to the free surfaces and interface between nanofilm layers. The duration of vortex motion of atoms is rather small (for the Cu-Ni system with a thickness of 10 and 30 atomic planes mades not more then several tens of picoseconds), herein the vortex displacement occur at distances from 8 to 15 lattice parameters.

The behavior of non-closed nanostructures under heating is investigated. The initial non-closed nanostructure is relaxed to 200K and then heated up to 300K or up to 500K by means of atom velocities scaling in order to study the transformation of supplied thermal energy into mechanical oscillation energy of its free edges. The efficiency estimation of this transformation is carried out.

The simulation of heating process is carried out for films with following sizes: the lengths are equal to 50, 100, 150 and 200 lattice spacing and the sicknesses are equal to 4, 6, 8, 10 monolayer for each kind of atoms. The efficiency of thermal energy transformation (η) into mechanical oscillation energy of all simulated films is calculated for different temperatures:

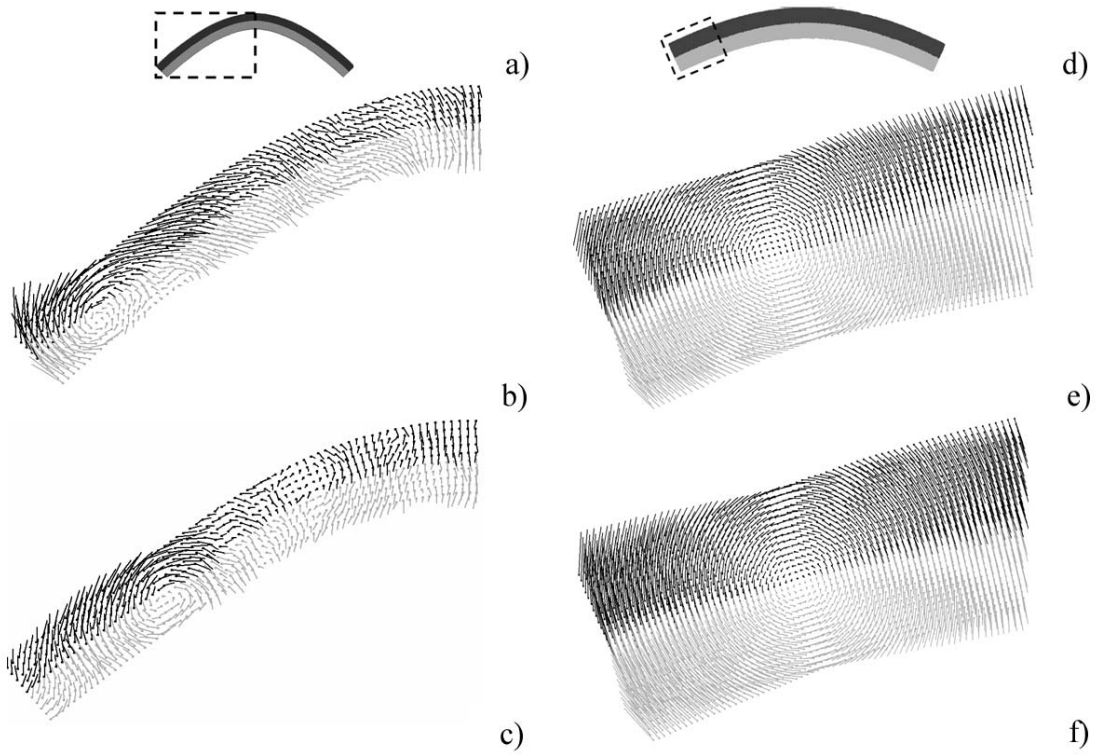

Fig. 5. The displacement fields of atoms for fragments (a), (d) of simulated Cu-Ni nanofilms, represented for different time cells: b– (43,54-44,02) ps; c– (44,02-44,50) ps; e– (254-266) ps; f– (268-280) ps. The displacements are represented for nanofilm fragments with length: a– 50 % d– 20 % from initial film length. The film thickness: a– 10 and d– 30 atomic planes

300 K (Fig. 6, a), 500 K (Fig. 6, b). This value is estimated as the fraction of thermal energy transformed into mechanical oscillations.

As demonstrated in Fig. 6 the transformation efficiency of thermal energy under heating increases with growth of heating temperature. Thus the variation of geometrical parameters of initial film allows purposefully having effect on transformation efficiency of thermal energy into energy of mechanical oscillations.

The behavior of non-closed nanostructure under heating subject to the mass increasing of its oscillated edge is investigated. The mass increasing is performed by applying of additional atomic layers on free edge non-closed nanostructure (Fig. 7, a), which other flat part is rigid fixed.

The resulting nanostructure is heated to about 300 K, which leads to the oscillations of its free edge. The calculations show that increasing the length of the free edge of the nanostructure at the same value of kinetic temperature leads to a decrease of the frequency of its oscillations, Fig. 7, b. Applying of additional atomic layers at the free edge increases the amplitude of their oscillations and virtually no effect on their frequency, Fig. 7, c. An increase in the total mass of the oscillating edge of 4% amplitude increased more than 4 times.

3. Conclusions

Thus, the performed calculations showed an opportunity of using the non-closed nano-sized structures as elementary energy converters. By means of matching the corresponding shape and elemental composition of non-closed nanostructure, pulsed heating mode, choice of

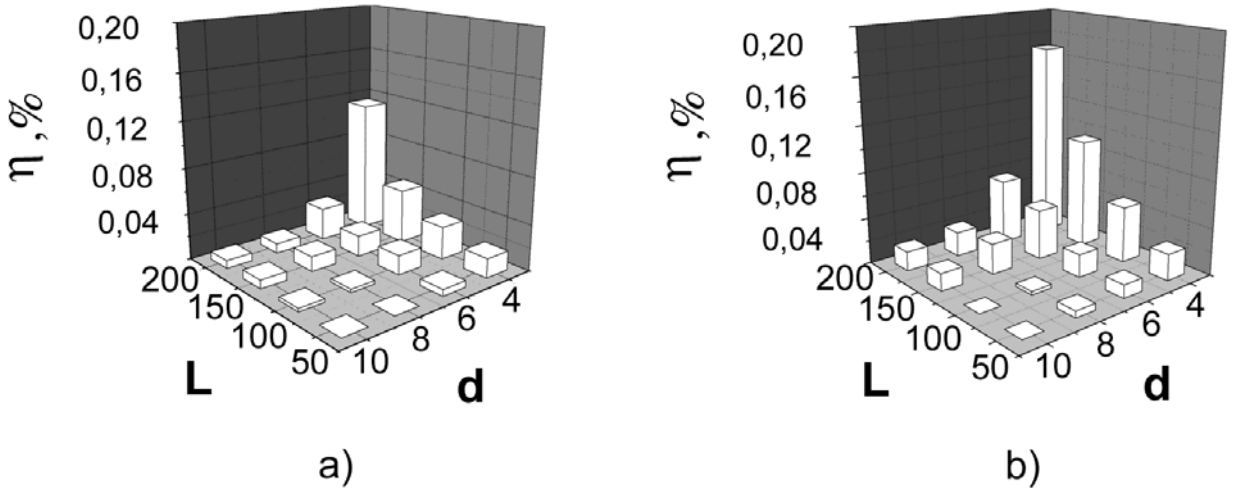

Fig. 6. The dependence of transformation efficiency of thermal energy into mechanical one for non-closed nanostructures on different lengths L and thicknesses d of the initial film (d is expressed as atomic plane number, L – as lattice constant number) under heating up to temperatures: a – T = 300 K; b – T = 500 K

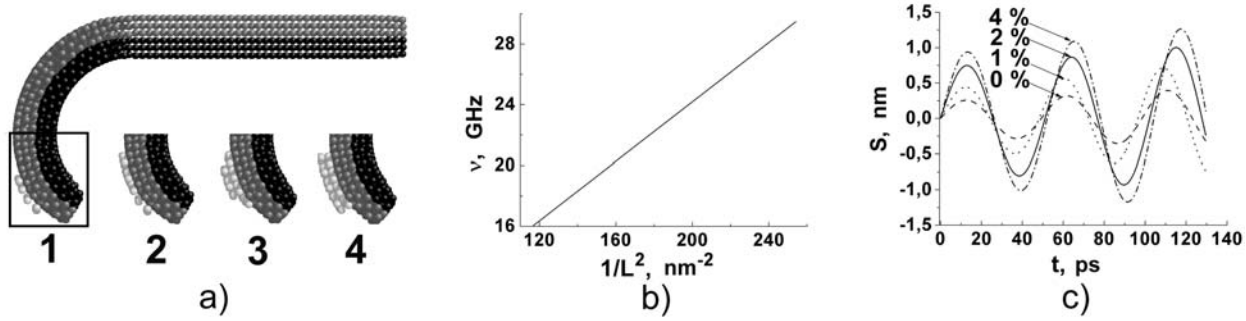

Fig. 7. Non-closed nanostructure with applied additional layers of Al atoms: *1*– 1%, *2*– 2%, *3*– 3%, *4*– 4% from weight of free edge of nanostructure (the Cu atoms are shown by black color; the Al atoms– by dark-grey color; the additional applied Al atoms– by light-grey color) (a); the dependence of nanostructure oscillation frequency on the length L of its free edge (b); the dependence of nanostructure free edge displacement S from equilibrium position on time under increasing of edge mass on 1, 2, 4 % (c)

the medium viscosity characteristics, one can significantly recover the oscillation amplitudes of the non-closed nanostructure edges. Relaxation and redistribution of elastic stresses in the initial film at rolling is carried out due to the collective motion of atomic groups. It is shown that there are two types of collective motions of the atomic system, determining the behavior at formation and subsequent oscillations.

Acknowledgements

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