Molecular-dynamics investigation of the nano-bar stability

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Abstract. This paper presents the analysis of the Eulerian instability of the nano-bar by the molecular dynamics method. The results shows that the same critical value of the external compressive stress is the bifurcation point both for the quasi-static structure contraction (alternation of the modes of instability and further fracture) and for the impact action (alternation of the energy absorption modes and occurring wave of transformation defects).

1. Introduction
The series of works \cite{1–3} are address to the analysis of the wave processes in nano-structures under the action of the external compressive stress within the range up to 4 GPa.

Performed analysis gave three intervals of the external compressive stresses. In the first interval, below 2.6 GPa, the total energy absorbed by the system is described by the quadratic dependency in the applied stress. In the second interval, from 2.6 to 2.8 GPa, the process of linear wave propagation incrementally transits to the mode of formation of transformation (or amorphization) waves. And in the third interval from 2.8 GPa to 4 GPa, this dependency was close to the linear one.

It stimulated the research of the Eulerian stability of nano-structures, but on the atomic scale, to avoid initial preset of any phenomenological models aside for the interatomic interaction potentials. By now, there are considerable amount of works addressed to the stability of various nano-size structure.

Note that this term means for the authors the structure stability in respect to its chemical composition, shape, size \cite{4–8}. In some papers, the molecular dynamics (MD) method was used to study the chemical structure stability, like \cite{9}. Moreover, under study is the thermodynamic stability \cite{10–11} and the non-linear response of the structure to the external action \cite{12}. The authors \cite{13} research the plastic deformation in stressed crystallites under irradiation by MD simulation. MD method got broad areas of applications in last decades, so in the work \cite{14}, scattering processes of argon beam impinging on tungsten surface are investigated numerically by applying MD simulations.

However, almost no works are devoted to the analysis of the Eulerian stability of the bar. And especially few works are addressed to the solution of this task by the molecular dynamics method. Quite frequently the continuum methods are used when considering nano-objects and stating the task of Eulerian stability definition, like \cite{15–18}. In \cite{15}, under consideration are spinning nanotubes under the action of the tangential stress. The motion equations have been obtained on the base of the Hamilton principle in the nanotube energy terms, regarding the rotational speed and compressive...
tangential stress. The authors compare the results obtained within the Euler theory with the ones obtained within the Timoshenko theory (the Euler–Bernoulli beam theory (EBT) and Timoshenko beam theory (TBT)). Thus this task has been solved here in the framework of the continuum mechanics. In [16], they applied the Galerkin finite-elements method. Multi-layer carbon nanotubes are the object of analysis in [17]. There, the nonlocal Euler Bernoulli beam theory is proposed for the free vibration and stability analyses of a multiple-nanobeam system (MNBS) using the Eringen nonlocal continuum theory.

The work [19] is the particular case. Here, the molecular dynamics method is used to analyze the nano-mechanical behavior of the β-SiC nano-wire at the extension, compression, spinning, combined extension and rotation, and combined compression and rotation. The Tersoff potential is used, the crystal orientation is chosen [111]. It is discovered that the defect depends on the size and temperature. At the uniaxial compression, the SiC nano-bar is crumpled by the column settling or bending regarding the length and diameter of the nano-bar, which agrees with the analysis of the equivalent continuum structures, on the base of the Euler theory of bar bending. The nano-bars are crumpled via the phase transition from the crystal structure to amorphous one in several atomic layers at the uniaxial spinning extension. Under the combined load, the spinning with the low spinning speed does not influence the defect and bending modes, but the critical stress decreases as the spinning speed rises. The plastic deformation occurs in the bending zone at the further rise of the combined load.

The nano-bars of various cross section shapes were considered: the hexagonal, triangular, rectangular, rhombohedral, octagonal, circular ones. But the length of the supercell was always similar. The authors found that the bars with the hexagonal cross section had the minimal potential energy, i.e. the most stable structure. It agrees with the experimental data wherein it is shown that the structures with the natural shape of the cross section are most stable. Moreover, σ-ε diagrams were plotted for the nano-bars of various diameters and at various temperatures.

The criticism of [19] includes the fact that the supercell length (supercell, 3.02, 4.53 nm) is too small to avoid the cross of the disturbance wave and the disturbance wave reflected from the opposite side of the nano-bar. The other difference of the results presented in this paper is that under consideration is metal, not ceramics. What is especially important, the aim of the work is to study not only the Eulerian stability of the bar, but the effect of the loss of bar stability on the transformation of the sample crystal structure.

This work is devoted to the analysis of the relation between the synergetic transition in the intensive dynamic process with the stability loss in the quasi-static process under the action of the compressive stress.

To do this, the specific task of compression of metal nano-structures shaped as rectangular parallelepipeds and getting of uniform states along the nano-structure length was solved.

The characteristic scale of the studied phenomena in the space and time is about $10^{-9}$ cm – $10^{-12}$ s, respectively. Hence, experimental investigation of such processes is impossible now. It caused the application of the molecular dynamics method based on the first principles. The method is based on the calculation of atom trajectories in the phase space on the base of the classic motion equations, but in the potential fields found in the framework of the quantum theory regarding electronic states. The calculations gave the fullest information on the system: the coordinates and impulses of every atom at every time instant. It permits performing detained investigations of the process.

2. Physical system and mathematical model

The technique and software complex for the MD analysis of the disturbances propagation in the nano-structures were adjusted on the example of a copper cluster shaped as the rectangular parallelepiped, its sizes were 50*5*5 and 200*5*5 crystal cells along the coordinate axes XYZ, respectively. The crystal orientation was chosen (1,0,0). To describe the interatomic interaction, the widely approved A. Voter EAM potential [20] for metals was chosen.
Initially, the atoms were in the nodes of the perfect crystal FCC lattice. Then, the system coordinates and impulses were found in the minimal potential energy state by the artificial viscosity method. Then the found values of the coordinates and impulses were used as initial data.

The calculation of macro- and meso- characteristics of the crystal is described in detail in [1].

The well-known velocity Verlet modification of the second accuracy order, with the time step $10^{-16}$ s was used as the numerical scheme [21]. It should be just stresses that in the case of the isolated system, the energy error is no more than $10^{-5}$ % within the time gap of 50 ps.

3. Calculation results

3.1. Adiabatic compression of the nano-structure

The value of the external compressing stress acting on the left side edge lying at the initial time instant in the $X = 0$ plane rose linearly within a certain time interval $T_o$ up to $\sigma_o$. Since the forces $\vec{f}_a$ acting on individual atoms are specified in the MD model as the initial value, they were calculated in the program by the simple formula

$$f_{ai} = \sigma_0 S_1 / n_1$$

where: $S_1$ is the area of the crystal left edge, and $n_1$ is the number of atoms on this edge. Since the edge area may vary somehow during the compression, it was re-calculated at each time step, similarly to the external forces acting on the atoms, providing that $\sigma_0 = \text{const}$. In other aspects, the movable clamp atoms were free.

To simulate the structure stop over the wall, the right edge (immovable clamp) was fixed in the space by means of the generalized potential

$$V(\vec{r}) = \frac{k}{2}(x_i - x_i^0)^4$$

where $(x_i^0, y_i^0, z_i^0)$ are the coordinates of the $i^{th}$ atom after cooling. Such a fixation enables to atoms to move freely in the $YZ$ plane, but limits their motion along the $X$ axis.

Mass calculations are carried out for the external compressing stress $\sigma_0$ values within the range up to 4 GPa with the step 0.1 GPa.

The preliminary method proposed by the authors was the quasi-static loading of the system resulting in the stationary and spatially uniform state of the system [22]. The monotony rise of the external load (under the condition of smallness of its time derivative) and artificial viscosity are the necessary conditions of such an action.

For the structure compression, the external stress $\sigma_{ext}$ linearly rising within 10 ps up to the preset value $\sigma_0$ was supplied to the crystal left edge.

The viscous force model was used at the growing external loads

$$\vec{f}_i = -\nu \vec{p}_i,$$

acting on each $i$-th atom ($\vec{p}_i$ is the impulse of the $i$-th atom). The value of the viscosity coefficient is $\nu = 0.1$ in the program entities. It enabled to simulate the quasi-static growth of the external load and remove the wave processes in the nano-structure.

At the same time, the dependency of the potential energy on time shows that the time of system relaxation is above 100 ps for the chosen parameters of the external stress relaxation and viscosity value.

All these factors caused the check of the interval duration of the system relaxation into the equilibrium state. Figure 1 shows the dependency of external forces deflection on the clamps.
\[ errF = 10 \log \left( \frac{|F_{ext1}| - |F_{ext2}|}{|F_{ext}|} \cdot 100\% \right) \]

on the time within the gap of 500 ps.

**Figure 1.** External forces on clamps versus time. External stress amplitude 1 GPa.

Evident that the deflection linearly decreases within this interval from 100% to $10^{-6}$%. It means that the sum of the external forces acting on the system equals to zero accurate to the eighth place.

### 3.2. Analysis of instability characteristics at the adiabatic compression of the x nano-structure

Since the major task of this stage is the sought of the critical compressive stress at which the structure does not break, the numerical experiment was performed with the external load interval from 1 GPa to 4 GPa. It was preconditioned that the system should survive the time gas of 500 ps without fracture. The pre-check showed that by this time, the parameter distribution over the structure was quite uniform. As a result is was shown that the structure did not break up to 2.3 GPa within this time interval. Figure 2 presents the illustration of the sought of this utmost stress.

To illustrate the behavior of the system stability within the interval of the external stresses causing the propagation of the transformation wave in the structure [1], figure 3 shows the dependency of the potential energy on time for the external stress above 2.7 GPa.

**Figure 2.** Potential energy versus time. 1 – 2.69 GPa, 2 – 2.6 GPa, 3 – 2.5 GPa, 4 – 2.4 GPa, 5 – 2.3 GPa

**Figure 3.** Potential energy versus time. 1 – 4 GPa, 2 – 3.5 GPa, 3 – 3.0 GPa, 4 – 2.75 GPa

Figures 4–5 give the results of such detailed processing: the critical time instants of the fracture and accumulated potential energy versus the external applied stress.
For convenience, the calculated points are charted in the graphs. Evident that this technique of data processing enables to determine the critical value of the external stress (the bifurcation point), at which the modes of energy absorption alternate at the impact action [1] accurate to 0.01 GPa. Its value is 2.70 GPa. For the stresses below this value, the linear section of time reduction and linear growth of the potential energy variation are observed as the stress grows. Then both the time and critical potential energy decrease as the applied stress rises in rough accordance with the hyperbolic law.

4. Conclusions
Thus, the same critical value of the compressive external stress is the bifurcation point both for the quasi-static structure compression (alternation of the instability and further fracture modes), and for the impact action (alternation of the energy absorption modes and occurring wave of transformation defects).

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