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NUMERICAL SOLUTION OF NANOMECHANICS PROBLEMS. DEVELOPMENT OF THE HYBRID METHOD

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ABSTRACT

Work is devoted to the development of numerical methods for modeling of deformation and failure processes in a coating body. The coat contains a few layers of atoms, i.e., it is a nanocoat. Then we must use the molecular theory hypotheses [1] to describe the behavior of such system. If a coated body is modeled in the frame of molecular dynamic (quasi-static) too then the dimensionality of the problem will be huge. The new method is proposed to decrease this dimensionality. This method consists of the continuum approach to the deformed body far from the coat and far from the boundaries of the deformed body; the molecular quasi-static equations for coat and a layer of coating body near the coat and boundaries are used. This approach is called the hybrid method. Essentially the quasi-static problems are considered. A new numerical solutions were obtained before formulate the hybrid model; these solutions allow us find some peculiarities of the displacement and force distributions being a ground for the hybrid model. In all the cases the problems of nanomechanics are nonlinear ones. This nonlinearity has some peculiarities which follow from the special dependence of the force interaction $F(r)$ on the distance r between the atoms: existence of the maximum of $F(r)$, decreasing of $F(r)$ to zero with $r \to +\infty$, and to minus infinity when $r \to 0$.

First numerical solutions were obtained for the chains composed from one or two kind of atoms. The Newton - Rafson iterations were used for solution of the quasi-static problems. Molecular dynamic equations were solved with Verlet's algorithm, and used as a test for quasi-static solutions. Enumerate some quantitative results. In a homogeneous chain composed from the finite number of particles with zero external loads (free chain) the internal forces arise due to the long distance force interactions – see Fig. 1; K, L are the numbers of

atoms, K for 40 atoms, L for 80. Values of these "self-compression" forces do not depend on the atom quantity.

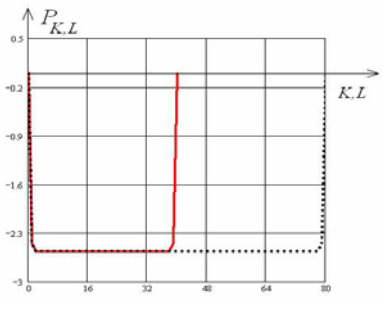

Fig. 1: Self-compression forces

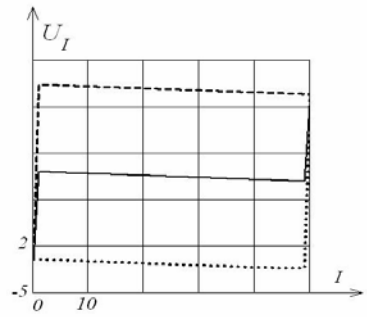

Fig. 2: Multiple solutions

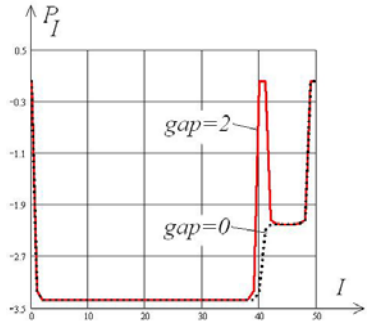

Fig. 3: Heterogeneous chain

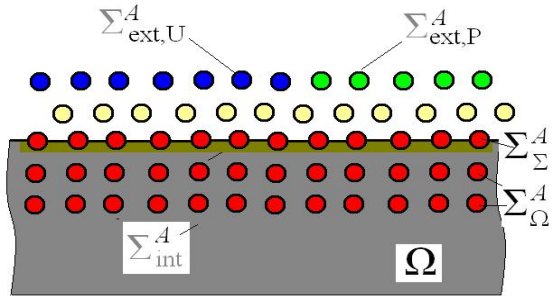

Fig.4: Scheme of a hybrid model

Curves at the Fig. 2 illustrate an effect of no uniqueness: for the same peak value of the end atom displacement there exists three solutions. First solution corresponds to the separation of the atom «1» from atom «0», 2nd - separation of the atom number $I = 50$ from atom 49 , and the 3rd - simultaneous separation of two pointed types – this case corresponds to the symmetrical failure of the chain. Distributions of the forces in a heterogeneous chain are given at the Fig. 3. The solid curves correspond to the gap between two metals equal to 2, dashed curve - zero gaps. All results were confirmed by solution of 2D problems. An analysis of stability and bifurcation is proposed with calculation of eigenvalues of the tangent matrix.

Scheme of the hybrid model is shown at the Fig. 4. The notations are the following: $\Sigma^A_{ext,U}$; $\Sigma^A_{ext,P}$ is the set of atom numbers at the boundary, Σ^A_{int} is the set of atom numbers contacting the continuum Ω; $\Sigma^A = \Sigma^A_{\text{int}} \bigcup \Sigma^A_{ext}$; $\Sigma^A_{\text{int}} = \Sigma^A_{\Sigma} \bigcup \Sigma^A_{\Omega}$, Σ^A_{Σ} is the set of atom numbers at the boundary $\Sigma^{\Omega} \equiv \Sigma = \partial\Omega$, Σ^A_{Ω} are the atom numbers strict inside the domain Ω. The hybrid problem is formulated as follows: given external load - displacements for $p \in \Sigma^A_{ext,U}$ and forces applied to the atoms with $p \in \Sigma^A_{ext,P}$, find the displacement field $\vec{u}(\vec{x})$, $\vec{x} \in \Omega$ and displacements of the atoms with $p \in \Sigma^A \setminus \Sigma^A_{ext,U}$.

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