

# CONTINUUM-ATOMISTIC MODELING OF NANOMECHANICAL SYSTEMS

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## Introduction

The description of strains and stresses in materials and devices at the nanoscale range constitutes a current topic in mechanics and material science. Although quantum mechanics and molecular dynamics are a natural base for the description of mechanical phenomena at this scale level, it has been shown by many authors, that the continuum mechanics approach, modified by molecular equivalence, gives results being in good agreement with experiments (see [1]). Different methods and models have been developed up till now. In the present paper alternative mixed continuum – molecular model of stress and deformation states analysis will be considered. The main idea of the description lies in the assumption that the molecular structure of the material can be described in frame of continuum mechanics, provided that the constitutive stress-strain relations take molecular interactions into account. Large strain and many body potentials are considered. Molecular dynamics and static simulations are performed to verify the proposed model.

## Field quantities in discrete and continuum systems.

To couple molecular and continuum mechanics descriptions let us consider a system of material points with masses  $m_i$  and position vectors  $\mathbf{r}_i, i = 1, N$  referred to a fixed Cartesian frame  $\{0x_k\}, k = 1, 2, 3$ . Let the initial position vectors be denoted by  $\mathbf{r}_{0i}$ . The system is subjected to force actions resulting from the potential  $U(\mathbf{r}_1, \dots, \mathbf{r}_N) = U(r_{ij}, \theta_{ijk})$ , where

$r_{ij} = |\mathbf{r}_{ij}|, \mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$ , and  $\theta_{ijk}$  means the angle between bonds.

The molecular stress tensor resulting from the generalized Clausius virial theorem has the known form

$$i = \frac{1}{V_i} \sum \mathbf{f}_{ij} \otimes \mathbf{r}_{ij} \text{ where}$$

$$f_{ij} = \frac{1}{r_{ij}} \frac{\partial U}{\partial r_{ij}} \mathbf{r}_{ij} = \frac{\partial U}{\partial r_{ij}} \mathbf{e}_{ij}, \mathbf{e}_{ij} = \frac{\mathbf{r}_{ij}}{r_{ij}}. \text{ The advantage of}$$

using the continuum approach has been emphasized by many authors [2]. It leads to immense reduction of the number of unknowns in numerical computations. This property is enhanced by using many body potentials (e.g. Tersoff-Brenner, Stillinger-Weber etc.).

We assume that the nanostructure is a nanocontinuum subjected to large deformations (for the system of molecules finite rotations are particularly of great importance). The Voronoi tessellation of space, and hence the set of Delaunay tetrahedrons constitute a natural way to build the mesh of finite elements for any arrangement of molecules. Thus using the FEM

technique, by expressing the displacement field in the form  $u_k(\mathbf{x}, t) = \sum_{\alpha} N_{k\alpha}(\mathbf{x}) q_{\alpha}(t)$  one obtains the

equations of motion of the system in the standard matrix form [3]  $[M_{\alpha\beta}] [\ddot{q}_{\beta}] + [F_{\alpha}^{int}] = [F_{\alpha}^{ext}]$  where

$$M_{\alpha\beta} = \int_V \rho N_{i\alpha}(\mathbf{x}) N_{i\beta}(\mathbf{x}) dV,$$

$$F_{\alpha}^{ext} = \int_V \rho b_i N_{i\alpha}(x) dV + \int_S p_i N_{i\alpha}(x) dS,$$

$$F_{\alpha}^{int} = \int_V \sigma_{kl}(x) \frac{\partial N_{k\alpha}}{\partial x_l} dV,$$

$$\sigma_{kl} = \sum_i \sigma_{kl}^i = \sum_i \sum_j \frac{1}{V_i} \chi_{ij} r_k^{ij} r_l^{ij}, \chi_{ij} = \frac{1}{r_{ij}} \frac{\partial U}{\partial r_{ij}},$$

$$r_k^{ij} = r_{ok}^{ij} + u_k^{ij}(\mathbf{x}), u_k^{ij} = u_k^j - u_k^i, q_{\alpha} - \text{nodal}$$

displacements. The molecular stress tensor can be transformed into the form convenient for structure mechanical calculations. For this purpose let us assume molecular bonds as rods with circular cross-section area  $A$  and diameter  $d$ . Assuming further the volume of bonds being constant  $V^{bond} = Ar_{ij} = A_0 r_0^{ij}$  where  $A_0$  is the cross section area in the initial configuration, one can write

$$i = \frac{V^{bond}}{V_i} \sum_j \frac{1}{Ar_{ij}} \mathbf{f}_{ij} \otimes \mathbf{r}_{ij} = \frac{V^{bond}}{V_i} \sum_j \sigma_{ij}^{bond} e^{ij} \otimes e^{ij}$$

where  $\sigma_{ij}^{bond} = \frac{\partial U}{\partial r_{ij}}$ . Using now for generality the

Seth's and Hencky's finite strain measure, which in case of uniaxial stretch takes the form

$$\varepsilon_m = \frac{1}{m} \left[ \left( \frac{r}{r_0} \right)^m - 1 \right] \text{ for } m \neq 0 \text{ and } \varepsilon_m = \ln \left( \frac{r}{r_0} \right) \text{ for}$$

$m = 0$ , one obtains

$$\sigma_{ij}^{bond} = \frac{1}{A_0 r_0} r_{ij} \frac{\partial U}{\partial r_{ij}} = E_m^{bond}(r) \varepsilon_m = E_h^{bond}(r) \varepsilon_h$$

where  $E_m^{bond}$  and  $E_h^{bond}$  stand for the generalized Young's moduli related to the strains  $\varepsilon_m$  and  $\varepsilon_h$  respectively. The formula for virial stresses presented above is especially suitable for nanotubes and graphene sheets for which truss and frame models can be used. Thus for any node of the system it will be

$$\sigma = \frac{f_{ij}}{A} = \sigma^{bond}.$$

## Numerical results.

As an example of modeling we consider carbon bonds of nanotubes. Using the data for modified Morse potential from [4] and assuming an artificial (computational) bond diameter  $d = 0,147nm$  (from [1]) one obtains the moduli functions  $E^{bond}(r)$  for different strain measures presented in Fig. 1. The application of Tersoff-Brenner potential  $U^{TB} = U_R(r) - \bar{B}(\theta)U_A(r)$ , which is more accurate for carbon bonds, but simultaneously more complex in calculations, needs some remarks. The

expression  $E^{bond}(r, \theta) = \frac{1}{A_0 r_0} r \frac{\partial U}{\partial r} \varepsilon_m^{-1}$  possesses

points of indeterminacy at  $r = r_0(\theta)$  depending on the angle  $\theta$  i.e. on the configuration of neighbouring bonds. Thus keeping the angle  $\theta$  constant ( $\theta = 120^\circ$ ) one obtains results shown in Fig.2.

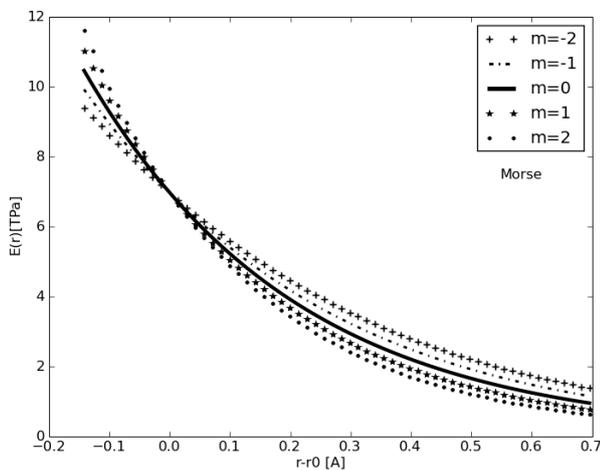


Fig.1 Young modulus of the bonds as a function of the distance r for the Morse potential. Data from [4].

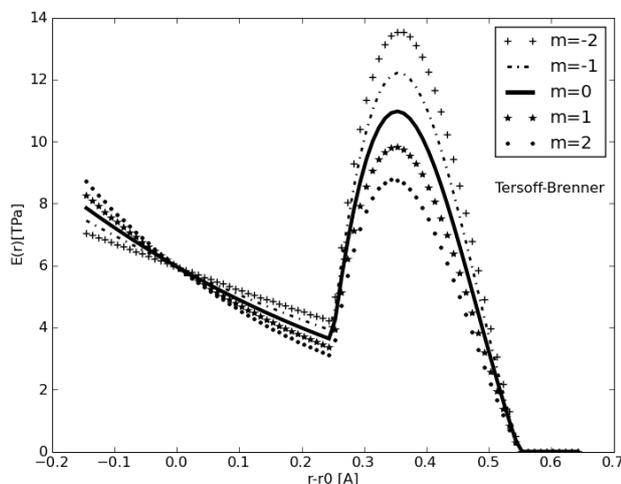


Fig.2 Young modulus for the Tersoff-Brenner potential. Data for carbon from [5].

The obtained results lead to the following corroboration: for small deformations the Young modulus of the bonds takes the value  $E^M = 6.0TPa$  for the Morse potential, and about  $E^{TB} = 5.8TPa$  for the Tersoff-Brenner potential function. These results are in good agreement with the value  $E=5.49TPa$  obtained in [1] for constant E. For large strains the values  $E(r)$  differ essentially for all the values of m. The function  $E(r)$  is decreasing for the Morse potential, whereas for the Tersoff-Brenner case the camelback effect takes place. Applying the structural approach presented above (which takes molecular interactions into account) different examples of graphenes, nanotubes and composites for various boundary conditions are considered. Using the ABAQUS code, with own elaborated UMAT subroutines, a series of computational simulations with data taken from [4] and [5] are performed.

## Conclusions

The diagrams of Young modulus and stresses depending on molecular interactions show the possibility and effectiveness of constitutive modeling at the nanoscale range. From Fig.1 results that for  $r > r_0$  the kind of strain measure doesn't affect essentially the Young modulus changeability. For the Tersoff-Brenner potential the known camelback effect of forces (see also [4]) is visible. The presented approach can be applied to constitutive modeling of 2D and 3D hyperelastic nanocontinuum elements by using Voronoi polyhedrals as a base for the finite element mesh.

## References

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