Nonlocal correlation functions and an integral model for nanomechanical properties of nanostructural complexes

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The mechanical properties of nanostructural materials is often considerably different in comparison with properties of isotropic medium with similar mechanical parameters. This fact caused extensive studies of computational methods for modeling nanomaterials and nature of its integral properties formation. Even for particular case of rheological properties modeling there is a long list of such computational methods, as lattice-Boltzmann, dissipative particle dynamics, Langevin dynamics and some continual assumption. All of these methods are proposed for using in so called multiscale models with molecular mechanics (MM) computational methods, frequently molecular dynamics or Monte-Carlo molecular simulation. The subject of theoretical interest here is finding such general set of parameters measured with molecular mechanics methods and allowed more accurately estimation of integral properties of the material. This issue has not been resolved for today.

Measurements of the same parameters for micro-scale and molecular-scale levels, as Young's modulus and the like are quite obvious and often used way. This method is associated with so-called "representative volume element (RVE)" which unfortunately usually turns out too big for MM simulation. For example, for the polymer matrix with 100nm length nanotube inclusion RVE will be about $1\mu m^3$.

In this research one new, more suitable and effective way of multiscale nanomaterials modeling is considered. In our model integral formulation of elasticity problem is used. It doesn't contain any integral parameters of media, which all described by integral core functions. The last are solutions of Kelvin-Somilyany, can be both estimate analytically, and measured directly with molecular dynamics method. From the point of view of statistical mechanics, integral core functions are just space and time-dependent correlation function for values of local deformation and mass velocity. Reduced requirement for volume of MM simulation and statistical-vested method of MM measurements are main advantages of this molecular- to micro-scale bridge.

We considered rheological properties of polymer nanocomposite material with inclusion of carbon nanotube. At micro-scale level, considered system was represented as continual polymer matrix with included nanotubes modeled as continual 1D objects. We also assume tube slipping relative to the polymer matrix. All necessary properties of medium were measured with MD simulation method.

For the control the quality and universality of suggested model, we also consider a problem about nanotube flow. This problem is well studied, simple in formulation and most similar for testing of nanomechanical models. Poisson equation for problem of stationary flow in cylindrical tube could be written in integral formulation by the same way. The grin functions of Poisson equation were considered as a space correlation function for liquid velocity in different points of real space. At the center of tube measured correlation function was similar to well-known analytical form, but near the wall considerably difference was found. However, just measured correlation function gave velocity profile similar to given directly by MD simulation.

Therefore, integral formulation of nanomechanical problem turns out not only more suitable, but also more general model. Integral formulation of tube flow problem, for example, allows correctly slip boundary condition describing, which is impossible in a differential model.