MODELING OF MECHANICAL BEHAVIOR OF NANOPARTICLE

O.I.. Manevitch[1*], G.C. Rutledge[2] and M.A. Mazo[1]
[1] *Institute of Chemical Physics Russian Academy of Science, Kosygin str., 4, Moscow, 119991, Russia*
[2] *Massachusets Institute of Technology, Cambrige, MA 02139*

We present molecular dynamics simulation for estimation of mechanical behavior of crystalline nanoparticle consisting of two tetrahedral layers and intermediate octahedral layer. Mechanical model of the crystal is elaborated using potentials of atomic interaction adapted for aluminosilecates.

On the basis of this model the stress-stain relations are determined in NPT ensemble for different conditions of loading.

We examined the effect of the particle size and the rate of loading on the final results. Methodological problems relating to applicability of continuum models have been discussed.

*Phone: 07 095 939 7515; Fax: 07 095 137 8284;
E-mail: *omanev@ polymer.chph.ras.ru*