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# Computer study of elastic properties of small nanoparticles

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The density functional theory and the method of pseudopotentials (quantum mechanical calculations from first principles) were used to study reactions of small nanoparticles aluminum (2－13 atoms), silicon (5－18 atoms) and zirconia (18－30 atoms) on compression and tension. It has been found that elastic modules (Young modules) decrease with increasing of the number of atoms in nanoparticles, however their values overestimate those typical for bulk materials. Differences of atomic structures and elastic properties of metallic, semiconductor and dielectric nanoparticles are discussed.

To analyze elastic properties of nanoparticles a special methodics has been used. Namely, the elastic module $K$has been calculated from a second derivation of the total energy $E$of the particle as a function of a deformation (compression and tension) along some direction $d$:

$$K=\frac{\partial^2 E}{\partial d^2}\cdot\frac{{d_0}^2}{V_0},$$

where $V_0$ and $d_0$ are the equilibrium value and length of a nanoparticle. A nanoparticle's value was calculated as a sum of atomic values $V_A$($V_A=\frac{3}{4}\pi\cdot R_A^3$), where $R_A$ is an atomic radius.

Calculations show that nanoparticles with metallic, covalent and ionic bondings have different reactions on mechanical deformations. Elastic module of aluminum (metallic) particles depends non-linearly on deformation; the dependence of elastic module for silicon particles (with covalent bonds) on deformation is linear; while elastic module for nanoparticles of zirconia is a constant. At the whole, one can say that elastic characteristics for nanoparticles overestimate significantly (several times) those for bulk materials, however the elastic module for silicon nanoparticles quickly aspires to the bulk Young module as the number of atoms in a particle increases.

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