Nanocomposites and nanomaterials

The Role of Chemical Bonds in Dimensional Effect of Nanomaterials

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The properties of nanomaterials depend on size of constituting nanoparticles (dimensional effect), the nature of which has not been understood so far because there are offered different mechanisms for explanation of the change of separate properties of nanomaterials. In presented work, a new mechanism of this effect is given which explains the change of different properties from the single point of view. The mechanism is based on the weakening of chemical bond between the atoms of nanoparticles with the reduction of their size. Earlier it was shown that the decrease of the energy of chemical bonds occurs because of the increase of concentration of antibonding electrons and/or holes on bonding levels (these quasi-particles are called antibonding quasi particles-AQP) due to thermal or non thermal (pressure, light, electric and magnetic field) action [1]. However, it turned out that the AQP concentration increases upon the reduction of nanoparticles volume beginning from their linear size compared with free path length of AQP in the given material. During their motion the AQP reaching the surface of nanoparticle reflect from them and remain in its volume increasing the probability of their appearance near the given atom unlike the compact solid body of the same volume, from where AQP can freely transfer to the neighboring region. This can be described by real concentration of AQP which is higher compared with the calculated at the given temperature and the bigger it is the less the nanoparticles size is. Due to the fact that in nanoparticles AQP appear more frequently near the given atom than in compact solid body, the weakening of their chemical bonds will be more. In subsurface region of the nanoparticle the AQPs appear more frequently near atoms than in its volume because of direct and reverse motion of AQPs in the reflection process which will cause additional weakening of chemical bonds in subsurface region of the nanoparticle.

Thus, with the reduction of nanoparticles size, the effective concentration of AQP and weakening of chemical bonds increase and it is more in the subsurface range. Based on this effect all physical-chemical properties of nanoparticles and nanomaterials which are determined by the energy of chemical bonds will be changed appropriately with the decrease of this energy. For example, in nanoparticles the interatomic distance and correspondingly, volume of element cell should increase; melting temperature decrease and in subsurface region more rapidly; diffusion and recrystallization rate increase, in nanomaterials hardness and fluidity point decrease, plasticity increase, etc. All these changes are observed experimentally and as was shown above, can be explained from a single point of view.

Gerasimov A.V., Principles of the molecular-potential theory. 2nd Intern. Conf. “Nanotechnologies”, Tbilisi, Georgia, Sept., 19-21, 2012, p.160-170.