Nanocomposites and nanomaterials

The alteration of structure of silver nanotube in the process of heating

O.V. Filatov, S.M. Soldatenko, O.M. Soldatenko

Physical Engineering Faculty, the Physics of Metals Department, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Prosp. Peremohy, 37, Kyiv-03056, Ukraine.
E-mail: oksana.hubina2811@gmail.com

After the discovery of carbon nanotubes, scientists from different scientific areas began to be interested in materials with similar structures. Nanotubes are important structural element and they brought a big breakthrough in science and technology, including electronics, mechanics, physics and chemistry. Metallic nanotubes also exhibit a range of properties that are superior to their bulk counterparts.

The aim of this work is to compare calculated parameters in molecular dynamics simulation with data obtained in physical experiments to test the correctness of the modeling of thermal properties and to study temperature stability of silver nanotubes.

There was modeled silver nanotube by molecular dynamics method with the following parameters: nanotubes length – 30 nm., the outer diameter - 3 nm., the internal diameter - 1 nm ..

During the simulation the nanotube was heated in the temperature range from 123 K to 323 K and the changing in linear dimensions of the structure along the axis of the nanotube was recorded. This modeling does not include resizing by the emergence of vacancies.

It is found out that silver nanotube is not stable if its axis coincides with the direction [100] of face-centered cubic lattice. The structure deforms and the atoms rearrange so that the axis coincides with the direction [110] of FCC-lattice, which is the densest direction of packaging for such structure. The resulting configuration is more stable.

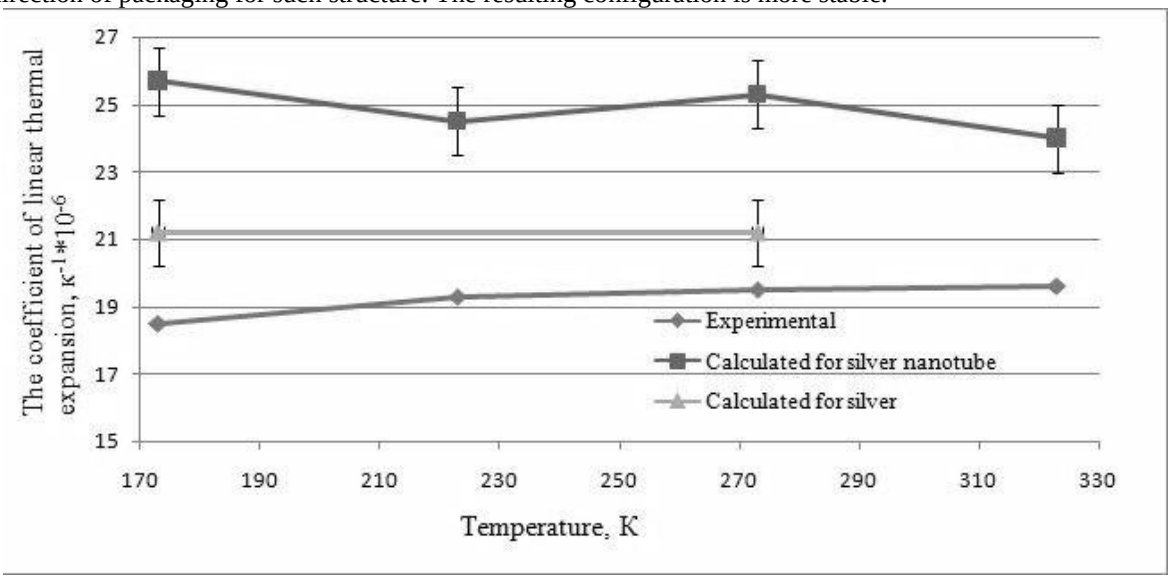

Figure 1 - The dependence of the coefficient of linear thermal expansion on temperature.

The study found that the coefficient of linear thermal expansion is also changing with the temperature. This corresponds to experimental data presented for bulk samples of silver [1]. Thus, at a temperature of 173 K the coefficient of linear thermal expansion of silver nanotube is $25{,}7*10^{-6}$ K^{-1}, and at temperature of 273 K is $25{,}3*10^{-6}$ K^{-1}.

The similar character of the theoretical and experimental curves indicates the correct simulation.

The calculated by MD coefficient of linear thermal expansion differs from experimental at 7% - for silver and at 20% - for silver nanotubes. The calculated coefficients of thermal expansion for silver differs from calculated coefficients of thermal expansion for silver nanotube at 15%.

To investigate the thermal stability of silver nanotube the structure was relaxed in different temperatures up to 600 K.

At a temperature of 550 K (corresponding approximately to a half of silver melting point) free ends of the nanotube close, while retaining a cavity inside nanostructure. This structure persists throughout the all simulation time (0.12 ns). We can assume that this effect occurs because of the dangling bonds of atoms located at the ends of the nanotube. Closing of free ends of nanotube reduces the surface energy of this nanostructure, making it more stable.

At the temperatures of 600 K the cavity in the nanotube structure disappears. It is indicating the instability of the structure at this temperature.

1. Callister W.D.,JR. Materials Science and Engineering: An introduction // 7^{th} edition. John Wiley &Sons, Inc. – 2007.