11th International Conference
on Advanced Materials
Rio de Janeiro Brazil
September 20 - 25
ICAM2009

Molecular dynamics calculations of InSb nanowires thermal conductivity

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Abstract – Non equilibrium molecular dynamics calculations were performed in order to obtain the thermal conductivity coefficients of InSb nanowires. In comparison with the bulk system value previously obtained (16 $Wm^{-1}K^{-1}$ which is in very good agreement with experimental value of 15 $Wm^{-1}K^{-1}$), the thermal conductivity of the 5 unit cells side square section nanowire is about 0,67 $Wm^{-1}K^{-1}$, almost two orders of magnitude smaller, and seems to diminish with the nanowire diameter. This result is in agreement with other simulations performed for other materials.

Indium antimonite (InSb) nanowires were modeled by non equilibrium molecular dynamics simulations, varying their lengths and diameters, to obtain the values of thermal conductivity coefficients. There are a large number of potentials used to model a very high number of materials with remarkable results in comparison with experimental data reported. In the case of the present report, which covers only InSb, it was used a very transferable potential developed by Vashishta-Kalia-Nakano[1], parameterized by Rino et. al. [2] and recently improved [3].

The non equilibrium molecular dynamics method is based on the Fourier law, where a heat current is generated through the nanowire by the imposition of a temperature gradient[4-7]. The gradient is imposed when two reservoirs, at different temperatures, are inserted in the system at a distance *L* from each other. The thermal conductivity coefficient is obtained by the relation between heat current and temperature gradient [5-7].

The systems modeled were: (i) a nanowire with 5 unit cells side square section and four different lengths (what means four different inter reservoir distance *L*), and (ii) a nanowire with 4 unit cells side square section and the largest length used in the case (i). In the case (i) four different lengths were used in order to performed an infinite extrapolation for *L*, obtaining a coefficient value for an infinite system [4]. In the case (ii) only one length was used to make a comparison between the thermal conductivity coefficients obtained for two different diameter nanowires whose lengths were the same, giving an idea about the behavior of thermal conductivity when the diameter is decreased. Calculations of the thermal conductivity for this thin nanowire and different length are in progress.

The obtained value, in the case (i), for a mean temperature of 300K, was about 0,67$Wm^{-1}K^{-1}$, in contrast with the obtained value of 16 $Wm^{-1}K^{-1}$ for a bulk system simulation and the experimental value of 15 $Wm^{-1}K^{-1}$. This result is in accordance with previous simulations made with other materials where the thermal conductivity coefficient, for a nanowires, is about two orders of magnitude smaller than that obtained for a bulk system[8]. This effect is known as phonon confinement[9]. The simulation of case (ii) shown an even smaller thermal conductivity coefficient in comparison with the case (i) for the same length.

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