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Praca doktorska

Wpływ ograniczeń geometrycznych i polidyspersji rozmiarów cząstek na przewodnictwo cieplne układów modelowych

Promotor

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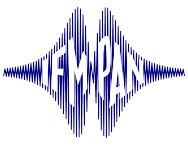

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Abstract

The dissertation presents results of the research on the thermal conductivity of model systems. The main subjects of this work are: thermal conductivity of liquid argon in nanochannels, thermal conductivity of argon nanowires and thermal conductivity of Yukawa crystals with size polydispersity of particles.

The methodological part is devoted to such topics as: definition of the thermal conductivity coefficient, the basics of the Molecular Dynamics method (including the methods to calculate thermal conductivity), and the models and potentials used. In this work, the interactions between the atoms of argon were described by Lennard-Jones's potential and the interactions of particles in colloidal crystals were described by the Yukawa potential. In the section, a modification of one of the calculation methods that allowed to determine the thermal conductivity of argon nanowires has been proposed. At the end of this part of the dissertation, all details of computer simulations were presented.

Computer simulations of the presented models have been performed. In the case of models of nanochannels and nanowires, the influence of the system transversal size as well as temperature and density on the thermal conductivity of the system have been studied. Moreover, theoretical models of thermal conductivity of bulk system and nanowires were discussed. The results of the calculations for these theoretical models have been compared with the computer simulations results and available experimental results. This allowed us to characterize qualitatively the phonon scattering in argon crystals and nanowires. Moreover, the research allowed us to determine how the thermal conductivity of liquid argon in nanochannels and argon nanowires scales with the cross-section area of the system and to determine the characteristic size of the systems below which the thermal conductivity deviates from that observed in the bulk system.

The study of colloidal crystals models has been involved determination of the influence of the Debye screening length and the polydispersity of particles size on the thermal conductivity of the crystal. The results of simulations of colloidal crystals revealed a strong dependence of the thermal conductivity coefficient on the size polydispersity of particles. These studies have shown that the increase of the screening length results in a decrease of the thermal conductivity coefficient.