Thermophysical properties of the phonon subsystem of gold in the solid–liquid phase transition region: Atomistic modeling

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Studies of recent years have shown that gold nanoparticles demonstrate excellent imitation of the activity of biological enzymes. Pulsed laser ablation (PLA) is one of the common methods for generating nanoparticles. The generation of gold nanoparticles by PLA is carried out in a temperature range, in which the phase transitions play a decisive role. Studies of the kinetics and dynamics of phase transformations are carried out mainly by methods of mathematical modeling. PLA is accompanied by the phenomena of thermodynamic nonequilibrium, which leads to the need to take into account the characteristics of two subsystems: electronic and phonon.
This report presents the results of atomistic modeling of the thermophysical properties of gold in the region of the melting–crystallization phase transition. The pressure dependencies of the specific heat of melting and equilibrium melting point, temperature dependencies of the density, linear size of the sample, coefficient of linear expansion, enthalpy, and heat capacity were determined. The obtained dependencies of the properties of gold are approximated by polynomials of low degrees. The results of comparing the obtained characteristics of this metal with experimental data show acceptable agreement. Numerical and graphical information about the obtained properties and the results of comparison with experimental data is presented.
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