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3D molecular dynamic simulation of thermodynamic equilibrium problem for heated nickel

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This work is devoted molecular dynamic modeling of the thermal impact processes on the metal sample consisting of nickel atoms. For the decision of this problem the continuous mathematical model on the basis of the classical Newton mechanics equations is used, the numerical method using in the basis the Verlet scheme is chosen, the parallel algorithm is offered and its realization within the MPI and OpenMP technologies is executed. By means of the developed parallel program the investigation of thermodynamic equilibrium of nickel atoms system under the conditions of heating a sample to desired temperature was executed. In numerical experiments both optimum parameters of a calculation procedure, and physical parameters of analyzed process are defined. The received numerical results are well corresponding to known theoretical and experimental data.

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