Calculated data on a cubic nickel cluster

Sergey V. Polyakov, Viktoria O. Podryga

Keldysh Institute of Applied Mathematics
Russian Academy of Sciences

The proposed data set relates to calculations of thermodynamic equilibrium of a cubic nickel cluster under normal conditions (T=273.15, p=101325 Pa). As an example, a cluster with dimensions of 24x24x24, measured in units of a lattice edge equal to a=0.35314 nm, is selected. The calculation was carried out using the molecular dynamics method. Details of the calculation procedure are presented in the work

V.O. Podryga, S.V. Polyakov. Molecular dynamic simulation of thermodynamic equilibrium problem for heated nickel // Preprints of KIAM RAS. 2014. № 41. 20 p. URL: http://library.keldysh.ru/preprint.asp?id=2014-41.

The data set is an archive containing data in text and binary formats, including the format of the scientific visualization package TecPlot.