QUANTUM MOLECULAR DYNAMICS CALCULATIONS OF SOLID AND LIQUID IRON IN THE VICINITY OF MELTING

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Iron is a widespread component in various types of structural materials, which are exposed to intensive thermal and mechanical loads. So, the equation of state of iron is of great importance due to its numerous technological applications. Nevertheless, thermal expansion of iron, especially in liquid state, is still a matter of debate. Actually, *ab initio* calculations may be used to obtain reliable data on properties of materials, if thermodynamic parameters are such that it is difficult or impossible to conduct an experiment or its results are hardly reproducible. Quantum molecular dynamics (QMD) based on density functional theory [1] can be used for modeling the behavior of metals in both solid and liquid states. In this work, we follow Redmer [2] in investigating the influence of spin polarization on the thermal expansion of solid and liquid iron in the vicinity of melting. Thermal expansion curve of solid iron is reconstructed both with and without taking spin polarization into account. Comparison with experimental data is presented. Special attention is paid to the dependence of thermodynamic and magnetic properties of solid iron on the initial distribution of magnetic moments and the type of crystal lattice.

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1. R. M. Martin. Electronic structure: basic theory and practical methods. Cambridge University Press, Cambridge, 2004.
2. J A Korell, A French, G Steinle-Neumann, and R Redmer. Phys. Rev. Lett., 122:086601, 2019.