Predicting high-PT melting curve of Fe using ab initio molecular dynamics and machine learning approach

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Iron is the main element that makes up the core of the Earth and terrestrial exoplanets. It is reliably known that under the conditions of the Earth's inner core (pressure of 330 to 360 GPa, temperature of 5 to 7 kK), iron is in a solid state, but its crystalline modification is a matter of debate. There is also significant variation in melting line estimates based on experiments with shock waves and diamond anvil cells, as well as theoretical estimates based on calculations using the density functional theory, classical and quantum molecular dynamics. Recent data from experiments are usually interpreted as evidence of stability of the hcp phase at high temperatures and pressures, while first-principles molecular dynamics calculations in ultra-large cells indicate the existence of the bcc phase. Small computational cells (less than 1000 atoms) lead to the destruction of the bcc structure. In this work, an analysis of densities, coordination numbers and structural factors of crystalline modifications of iron shows the coincidence of calculated and experimental data for the bcc phase (previously attributed as hcp or liquid phase). Based on two-phase simulations in the large cells with machine-learning potentials, the melting curve of iron in the range of 50–500 GPa is calculated. The work was carried out within the framework of the Fundamental Research Program of the National Research University Higher School of Economics.