Comparative estimation of the properties of liquid metals at high temperatures and pressures using the methods of classical and ab initio molecular dynamics

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One of the foreground tasks of computer simulation is the prediction of metal properties at high temperatures and pressures, for example, under shock compression conditions. Recently the embedded atom model (EAM) was applied to describe highly compressed states, as a result were calculated multiparticle interatomic potentials of metals. Another method for calculating properties under shock compression is the ab initio quantum mechanical method. It allows the properties calculation without attracting any model approximations but it requires a lot of power and is really time consumable. To estimate the forecasting power of both methods, we compared the data obtained for the same states under conditions of shock compression for four liquid metals Na (4000 K), Bi (10 000 K), Ni (4450 K) and Fe (6000 K). Both methods gave similar results for the coefficient of self-diffusion and the functions of the pair distribution of atoms but the pressure difference can reach up to 30%.

The reported study was funded by RFBR, project number 20-03-00370