THE APPLICATION OF EMBEDDED ATOM MODEL TO LIQUID METALS. URANIUM

D.K. Belashchenko, D.E. Smirnova
State Technological University “Moscow Institute of Steel and Alloys”
E-mail: dkbel@mail.ru

The embedded atom model potential (EAM) is applied for uranium. The calculation method is proposed where diffraction data of liquid metal near the melting temperature, thermodynamic data and the results of shock wave experiments are used. Molecular dynamics simulation with EAM potential leads to good accordance with experiment on the structure, density and energy of liquid U at the temperatures up to 5000 K and also for solid and liquid U along the shock adiabat up to ~220 GPa. The calculated compressibility module is in agreement with experimental one. The self-diffusion coefficients grow at heating via power law with the power ~2.103. The dynamic viscosity is evaluated up to 6000 K. The EAM potential calculated isn’t sufficiently good for the description of BCC uranium at normal conditions. The melting temperature is equal 1455 ± 2 K and is something higher than real one. It was necessary to propose that the specific term must be included in common EAM potential that accounts for the excitation of atomic electrons and causes the high thermal capacity. The value of this term may reach 100 kJ/mol at 5000 K. However this term isn’t revealed in strongly compressed states. It means that the compression evidently suppresses the electronic excitation processes. The thermodynamic properties of BCC and liquid uranium are calculated at the pressures up to 220 GPa and temperatures up to 12000 K.