

Application of the Embedded Atom Model to Liquid Metals: Uranium

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The embedded atom model (EAM) is applied to uranium using the thermodynamic properties of the liquid and the results of shock tests. Using the molecular dynamics method and the EAM potential, good agreement with experiment was obtained for the structure, density, and potential energy of liquid uranium for temperatures up to 5000 K, and also along the shock-compression Hugoniot curve up to ~220 GPa. Thermodynamic properties of BCC and liquid uranium are calculated at pressures up to 220 GPa and temperatures up to 12000 K. The bulk compressibility of liquid uranium calculated at 1406 K is close to experiment. Self-diffusion coefficients at isobar heating increase with temperature as a power law with exponent ~2.103. By means of the Stokes-Einstein equation, the dynamic viscosity is defined at temperatures up to 6000 K. The obtained potential is insufficient for the description of BCC uranium at normal conditions. The melting temperature of uranium with the EAM potential is equal to 1455 ± 2 K and is a little greater than the experimental value. The melting temperature increases monotonically with pressure and reaches 6015 K at 275 GPa. In order to reproduce experimental data for the energy along the $p = 0$ isobar, it is assumed that there is an additional electronic contribution to energy at high temperatures, which leads to a high heat capacity of uranium. The value of this contribution reaches almost 100 kJ/mol at 5000 K. This conception is applied also for strongly compressed states.