Application of the Embedded Atom Model to Liquid Metals: Sodium

David Belashchenko [C, S]
Moscow Institute of Steel and Alloys, Moscow, Russia

A special form of the embedded atom model (EAM), which was previously developed for liquid metals, is applied to sodium. This model uses diffraction structure data near the melting point. The parameters of the EAM potential were found using structural and thermodynamic data along the zero-pressure isobar with the shock compression data for pressures up to ~100 GPa. Using the molecular dynamics (MD) method and the EAM potential, good agreement with experiment was obtained for the structure, density, and potential energy of the liquid metal along the p ~ 0 isobar for temperatures up to 2300 K, as well as along the shock-compression Hugoniot curve up to ~100 GPa and ~30000 K. The melting temperature of a BCC sodium model with the EAM potential is equal to 358 ± 1 K which is close to experiment. The bulk modulus at 378 K is also close to experiment. For isobaric heating, the self-diffusion coefficient increases as the power 1.6546 of temperature. Pressure, energy, heat capacity, and the temperature derivative of pressure are calculated in a wide range of densities and temperatures. The volume dependence of pressure along the shock Hugoniot curve is close to experiment. Overall, the potential describes BCC sodium quite well. A change of structure of liquid sodium is discovered at the compression ratio of about 2, where nearest neighbors appear at short distances (~2.1 Å) but with low coordination number, thus forming bound groups (clusters). Their concentration grows when the volume decreases or the temperature increases. These neighbors are observed in particular due to the pre-peak of the pair correlation function whose height grows with compression and heating. In the region of the structural change, the pressure decreases during isochoric heating, similar to the water anomaly below 4 ^{o}C.

D.K. Belashchenko. // High Temperature. 2009. V. 47. In press.