An Application of the Embedded Atom Model to Liquid Metals: Non-Crystalline Iron in Earth's Core

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A method is proposed for the creation of an embedded atom potential that uses data for the structure and thermodynamic properties of liquid metals near their normal melting temperatures. This method is applied to liquid iron at temperatures up to 5000 K and pressures up to 360 GPa. A series of molecular dynamic models was created using this EAM potential at temperatures from 1820 to 5000 K, and densities from 8.00 to 12.50 g/cm^3. The thermodynamic, structural, diffusion, and viscous properties of iron are calculated. The self-diffusion coefficients diminish almost linearly with the decrease of the system volume, and become zero around a density of about 11.6 g/cm^3. In the region of the Earth's outer core, the iron behaves as a liquid, with the values of the self-diffusion coefficients on the order of 10^{-5} cm^2/s, and viscosities of about 10^{-3} to 10^{-2} Pa·s. At the boundary between the outer and inner Earth's cores, at densities of 11 to 12 g/cm^3, the iron behaves as in an amorphous phase, and the self-diffusion coefficients appear to be too small for evaluation using the molecular dynamics method. Under the conditions of the Earth's inner core, the iron model with the EAM potential crystallizes spontaneously.