Molecular Dynamics Modeling of Liquid Iron-Sulfur Solutions Using the Embedded Atom Model

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The Embedded Atom Model (EAM) potential was used in the molecular dynamics modeling of liquid iron-sulfur solutions. Parameters of the EAM potential for Fe-Fe, Fe-S, and S-S pairs were calculated using the thermodynamic and structural properties of iron near the melting point, and Fe-S melts (density, enthalpy, and distance between nearest neighbors). Iron-sulfur solutions with 0 to 18 at. % S were modeled, and thermodynamic, structural, and transport properties of solutions were calculated at temperatures from 1800 to 5000 K, and pressures up to 360 GPa. The densities of the solutions were in the range 12.3 - 10.7 g/cm^3. The viscosity was as high as tens of Pa·s; it decreased with increasing sulfur concentration from 0 to 6.2 at. %, and increased with further increase of the sulfur concentration. The solution composition had very little effect on the sound speed, which was equal to 12 to 13 km/s. The diffusion coefficient was on the order of 10^{-7} cm^2/s. At pressures near 360 GPa and temperatures near 5000 K, the pure iron crystallized spontaneously, while the iron – sulfur solutions could be characterized as "quasi-crystal," with slightly bent atomic planes which were seen in the model of the rotation as basic cubes. The true crystallization of iron-sulfur solutions is either not realized, or its realization requires a very long relaxation time.