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Density and sound velocity of liquid Fe-S alloys at Earth's outer core *P-T* conditions

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Abstract

Pressure-temperature-volume (*P-T-V*) data on liquid iron-sulfur (Fe-S) alloys at the Earth's outer core conditions (~136 to 330 GPa, ~4000 to 7000 K) have been obtained by first-principles molecular dynamics simulations. We developed a thermal equation of state (EoS) composed of Murnaghan and Mie-Grüneisen-Debye expressions for liquid Fe-S alloys. The density and sound velocity are calculated and compared with Preliminary Reference Earth Model (PREM) to constrain the S concentration in the outer core. Since the temperature at the inner core boundary (T_{ICB}) has not been measured precisely (4850~7100 K), we deduce that the S concentration ranges from 10~14 wt% assuming S is the only light element. Our results also show that Fe-S alloys cannot satisfy the seismological density and sound velocity simultaneously and thus S element is not the only light element. Considering the geophysical and geochemical constraints, we propose that the outer core contains no more than 3.5 wt% S, 2.5 wt% O, or 3.8 wt% Si. In addition, the developed thermal EoS can be utilized to calculate the thermal properties of liquid Fe-S alloys, which may serve as the fundamental parameters to model the Earth's outer core.

Keywords: Earth's outer core, liquid Fe-S alloy, first-principles molecular dynamics, sound velocity, equation of state