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Non-ideal thermodynamic mixing of sulfur with liquid iron-nickel alloys under the outer core conditions

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Great progress has been made on the nature of light elements in earth's core over the last decades. Considerable density deficit in earth's core relative to pure iron suggests possible lighter elements like hydrogen, carbon, oxygen, silicon, and sulfur alloyed with iron. Simple extrapolation of experimental data obtained at relatively low temperatures and pressures to the core conditions may not be sufficient to elucidate the effects of candidate light elements on the properties as it cannot account for abnormal changes in the interactions of light elements with Fe-Ni at the molecular level because of possible temperature and pressure-dependent molecular cluster formation within the outer core spanning a huge temperature and pressure range. To understand the effect of sulfur on the properties of the liquid alloy, thermodynamic mixing properties like excess volume (ΔV) and enthalpy (ΔH) were calculated as a function of molar concentration under core conditions. Thermodynamic mixing curves and excess properties of FeNiS systems give information about non-ideal mixing at the core-mantle boundary (CMB) and inner core boundary (ICB). The first principle molecular dynamics simulation was performed to simulate the liquid at 4050 K, 136 GPa, and 5530 K, 330 GPa conditions at sulfur concentrations in the range of 0-16 wt%S with 200 atoms in a cubical computational supercell. Pressure correction was applied and based on existing experimental data and thermodynamic model to account for discrepancies between experimental data and ab initio calculations due to systematic errors in the computation. The result shows the volume and enthalpy as a function of sulfur concentration becomes flat at low sulfur concentration. Deviations of ΔV and ΔH from the ideal mixing lines suggest non-ideal mixing of the liquid under the core conditions. The maximum negative ΔV and ΔH occur at ~10wt% S at the CMB, and decrease to ~5wt%S at ICB, suggesting that there is a unique and pressure-dependent concentration of sulfur where the interactions between Fe and sulfur are greatest. These results provide important clues on how sulfur is incorporated into Fe liquid and the role of sulfur as a candidate light element to accommodate the density deficit in the core.