Goldschmidt 2024 Abstract
https://doi.org/10.46247/gold2024.24317

Thermodynamic mixing model for liquid Fe-LEs alloys under the earth's outer core conditions

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The effect of light elements (LEs) like C, H, O, Si, S, and Ni on the geophysical properties of liquid Fe alloys under the core-relevant conditions is critical in understanding the earth's core composition and its dynamics. Significant progress has been made in understanding the geophysical properties of Fe-LEs alloys under earth's outer core conditions over the recent decades. Most experiments on the liquid are conducted at pressures or temperatures significantly below outer core conditions, necessitating extensive extrapolation of properties like density (ρ). These extrapolations may not accurately account for the effects of light elements on thermodynamic properties due to potential temperature- and pressure-dependent structural changes along core conditions as well as non-ideal mixing. It would be instrumental to have thermodynamic mixing models for the outer core from data obtained at the outer core conditions. In this study, the first principles molecular dynamics simulations were employed to quantify the mixing properties of binary Fe-LE alloy systems and their effect on the geophysical properties of the melts under the core conditions. Pressure correction was applied to reconcile discrepancies between experimental data and ab initio calculations. The molar volume, enthalpy, and excess properties of respective binary Fe-LE alloys were calculated at the temperatures and pressures of core adiabat and as a function of LE composition. Results showed that the volume and enthalpy of Fe-S and Fe-Si alloys increase non-linearly with their respective composition throughout core conditions. Conversely, the molar volume of Fe-H, Fe-O, and Fe-C alloys decreases with increasing concentration of respective LEs. For Fe-Ni, the molar volume change is nearly linear with increasing Ni concentration at core conditions. Based on this dataset, mixing models were established for the six Fe-LEs binary systems. The models were used to predict the molar volume, enthalpy, and density of any combination of Fe-LEs multi-component alloys along the outer core adiabat. The predicted volumes for quaternary alloys using the mixing models were within 0.06% error with respect to the first-principles calculations. The mixing models are expected to provide an essential tool for understanding LEs incorporation in liquid Fe-alloy and important insight into the outer core composition.