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# Effect of LEs on the diffusivity and viscosity of Fe-Ni alloy under the earth's outer core conditions

**JIANWEI WANG**[1], SAJIN SATYAL[1], FENG ZHU[2] AND BIN CHEN[3]

[1]Louisiana State University
[2]China University of Geosciences (Wuhan)
[3]University of Hawai'i at Manoa
Presenting Author: jianwei@lsu.edu

Properties of liquid Fe-Ni alloys under the earth's outer core conditions are crucial for understanding the composition, thermal state, dynamics, and evolution of the Earth's core. However, experiments on the liquids are often performed at pressures far below those of the outer core, prompting a long extrapolation of the experimental results to estimate the liquid properties under the core conditions. Such estimations can be complicated by light elements (LEs) such as H, C, O, Si, and S possibly forming subnormal pressure-dependent molecular clusters that can affect the thermodynamic properties of mixing of the LEs with Fe-Ni, leading to thermodynamics of non-ideal mixing in a large pressure range within the outer core. Such non-ideal mixing could significantly affect the dynamic properties of the liquid such as diffusivity and viscosity, which is the key for the core dynamo and core-mantle differentiation of terrestrial bodies. The focus of this contribution is to understand how LEs affect the diffusion coefficient and shear viscosity of liquid Fe-Ni alloy ($Fe_{90}Ni_{10}$) at 4050 K, 135 GPa (CMB) and 5530 K, 330 GPa (ICB). First-principles molecular dynamics was employed to compute the dynamic properties with the LE concentration from 0 mol% to 25 mol%, depending on the solubility and potential concentration range of the element in the core. The results show that the effect of LEs on the properties is complicated, depending on the nature and amount of the LEs, and controlled by how LEs are incorporated in the liquid alloy. A range of mixing behavior can occur, from close-to-ideal to non-ideal mixing with a large negative excess volume and enthalpy. Such non-ideal mixing is controlled the molecular structure described by covalency and compressibility of individual bonds and the short- and intermediate range structures (partial configurationally-decomposed distribution function). Activation energy and activation volume for diffusion and viscosity were estimated. The results provide fundemental basis on the level of turbulence in the couter core, percolation of the liquid alloy in the earth's deep mantle, and improve our understanding of the core dynamo and core-mantle differentiation of terrestrial bodies in large terrestrial body.