Effects of light-element impurities on transport properties of liquid Fe-Ni alloy at Earth's core conditions

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It is widely believed that the Earth's outer core consists of liqud iron (or liquid-nickel alloy) with light element impurities. Therefore, electrical and thermal conductivities of liquid iron-nickel alloys are important to understand magnetic and thermal behaviors of Earth.
Several experimental studies investigated the electrical conductivity or resistivity for iron under high pressure (Keeler, 1969 : Bi ,2002 : Ohta, 2016). Also, by using first principles calculations, electrical conductivity for liquid iron and mixtures with silicon and oxygen under high pressure has been investigated. (Pozzo, 2012, 2013 : de Koker, 2012)
Although first principles studies for liquid iron-oxygen and -silicon mixtures have been conducted so far, mixtures with other light elements such as hydrogen and carbon have not been investigated yet. Under this circumstance, in this study, we perform ab initio molecular dynamics simulations for liquid Fe-Ni alloy with H, C, O, S and Si. We calculate electronic and thermal conductivities at Earth's core conditions with using Kubo-Greenwood formulation. By comparing against results of pure system, we discuss effects of light element impurities on transport properties of liquid Fe-Ni alloy.

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