

Effects of light elements on transport properties of liquid Fe alloys under high pressure.

*Satoshi Ohmura¹, Taku Tsuchiya², Hiroki Ichikawa³

1. Hiroshima Institute of Technology, 2. Ehime University, 3. Tokyo Institute of Technology

It is believed that Earth's outer core consists of liquid iron (or liquid-nickel alloy) with light element impurities. For understanding magnetic and thermal behaviors of the Earth, it is required to investigate electrical and thermal conductivities of liquid iron and influence of the light elements on these properties. Several experimental studies investigated the electrical and thermal conductivities under high pressure by shock compression experiments (Keeler, 1969 : Bi, 2002) and by experiments in a laser-heated diamond anvil cell (Ohta, 2016 : Konôpková 2016). First principle calculations also have been used to investigate transport properties of liquid iron and mixtures with silicon and oxygen. (Pozzo, 2012, 2013 : de Koker, 2012)

Under this circumstance, we have investigated effects of light elements (including all candidate other than silicon and oxygen) on transport properties of liquid Fe alloy under high pressure by using *ab initio* molecular dynamics simulations. To provide further details of the effects of light-element, in addition to the type of light element, we have investigated how much transport properties are affected by the amount of light elements. This time, we discuss effects of the light element on transport properties of liquid Fe alloys in terms of the type and amount of light elements.

Reference

- R.N. keeler and A.C. Mitchell, *Solid state Commum.* **7**, 271 (1969)
Y. Bi, et al., *J. Phys. Condens Matter* **14**, 10849 (2002)
M. Pozzo et al., *Nature* **485**, 355 (2012)
N de Koker, et al., *Proc. Natl., Acad. Sci.* 109 4070 (2012)
M. Pozzo, et al., *Phys. Rev. B* **87** 014110 (2013)
K. Ohta et al., *Nature* **534** 95 (2016)
Z. Konôpková et al., *Nature* **534** 99 (2016)

Keywords: electrical conductivity, thermal conductivity, liquid Fe alloys, high pressure, ab initio molecular dynamics simulation