The Equation of State of Liquid Pure Fe and Fe-light Elements Alloys by Ab Initio Molecular Dynamics Simulations to confine the outer core composition

HIROKI ICHIKAWA[1,2]*, TAKU TSUCHIYA[1,2], AND MASANAO OHSUMI[1]

[1]Geodynamics Research Center, Ehime University, 2-5, Bunkyocho, Matsuyama, Ehime, 790-8577, Japan

[2] Earth-Life Science Institute, Tokyo Institute of Technology, Ookayama 2-12-1, Megro Tokyo, 152-8551, Japan

(*correspondence: h-ichikawa@sci.ehime-u.ac.jp)

The equation of state (EoS) of pure Fe and Fe-light elements alloy liquids were calculated by means of ab initio molecular dynamics (AIMD) simulations at the outer core *P-T* conditions. In the outer core, many light elements, such as carbon, nitrogen, oxygen, hydrogen, sulfur, and silicon, have been proposed as possible constituents. The concentrations of these elements have been strongly debated for years.

The density and the adiabatic bulk and shear modulus of iron and iron-light element alloys are essential to interpreting seismological observations and to constructing a mineralogical model of the core. On this subject, AIMD simulations have successfully clarified density and bulk sound velocity at the outer core conditions for various Fe-light elements systems [e.g. 1, 2]. However, the data points are limited at several *P*, *T* conditions. Meanwhile, several studies have been performed throughout the whole outer core *P-T* conditions for pure Fe [3, 4], Fe-S [5], and Fe-H [6]. In these studies, Grüneisen parameter, whose value is required for the calculation of bulk sound velocity, is obtained as a consequence of the evaluation of the equation of state. However, different formulations of Grüneisen parameter are employed in all the studies.

In this study, we investigated energy (*E*)-pressure (*P*)-volume (*V*)-temperature (*T*) relationships of liquid Fe-light elements systems in the Earth's core condition by AIMD simulations and proposed a new *P-V-T* EoS under the whole outer core conditions. We also confined plausible outer core compositions, which reproduce seismological values reasonably throughout the whole outer core conditions.

[1] Pozzo *et al*. (2013) *PRB* **87**, 014110. [2] Badro *et al*. (2014) *PNAS* **111**, 7542-7545. [3] Vočadlo *et al*. (2003) *PEPI* **140**, 101-125. [4] Ichikawa *et al*. (2014) *JGR* **119,** 240-252. [5] Umemoto *et al*. (2014) *GRL* **41**, 6712-6717. [6] Umemoto & Hirose (2015) *GRL* **42**, 7513-7520.