Japan Geoscience Union Meeting 2014
(28 April - 02 May 2014 at Pacifico YOKOHAMA, Kanagawa, Japan)

SIT39-10 会場:416 時間:5 月 2 日 11:30-11:45

第一原理分子動力学法による鉄・軽元素系液体合金の状態方程式の決定
The P-V-T equation of state of liquid pure Fe and Fe-light elements alloys by ab initio molecular dynamics simulations

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The equation of state (EoS) of pure Fe and Fe-light elements alloy liquids were calculated by means of ab initio molecular dynamics 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. In this study, internally consistent thermodynamic and elastic properties of pure Fe and Fe-light elements alloys, in particular density, adiabatic bulk modulus, and P-wave velocity were analyzed in order to clarify the effect of light elements incorporation on seismically observable data. Then the results were compared with the seismological data of the Earth's outer core to confine the plausible compositions of the outer core. The new EoS model of liquid iron alloys as a function of pressure, temperature and fraction of light elements may serve as fundamental data for the composition model of the Earth's core.