沈み込み帯で起こる海洋プレートによるアルゴンのインプット Inputs of Argon on oceanic plate at subduction zones

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It is known that noble gases are key tracers to understand the evolution of the mantle because of their inertness nature and isotope variations. However, a mechanism of recycle of noble gases in the deep mantle is still open question. Argon is one of noble gases and has three isotopes, ³⁶Ar, ³⁸Ar, and ⁴⁰Ar. Holland and Ballentine [2006] proposed that Ar from the mantle is identical to seawater component. This indicates that the seawater recycling dominates a behavior of Ar in the mantle. In contrast, the systematic analysis for noble gases indicates that ocean island basalt has a primordial signature which is different from atmosphere component [Mukhopadhyay 2012]. The recycling of Ar between the Earth's surface and the deep mantle has been discussed using the isotope data of noble gases. However, it is difficult to understand a mechanism of recycling of Ar because of a lack of knowledge for physical and chemical properties of Ar at high pressure and high temperature.

In this study, we used density functional theory to investigate the melting temperature and thermal pressure of Ar. We also performed the high-pressure experiments to determine the room-temperature equation of state for Ar. The combination of the first-principles molecular dynamics calculations and the high-pressure experiments led us to determine reliable physical properties, such as the equation of state and the melting temperature, over a wide range of pressures and temperatures.

The equation of state of Ar has been investigated to 382 GPa and 3000 K using the diamond anvil cell experiments and the first-principles molecular dynamics method. A large volume dependence of the thermal pressure of Ar was revealed at pressures higher than 200 GPa. A significant temperature dependence of the calculated effective Grüneisen parameters was confirmed at high pressures. This indicates that the conventional approach to analyze thermal properties using the Mie-Grüneisen approximation is likely to have a significant uncertainty in determining the equation of state for Ar, and that an intrinsic anharmonicity should be considered to analyze the equation of state. A melting temperature of Ar was estimated from calculation data, and a significant pressure dependence was confirmed. If the pressure-temperature path of the subducted slab is lower than critical condition, ~750 K and ~7.5 GPa, solid Ar can be carried down into the deep mantle. Melting of solid Ar in the upwelling mantle plume occurs at the bottom of the transition zone.

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