

Ab initio molecular dynamics study on a phase separation in liquid Fe-O

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The Earth's outer core is mainly composed of liquid Fe-Ni alloy. The density of the outer core is, however, ~10% smaller than this alloy. The density deficit indicates that substantial amount of light elements are present in the outer core [Birch, 1964]. Recent seismological observations proposed that seismic wave velocity is ~3% slower than PREM below a few hundred kilometers of the CMB [Helffrich and Kaneshima, 2010]. The low-velocity anomaly is considered to be caused by stratification. However, mechanisms of the stratification have not been clarified yet. One possible cause is phase separation into Fe-rich and light element-rich liquid. Oxygen is one of the most important light elements, because an iron-oxygen phase separation was observed experimentally at low-pressure condition [Tsuno et al., 2007]. This immiscible behavior is, however, still unclear at the outer core pressure.

In this study, we calculated liquid Fe-O alloy at the outer core condition by means of *ab initio* molecular dynamics simulations. First, we analyzed local structures of liquid Fe-O alloy to detect signs of phase separation. Second, we evaluated its excess enthalpy. Both indicate that the liquid was well-mixed. Finally, we computed P-wave velocity in liquid Fe-O alloy. P-wave velocity was found to increase with increasing the oxygen concentration. All these results suggest that the simple enrichment process is less suitable to explain the low-velocity anomaly.

Keywords: ab initio molecular dynamics simulation, phase separation, liquid Fe-O alloy