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The effect of carbon on density and elastic property of liquid Fe-C under high pressure

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The Earth's outer core is composed of the molten Fe alloys. Seismological and experimental studies show that the Earth's outer core is approximately 10% less dense than molten iron at the core pressure and temperature conditions, implying that some light elements, such as S, Si, O, H and C, exist in the outer core. Carbon is one of the plausible candidates of the light element in the core. Based on the effect of pressure on carbon solubility into molten iron and its thermodynamic calculation, carbon is expected to exist in the Earth's core. In this study, we measured the density of liquid Fe-3.5wt%C using X-ray absorption method and discussed the effect of carbon on the molar volume and elastic parameter (i.e. bulk modulus and thermal expansion coefficient)

High-pressure experiments were performed using a DIA-type cubic anvil press (SMAP-I) installed at the in-vacuum undulator beamline BL22XU at SPring-8 synchrotron radiation facility in Japan (Sakamaki et al., 2009, 2011; Nishida et al., 2011). We clarified the effects of pressure and temperature on the liquid density in the pressure and temperature range of 1.8-6.5 GPa and 1600-2200 K. The present results revealed that the density of liquid Fe-C shows an abrupt change at 5.5 GPa and 1800 K. This abrupt density change may be caused by the phase change of Fe_3C side. Incongruent melting takes place in Fe_3C and a solid phase (i.e., liquidus phase) coexists with the melt changes from graphite to Fe_7C_3 at around 5 GPa (Nakajima et al., 2009). This change in liquidus phase at 5 GPa may also affect the structure of liquid Fe-C. The effect of the structural change of the liquid Fe-C is important for considering an abundance of carbon in Earth's outer core.

We fitted the present data below 5 GPa using the Birch-Murnaghan EOS and obtained $K_{0,1500K}$ = 55.3(2.5) GPa, $(dK_0/dP)_T$ = 5.2(1.5), and thermal expansion coefficient = 0.86(4)$*10^{-4}$ K^{-1}. The estimated K_{0T} of liquid Fe-3.5wt%C (55.3 GPa) was lower than that of liquid iron (K_{0T}=85.1 GPa)(Anderson and Ahrens, 1994).

Comparing the present density with that of the previous studies which reported by Terasaki et al. (2010, JGR) for C=6.6 wt% and Sanloup et al. (2011, EPSL) for C=5.7 wt%, the compositional dependency of the liquid density can be estimated, The molar volume variation with C content is concave from the tie line between molar volumes of Fe and C end members (i.e., ideal mixing line), suggesting that excess molar volume (V_{ex}) of liquid Fe-C is negative at high pressure. This tendency is consistent with that observed at 1 atm (Ogino et al., 1984). The negative excess molar volume may indicate that inter-atomic distance of Fe decreases by occupying of carbon at the interstitial site. The density of liquid Fe-C shows non-ideal mixing behavior. Thus, the amount of carbon in the core may possibly be larger than the previous estimates if the non-ideal mixing behavior is maintained up to the core condition.

Keywords: High pressure and High temperatute, density, liquid Fe-C, molar volume, bulk modulus, thermal expansion coefficient