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X-ray diffraction study on structure of liquid Fe-C under pressure

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1 Introduction

Physical properties of molten iron alloys, such as density and viscosity, are fundamental to understand the dynamics of core of terrestrial planets. Structural study of molten iron alloys is fundamental to understand those properties. Sanloup et al. [1] reported that compressibility of liquid Fe-$_{5.7wt\%}$C increases around 5 GPa. They interpreted it as a result of liquid-liquid transformation in the vicinity of the δ–γ-liquid triple point of Fe (5.2 GPa) There is, however, no direct study of structure of liquid Fe-C at high pressures. Here we report the results of the first study of the structure of Fe-$_{3.5wt\%}$C melt under pressure using synchrotron radiation.

2 Experiment

High-pressure and high-temperature X-ray diffraction experiments were conducted by energy-dispersive x-ray diffraction method using the cubic-press MAX 80 at AR-NE5C. Diffraction patterns of Fe-C melt were acquired at fixed Bragg angles between 3° to 20°. Data were collected at the pressure range from 2 to 6.5 GPa.

3 Results and Discussion

Diffraction patterns acquired at different Bragg angle are connected to derive the structure factor $S(Q)$ shown in Fig.1. Structure factor of liquid Fe-C at high pressures resembles those at 0.1 MPa [2] and does not change much with pressure. Correlation function $g(r)$, which was obtained by Fourier transform of $S(Q)$, are also shown in Fig. 1. The first peak of $g(r)$ is a mixed correlation of pairs Fe-C and Fe-Fe [3]. The first peak position r_1 of $g(r)$ corresponds to a Fe-Fe correlation. Small hump around 2.2 Å is related to a pair Fe-C. The correlation function does not change much with pressure, except for r_1. The first peak position decreases clearly with increasing pressure.

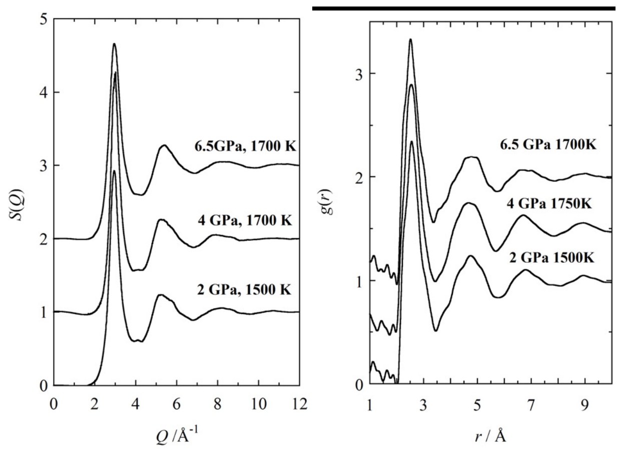

Fig. 1: Structure factor $S(Q)$ and total correlation function $g(r)$ for liquid Fe-$_{3.5wt\%}$C.

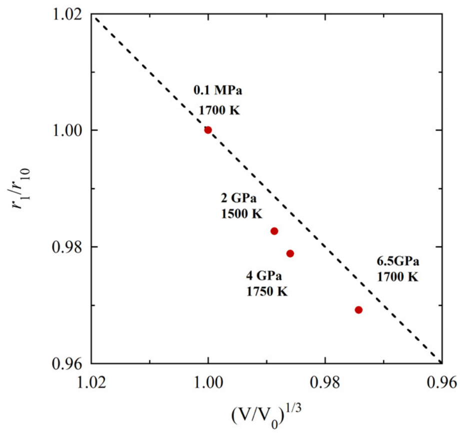

Fig. 2: Relationship between nearest neighbor distance and volume for liquid Fe-$_{3.5wt\%}$C.

The near neighbor distance r_1 of liquid Fe-C decreases linearly with $V^{1/3}$, indicating the uniform compression of this liquid (Fig. 2). The coordination number of nearest neighbor of liquid Fe-C is nearly constant to be about 13 within this pressure range.

Thus, we have not found any evidence of liquid–liquid transition in Fe-$_{3.5wt\%}$C composition up to 6.5 GPa, while the compressibility change was reported for more C-rich composition [1].

References

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