Light-element dependences on structure of liquid Fe at high pressure

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Abstract

The Earth's core consists of a roughly 96% liquid outer core and 4% solid inner core by volume. Presence of liquid core has been identified not only in the Earth but also in other planets such as Mercury, Mars, and the Moon. The planetary liquid core is considered to be composed of metallic iron with some light elements such as sulfur, silicon, and carbon. Therefore, knowledge on the liquid iron-light element alloys at high pressures is the most fundamental to understand dynamic processes of the core such as core formation and dynamo process which closely relate with nature of liquid iron alloys. In this work, we investigated structure of liquid Fe-Si, Fe-C, and Fe-S alloys at high pressure to understand influence of the light elements on structure of liquid Fe.

We measured structures of liquids Fe, Fe-18.1at.% Si, Fe-28.9at.% Si, Fe-50at.% Si, Fe-14.4at.% C, Fe-25at.% C, Fe-16.2at% S, Fe-23.5at.% S, and Fe-30.3at.% S at the pressures of 3-5 GPa using multi-angle energy-dispersive X-ray diffraction (EDXD) technique with a Paris-Edinburg type large volume press at the beamline 16-BM-B at the Advanced Photon Source.

Structures of liquid Fe-C alloys are basically similar to that of liquid Fe. Liquid Fe-16.2 at.% S also exhibits basic structure similar to liquid Fe, while, at higher S contents, the local structure changes to poorly ordered structure, similarly to those obtained in previous studies. Structures of liquid Fe-Si alloys show mixing behavior between the end member liquids Fe and FeSi. The dissolution of C expands the nearest neighbor distance, indicating that the incorporation mechanism of C into liquid Fe is interstitial type. Similarly, incorporation of small amount of S expands the nearest neighbor distance, while, at high S content, the nearest neighbor distance significantly decreases with increasing S content. In contrast, incorporation of Si shortens the nearest neighbor distance. Our results indicate different nature of incorporation of S, C, and Si in liquid Fe at 3-5 GPa, which may be a key to understand physical properties of liquid iron-light element alloys.

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