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In-situ XRD measurements of Fe encapsulated in carbon nanotubes under high pressure

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1 Introduction

Carbon nanotube (CNT) hollow cores provide strong interaction potential field to molecules encapsulated in CNTs. So far, many encapsulation systems including C_{60} peapods have been prepared. Due to the strong potential field and the restricted space, the encapsulated molecules sometimes have unique structures which are different from the structures of bulk states. In some cases, the atom-atom distances are much smaller than those of the bulk states. Such effect is called “pseudo high pressure effect”. However, it is not very clear whether this effect is universal effect for all the encapsulation system. Furthermore, we don’t have much knowledge about structural phenomena of the encapsulated molecules for external pressure.

2 Experiment

CNTs encapsulating Fe were prepared by metal organic chemical vapor deposition (MOCVD) method using ferrocene. The encapsulated Fe and CNTs were characterized by TEM. The tube diameter and hollow core diameter were about 20-40 and 10-20 nm, respectively. In situ XRD measurements of Fe encapsulated in CNTs under high pressure were performed with a diamond anvil cell. A 4:1 mixture of methanol and ethanol was used as the pressure transmitting medium. The pressure was determined by the ruby fluorescence method.

3 Results and Discussion

At ambient pressure, we observed wide angle diffraction pattern and performed Rietveld analysis for the obtained pattern. We found two types of crystals were encapsulated: α-Fe and cementite FeC_3. Fig. 1 shows the observed and simulated patterns. As shown Fig. 1, the accordance of these two patterns is very good. Since the calculated lattice parameters are in good agreement with the previously reported values, we cannot find the pseudo high pressure effect for this system. Fig. 2 shows the change in XRD pattern with pressure. By analyzing the observed patterns, we could determine the bulk moduli of both α-Fe and cementite FeC_3 phases. The determined values are not deviated from the values reported for the bulk crystals.

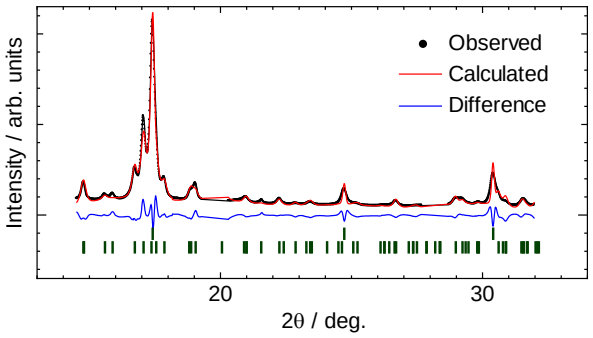

Fig. 1 Rietveld analysis of the observed XRD pattern of Fe@SWCNT.

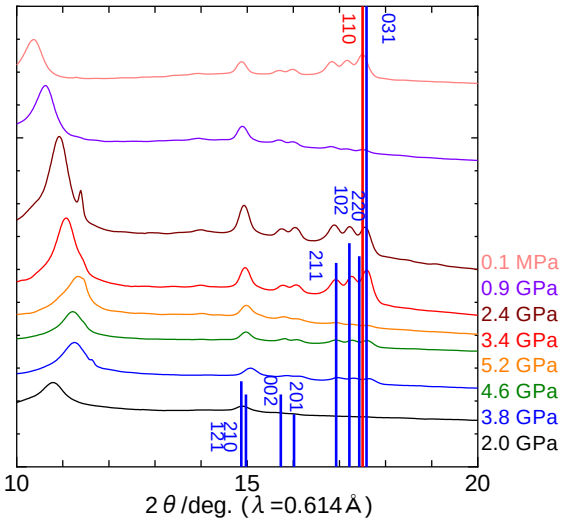

Fig. 2 The observed XRD patterns at several pressures. The blue and red vertical lines indicates the diffraction line positions of FeC3 and α-Fe at ambient pressure, respectively.

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