



Structure and properties of iron carbide at the Earth's mantle and core conditions

V. Prakapenka, M. Rivers and S. Sutton

CARS, University of Chicago, Chicago, Illinois 60637, USA (prakapenka@cars.uchicago.edu)

Recent seismological investigations are revealing a very complex texture and/or heterogeneity of the Earth's core and core-mantle boundary (Vidale, 2000). The knowledge of the chemical composition of the core is one of the key factors in understanding the Earth's structure. Among the number of candidate elements considered as light constituents in the metallic core, carbon and its alloys are most challenging for direct high pressure high temperature studies. At the same time, the presence of even a small amount of carbon can drastically change the path of multi elemental chemical reactions and thereby physical properties of the end products. Hence, the influence of carbon on the phase transformations, chemical reactions, partitioning, melting temperatures etc of the core-mantle forming elements is essential for understanding of the Earth's evolution.

One of the carbon compounds, Fe_3C has been suggested as a major phase of the Earth's inner core (Wood, 1993). A number of experimental studies of its equation of state at room temperature led to a density of this material at inner core pressures in excellent agreement with the PREM (Scott, 2001; Li, 2002). However, first-principles computer simulations and measurements of the thermal expansion of Fe_3C below and above the ferromagnetic phase transition by neutron powder diffraction at ambient pressure have suggested that the physical properties of Fe_3C are incompatible with the probable range of inner core density determined from seismic data (Vocadlo, 2002; Lin, 2004). Disparate conclusions might be a result of fact that these studies were conducted at either at room temperature or at ambient pressure. For correct modelling of the carbon budget in the lowermost Earth's mantle and core the studies should be performed in-situ under appropriate core-mantle conditions.

In this work we have studied in-situ the chemical stability and physical properties of the iron-carbon system under relevant Earth's lower mantle and core conditions. The double-sided laser heating technique combined with high resolution angle-dispersive micro x-ray diffraction system at GSECARS (Sector 13, APS, Argonne) was used to characterize samples in the diamond anvil cell (DAC). Iron carbide was synthesized in-situ in the DAC from various mixtures of Fe and C powders with different atomic ratios: 1:3, 1:2 and 1:1. We have found that chemical reaction between iron and carbon does not depend on the starting phases of Fe (*fcc* or *hcp*) and C: (graphite or diamond). The reaction temperature increases gradually from ~ 1000 K to ~ 1700 K as pressure increased from ~ 6 GPa to ~ 155 GPa respectively. We did not observe dissociation of iron carbide in the entire pressure-temperatures range studied: up to ~ 170 GPa and ~ 4000 K. Thus, the high-pressure high-temperature stability and physical/chemical properties of iron carbide phases at the relevant Earth's mantle and core conditions provide important constraints on interpretation of the reported seismic anomaly in the D'' layer and are essential for understanding the differentiation of the early Earth. Implications of these results for the composition of the Earth's interior will be discussed.