Compressional and shear wave velocities for polycrystalline bcc-Fe up to 6.3 GPa and 800 K

YUKI SHIBAZAKI1,2,*, KEISUKE NISHIDA3, YUJI HIGO1, MAKO IGARASHI2, MASAKI TAHARA2, TATSUYA SAKAMAKI2, HIDENORI TERASAKI6, YUTA SHIMOYAMA5, SOMA KUWABARA5, YUSAKU TAKUBO5, and EIJI OHTANI2

1Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, 6-3 Aoba, Aramaki, Aoba-ku, Sendai 980-8578, Japan
2Department of Earth and Planetary Material Sciences, Tohoku University, 6-3 Aoba, Aramaki, Aoba-ku, Sendai 980-8578, Japan
3Department of Earth and Planetary Science, University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113-0033, Japan
4Japan Synchrotron Radiation Research Institute, 1-1-1 Kouto, Sayo 679-5198, Japan
5Department of Earth and Space Science, Osaka University, 1-1 Machikaneyama-cho, Toyonaka, Osaka 560-0043, Japan

ABSTRACT

The cores of the Earth and other differentiated bodies are believed to be comprised of iron and various amounts of light elements. Measuring the densities and sound velocities of iron and its alloys at high pressures and high temperatures is crucial for understanding the structure and composition of these cores. In this study, the sound velocities (v_P and v_S) and density measurements of body-centered cubic (bcc)-Fe were determined experimentally up to 6.3 GPa and 800 K using ultrasonic and X-ray diffraction methods. Based on the measured v_P, v_S, and density, we obtained the following parameters regarding the adiabatic bulk K_0 and shear G moduli of bcc-Fe: K_0 = 163.2(15) GPa, ∂K_0/∂P = 6.75(33), ∂K_0/∂T = −0.038(3) GPa/K, G_0 = 81.4(6) GPa, ∂G/∂P = 1.66(14), and ∂G/∂T = −0.029(1) GPa/K. Moreover, we observed that the sound velocity–density relationship for bcc-Fe depended on temperature in the pressure and temperature ranges analyzed in this study and the effect of temperature on v_P was stronger than that on v_S at a constant density, e.g., 6.0% and 2.7% depression for v_P and v_S, respectively, from 300 to 800 K at 8000 kg/m^3. Furthermore, the effects of temperature on both v_P and v_S at a constant density were much greater for bcc-Fe than for ε-FeSi (cubic B20 structure), according to previously obtained measurements, which may be attributable to differences in the degree of thermal pressure. These results suggest that the effects of temperature on the sound velocity–density relationship for Fe alloys strongly depend on their crystal structures and light element contents in the range of pressure and temperature studied.

Keywords: bcc-Fe, high pressure, planetary core, sound velocity, ultrasonic method

INTRODUCTION

Observations of seismic wave propagation and normal mode oscillation are the most powerful probes for examining the Earth’s interior, allowing us to obtain physical information on the Earth’s interior such as distributions of densities and sound velocities [both compressional (v_P) and shear (v_S) wave velocities] [e.g., Preliminary Reference Earth Model (PREM), proposed by Dziewonski and Anderson (1981)]. According to observation-based geophysical data and laboratory-based studies, the Earth’s core is considered to comprise metallic iron (Fe) with various amounts of light elements, such as hydrogen (H), carbon (C), oxygen (O), silicon (Si), and sulfur (S) (e.g., Birch 1952; Poirier 1994). Thus, iron alloyed with light elements is widely accepted as a basis for the chemical models of other planetary cores (e.g., Zharkov et al. 2009; Dumberry and Rivoldini 2015).

To constrain the species of major light elements and their abundances in the core, many studies have investigated the density and sound velocity of Fe as well as its alloys with light elements at the high pressures and high temperatures characteristic of interior planetary conditions (see the review by Li and Fei 2014). At high pressure and temperature, sound velocities have been measured mainly using shock compression (e.g., Brown and McQueen 1986), high-energy resolution inelastic X-ray scattering (IXS) (e.g., Fiquet et al. 2001; Badro et al. 2007), and nuclear resonant inelastic X-ray scattering (NRIXS) (e.g., Mao et al. 2001; Lin et al. 2003). Most recently, measurements by picosecond acoustics have been reported (Decremps et al. 2014). However, to estimate v_S (and also v_P in the case of NRIXS), those measurements require other physical quantities (e.g., density and bulk modulus) that must be obtained in separate experiments. That is, v_S (and v_P of NRIXS) must be obtained indirectly, and thus the accuracy of the estimated value depends on the uncertainties of these physical quantities as well as the velocity measurement itself. Therefore, most core compositional models have been developed using only v_P data, although the proposed physical models for the Earth’s interior (e.g., PREM) provide us with both v_P and v_S for the solid inner core. To constrain the abundances of light elements in the core more tightly, direct measurements of v_S for Fe and Fe alloys and core compositional analyses using

* E-mail: yshibazaki@m.tohoku.ac.jp