**Thermoelasticity of ε-FeSi to 8 GPa and 1273 K**

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**ABSTRACT**

The elastic properties of ε-FeSi were investigated at high temperature and pressure using a combination of ultrasonic interferometry and synchrotron radiation up to 8 GPa and 1273 K. The unit-cell volumes and sound velocity data were fit to third-order finite-strain equations with adiabatic temperature conversions to maintain a thermodynamically internally consistent data set. The adiabatic zero-pressure bulk and shear moduli and their first pressure and temperature derivatives were obtained from this fitting: \( K_0 = 168.9(7) \) GPa, \( G_0 = 116.5(3) \) GPa, \( K_0' = 6.6(2) \), \( G_0' = 2.9(1) \), \( \partial K_0/\partial T_p = -0.023(1) \) GPa/K, \( \partial G_0/\partial T_p = -0.030(1) \) GPa/K. This study presents the first complete thermodynamically consistent set of elastic moduli and their temperature and pressure derivatives.

**Keywords:** Ultrasonic interferometry, equation of state, iron silicide, elastic properties, high pressure, high temperature

**INTRODUCTION**

Many previous investigations have been directed at unraveling the possible composition of the Earth’s core (i.e., McDonough and Sun 1995). It has long been accepted that the core is made up of a predominantly metallic iron, or iron-nickel, alloy; however, several studies have shown that both metallic Fe and Fe-Ni alone are too dense to be the sole element in the Earth’s core, particularly the solid inner core (i.e., Dziwonsky and Anderson 1981; Jephcoat and Olson 1987; Mao et al. 1998). These studies, as well as several others, suggest that there must be some amount of some light element(s) in the core.

Silicon has been strongly suggested by previous studies to be a possible light-element constituent of the Earth’s core based on both density and velocity data (Badro et al. 2007), as well as on isotopic and geochemical data (Georg et al. 2007). To assess the possibility of Si as a constituent of the core, physical properties of Si-bearing iron phases under extreme conditions must be determined. This study is part of a continuing effort begun in Whitaker et al. (2008) that is designed to address this issue by studying ε-FeSi at high pressure and high temperature.

Under ambient conditions, FeSi occurs as ε-FeSi, which is a cubic material (B20 structure) in which the coordination numbers of both Si and Fe are seven (Pauling and Soldate 1948), and has a modified NaCl structure wherein the silicon and iron atoms are displaced along the [111] directions (Knittle and Williams 1995). Considerable debate exists over the behavior and physical properties of ε-FeSi under extreme conditions in spite of several previous studies that have been conducted on this material (Guyot et al. 1997; Knittle and Williams 1995; Lin et al. 2003; Sarrao et al. 1994; Whitaker et al. 2008; Wood et al. 1995). Some of this debate was clarified by Whitaker et al. (2008) in a study on the high-pressure elasticity of ε-FeSi at ambient temperatures, which presented the first complete data set on the bulk and shear moduli and their first pressure derivatives. However, despite all of these previous experimental studies on fersilicite, there is no available data on the temperature dependence of the elastic properties of this phase. This study sets out to determine the elastic properties of ε-FeSi in situ under high pressure and temperature, and examines the pressure and temperature dependence of these properties by using ultrasonic interferometry combined with synchrotron-based X-ray diffraction and X-radiographic imaging.

**EXPERIMENTAL METHODS**

The starting material for this study was powdered FeSi (99.9% pure) purchased from Alfa Aesar. X-ray powder diffraction of this material indicated that the powder was homogeneous and pure ε-FeSi. The bulk powder was then hand-ground with an agate mortar and pestle for ~30 min, resulting in a fine powder with an average grain size on the order of a few micrometers. This fine powder was loaded into a gold capsule and dried at 150 °C for 2 h, after which the capsule was pressure-sealed so as to prevent moisture adsorption. This capsule was then placed into the standard COMPRES 14/8 octahedral cell assembly for a hot-pressing experiment. The sample was sintered at 700 °C and 7 GPa in a Kawai-type 1000 ton uniaxial split-cylinder apparatus for exactly 1 h before temperature quenching and decompression. Visual inspection, X-ray diffraction, and SEM analysis of the finished run products all suggest that no oxidation of the FeSi occurred at any step during these sample preparation procedures.

The resulting sintered cylindrical sample was then analyzed at beamline X17B2 at the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL) to check for heterogeneity in grain size and/or composition. X-ray diffraction patterns of the sample were collected at a series of points while under ambient conditions by changing its position in the beam laterally and vertically; the diffracted X-rays were collected by four detectors (two aligned vertically and two horizontally) positioned at \( \chi = 0°, 90°, 180°, \) and 270° (Fig. 1). The diffraction patterns recorded by the horizontal (3 and 4 in Fig. 1) and vertical detectors (1 and 2 in Fig. 1) were virtually identical for each point analyzed, and all points analyzed gave similar diffraction patterns to those in Figure 1; this indicates that there was no detectable preferred orientation of the grains in the sample, and in conjunction with SEM analyses of the sample, suggests a uniform grain size and a pure and homogeneous ε-FeSi composition. Small unlabelled peaks in these diffraction patterns were either sample peaks not used for refinement or parasitic peaks from the surrounding cell assembly.

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