

Sound velocities of iron-nickel and iron-silicon alloys at high pressures

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[1] Understanding the alloying effects of nickel and light element(s) on the physical properties of iron under core conditions is crucial for interpreting and constraining geophysical and geochemical models. We have studied two alloys, $\text{Fe}_{0.92}\text{Ni}_{0.08}$ and $\text{Fe}_{0.85}\text{Si}_{0.15}$, with nuclear resonant inelastic x-ray scattering up to 106 GPa and 70 GPa, respectively. The sound velocities of the alloys are obtained from the measured partial phonon density of states for ^{57}Fe incorporated in the alloys. Addition of Ni slightly decreases the compression wave velocity and shear wave velocity of Fe under high pressures. Silicon alloyed with Fe increases the compressional wave velocity and shear wave velocity under high pressures, which provides a better match to seismological data of the Earth's core. **INDEX TERMS:** 1015 Geochemistry: Composition of the core; 3909 Mineral Physics: Elasticity and anelasticity; 3924 Mineral Physics: High-pressure behavior; 3939 Mineral Physics: Physical thermodynamics; 8124 Tectonophysics: Earth's interior—composition and state (1212). **Citation:** Lin, J.-F., V. V. Struzhkin, W. Sturhahn, E. Huang, J. Zhao, M. Y. Hu, E. E. Alp, H.-k. Mao, N. Boctor, and R. J. Hemley, Sound velocities of iron-nickel and iron-silicon alloys at high pressures, *Geophys. Res. Lett.*, 30(21), 2112, doi:10.1029/2003GL018405, 2003.

1. Introduction

[2] Iron-nickel (Fe-Ni) alloy is believed to be the most abundant constituent of the Earth's core [Birch, 1952]. The amount of Ni in the core is about 5.5 wt%, based on geochemical and cosmochemical models [McDonough and Sun, 1995]. On the other hand, the density of the outer core is about 10% lower than the density of Fe at core pressures and temperatures [Birch, 1952], while the bulk sound velocity of the outer core is 3% higher than that of liquid Fe [Anderson and Ahrens, 1994], suggesting the presence of light element(s) (such as H, C, O, Si, or S) in the outer core [Poirier, 1994; Hemley and Mao, 2001]. A certain amount of light element(s) may also be present in the Earth's inner core, because the differences in the density and compressional wave velocity between solid Fe and the inner core may be as much as 5% [Stixrude et al., 1997; Fiquet et al., 2001; Hemley and Mao, 2001]. Therefore, understanding the alloying effects of Ni and potential light element(s)

on the physical properties of Fe under core conditions is crucial for geophysical and geochemical models of deep Earth.

[3] Silicon is a candidate light element component based on geophysical and geochemical arguments [Lin et al., 2003a, and references therein]. Here we have used an Fe-rich Fe-Si alloy, $\text{Fe}_{0.85}\text{Si}_{0.15}$, as an example to understand the alloying effects of a light element on the physical properties of Fe. We do this for the following reasons: (1) the abundance of light element(s) in the core is only as much as 10 wt% [Anderson and Ahrens, 1994]; (2) most light elements, such as oxygen and sulfur, have limited solubility in Fe and form intermediate compounds with Fe (such as FeO, FeS, Fe_3S_2) at least over a modest pressure-temperature range [Fei et al., 1997; Li et al., 2001]; (3) silicon readily forms alloys with Fe under ambient conditions; (4) Fe-rich Fe-Ni and Fe-Si alloys adopt the hexagonal close-packed (hcp) structure at high pressures [Mao et al., 1990; Lin et al., 2003a], which provides an important constraint on the crystal structure of the phase of the inner core [Hemley and Mao, 2001].

[4] The alloying effects of Ni and Si on the crystal structures and equation of state (EOS) of Fe under high pressures and temperatures have been extensively studied [Mao et al., 1990; Lin et al., 2002a, 2002b, 2003a]. The addition of Ni does not appreciably change the compressibility of hcp-Fe under high pressures [Mao et al., 1990]. Studies of the phase relations of Fe and Fe-Ni alloys indicate that Fe with up to 10 wt% Ni is likely to be in the hcp structure under inner core conditions [Lin et al., 2002b]. On the other hand, adding Si into Fe strongly stabilizes the body-centered cubic (bcc) structure to much higher pressures and temperatures. The presence of Si in the outer core may have substantial effects on the structure and other physical properties of the liquid [Sanloup et al., 2002].

[5] Nuclear resonant inelastic x-ray scattering (NRIXS) has been used to determine the phonon density of states (DOS) of Fe under high pressures [Mao et al., 2001]. The vibrational, elastic, and thermodynamic parameters of bcc- and hcp-Fe have been obtained from the DOS [Mao et al., 2001]. Here we have studied two iron alloys, $\text{Fe}_{0.92}\text{Ni}_{0.08}$ and $\text{Fe}_{0.85}\text{Si}_{0.15}$, with NRIXS in a diamond anvil cell (DAC). The sound velocities of the alloys are obtained from the measured partial phonon density of states (PDOS) for ^{57}Fe incorporated in the alloys and then compared to those of Fe [Brown and McQueen, 1986; Mao et al., 2001; Fiquet et al., 2001] and the inner core [Dziewonski and Anderson, 1981].

2. Experiments

[6] The starting material, ^{57}Fe -enriched $\text{Fe}_{0.92}\text{Ni}_{0.08}$ (95% ^{57}Fe enrichment or better) in the bcc structure, was synthe-

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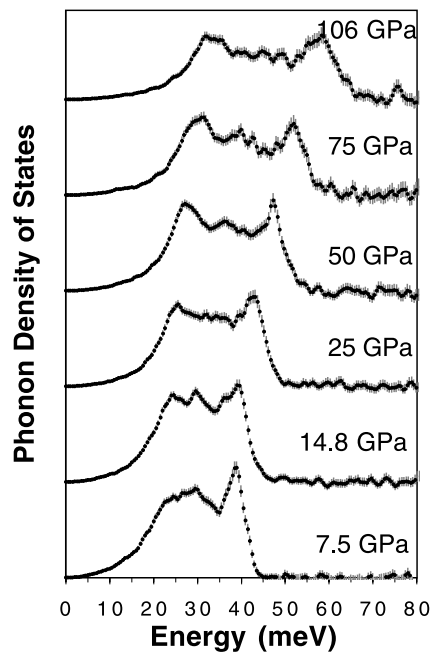


Figure 1. PDOS of $\text{Fe}_{0.92}\text{Ni}_{0.08}$ alloy under high pressures. Gray bars represent errors. The alloy was assumed to be in bcc structure at 7.5 GPa, in bcc + hcp phases at 14.8 GPa, and in hcp structure at 25, 50, 75, and 106 GPa [Mao *et al.*, 1990].

sized at the Geophysical Laboratory. The ^{57}Fe and Ni metals were reduced in a hydrogen atmosphere at 978 K to remove any surface oxidation. The two metals were mixed thoroughly and heated at 1800 K in a furnace equipped with a gas-mixing apparatus at an oxygen vapor pressure three log units below the Fe-FeO buffer for two hours, followed by annealing at 1678 K for five days. The ^{57}Fe -enriched $\text{Fe}_{0.85}\text{Si}_{0.15}$ alloy (95% ^{57}Fe enrichment or better) was synthesized by arc melting at Argonne National Laboratory (ANL). The crystal structures and chemical homogeneity of the alloys were examined by x-ray diffraction and electron microscope analyses. Both alloys crystallized in the bcc structure. Electron microprobe analyses showed that the starting materials contained 7.5 (± 0.3) wt % Ni and 7.9 (± 0.1) wt% Si, respectively, as averaged from at least 11 analyses. In Fe-Ni alloy experiments, a Be gasket was pre-indented to a thickness of 30 μm , followed by a 50 μm hole drilled in it. A small piece of the sample was loaded into the 50 μm hole. In Fe-Si alloy experiments, an amorphous boron and epoxy mixture (4:1 by weight) was inserted into the drilled 100 μm hole of the Be gasket, and then a smaller hole of 50 μm in diameter was drilled and used as the sample chamber. The high shear strength of the amorphous boron maximizes the thickness of the sample chamber and increases the pressure homogeneity [Lin *et al.*, 2003b]. A few ruby chips were placed on top of the sample for pressure measurement. Pressures were measured using the R_1 ruby fluorescence peak with a nonhydrostatic pressure scale [Mao *et al.*, 1978]. The pressure uncertainty (1σ) was estimated from multiple pressure measurements from at least three ruby chips.

[7] The NRIXS experiments were performed at undulator beamline 3-ID of the Advanced Photon Source (APS),

ANL. We used a high-resolution monochromator (1 meV resolution for the $\text{Fe}_{0.85}\text{Si}_{0.15}$ and 2.2 meV resolution for the $\text{Fe}_{0.92}\text{Ni}_{0.08}$) scanning the range of ± 100 meV in the vicinity of the nuclear resonance energy of 14.413 keV of ^{57}Fe . The x-ray beam diameter was less than 10 μm . The Fe K-fluorescence radiation was collected by three avalanche photodiode detectors; the counting time for each spectrum was approximately one hour, and 10–20 spectra were collected at the same pressure and added. The high-energy resolution is essential for deriving accurate Debye sound velocities from the PDOS (the Debye parabola is best constrained at the lower energy limit). The details of the DAC and the experimental setup are reported elsewhere [Mao *et al.*, 2001]. The measured spectra (count rate as a function of energy) were converted to a PDOS profile according to the procedure described by Sturhahn *et al.* [1995] and Sturhahn [2000].

3. Experimental Results and Calculations

[8] The PDOS of $\text{Fe}_{0.92}\text{Ni}_{0.08}$ and $\text{Fe}_{0.85}\text{Si}_{0.15}$ alloys were measured up to 106 GPa and 70 GPa at room temperature, respectively (Figures 1 and 2). Nuclear forward spectra revealed that bcc- $\text{Fe}_{92.5}\text{Ni}_{7.5}$ and bcc- $\text{Fe}_{0.85}\text{Si}_{0.15}$ are magnetic, while the hcp phases are nonmagnetic. A harmonic model was used to reduce the PDOS [Sturhahn *et al.*, 1995]. The Debye sound velocity was derived from parabolic fitting of the low-energy slope of the PDOS in the range of 3.5 meV to 14 meV. While the obtained PDOS only gives part of the lattice dynamics of the material, the low-energy portion of the PDOS provides an approximation to the bulk Debye sound velocity [Hu *et al.*, 2003]. The Debye sound velocity of the alloys was then obtained by applying a correction factor, the cube root of the ratio of the mass of the nuclear resonant isotope (^{57}Fe) to the average atomic mass

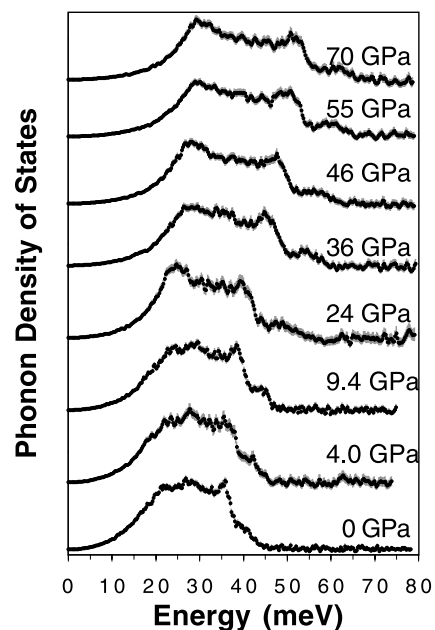


Figure 2. PDOS of $\text{Fe}_{0.85}\text{Si}_{0.15}$ alloy under high pressures. The alloy was assumed to be in bcc structure at 0, 4, and 9.4 GPa, in bcc + hcp phases at 24 GPa, and in hcp structure above 36 GPa [Lin *et al.*, 2003a].

of the sample [Hu et al., 2003]. The method of extracting the Debye sound velocity from PDOS, based on the harmonic approximation, has been tested for different Fe-bearing materials with Debye-like low-frequency dynamics [Hu et al., 2003]. The vibrational kinetic energy (E_k), zero point energy (E_z), vibrational heat capacity (C_{vib}), vibrational entropy (S_{vib}), and other thermodynamic and vibrational parameters were also calculated by integrating the PDOS [Sturhahn, 2000].

[9] The EOS of Fe-rich Fe-Si and Fe-Ni alloys have been previously determined by x-ray diffraction [Jephcoat et al., 1986; Mao et al., 1990; Zhang and Guyot, 1999; Lin et al., 2003a]. Since the EOS of Fe and Fe_{0.8}Ni_{0.2} alloy are almost identical [Mao et al., 1990], the EOS of Fe is used for Fe_{0.92}Ni_{0.08}. The adiabatic bulk modulus at zero pressure (K_{0S}) is calculated as:

$$K_{0S} = K_{0T}(1 + \alpha\gamma T), \quad (1)$$

where K_{0T} is the isothermal bulk modulus at zero pressure, α is the thermal expansion coefficient, γ is the Grüneisen parameter, and T is temperature (300 K) (these parameters are given in Table 7 of Lin et al., 2003a). The adiabatic bulk modulus at high pressures (K_S) is then calculated using the Birch-Murnaghan EOS [Birch, 1978]. The K_S , density (ρ), and Debye sound velocity (V_D) of the alloys are used to solve for the aggregate compressional wave velocity (V_P), shear wave velocity (V_S), and shear modulus (G) by the following equations (Figures 3) (See online supplementary materials¹ for details) [Dziewonski and Anderson, 1981; Brown and McQueen, 1986; Fiquet et al., 2001; Mao et al., 2001]:

$$\frac{K_S}{\rho} = V_P^2 - \frac{4}{3}V_S^2 \quad (2)$$

$$\frac{G}{\rho} = V_S^2 \quad (3)$$

$$\frac{3}{V_D^3} = \frac{1}{V_P^3} + \frac{2}{V_S^3} \quad (4)$$

4. Discussion

[10] Our results for the V_P and V_S of Fe_{0.92}Ni_{0.08} and Fe_{0.85}Si_{0.15} alloys, together with that of Fe from previous static and shock wave studies [Brown and McQueen, 1986; Fiquet et al., 2001; Mao et al., 2001], show that Fe, Fe-Ni and Fe-Si alloys follow a Birch's law trend for V_P in the hcp phase, i.e., the sound velocity is linearly related to the density and mean atomic weight [Birch, 1961] (Figure 3). The representation of the compressional wave velocity as a function of density in shock wave study probably incorporates much of the influence of temperature and pressure on the velocity through its volume dependence [Brown and

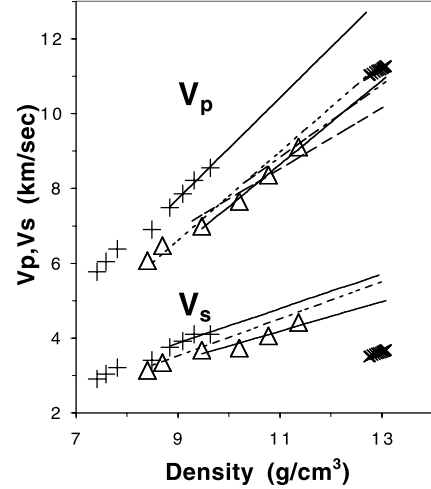


Figure 3. Comparison of aggregate compressional and shear wave velocities of Fe, Fe_{0.92}Ni_{0.08}, Fe_{0.85}Si_{0.15} at high pressures. Open triangles: Fe_{0.92}Ni_{0.08}; crosses: Fe_{0.85}Si_{0.15}; solid lines: extrapolation of hcp-Fe_{0.92}Ni_{0.08} and hcp-Fe_{0.85}Si_{0.15} to inner core density; short dashed line: hcp-Fe from NRIXS experiments [Mao et al., 2001]; long dashed line: hcp-Fe from inelastic x-ray scattering experiments [Fiquet et al., 2001]; dashed line with dots: hcp-Fe from shock wave experiments [Brown and McQueen, 1986]; x: PREM model [Dziewonski and Anderson, 1981].

McQueen, 1986]. Since Birch's law does not appear to hold through a phase transformation [Campbell and Heinz, 1992], only the sound velocity of the hcp phase is used for extrapolation to the pressure of the Earth's inner core. The shear wave velocity of the alloys appears to follow a linear relation of density but is much higher than that of the inner core. Since the bulk sound velocity, at a fixed density, is not known to increase with temperature, a strong temperature dependence on the V_P and V_S has to be further considered. Addition of Ni slightly decreases the V_P , V_S , and G of hcp-Fe under high pressures, but the changes are small. The slope of V_P for Fe_{0.92}Ni_{0.08} is more or less parallel to that of Fe from shock-wave experiments [Brown and McQueen, 1986] and from NRIXS experiments [Mao et al., 2001], while the V_P of hcp-Fe from inelastic x-ray scattering is slightly lower [Fiquet et al., 2001]. Extrapolation of the V_P for Fe_{0.92}Ni_{0.08} to inner core densities indicates that the V_P for Fe_{0.92}Ni_{0.08} is slightly lower than that of the inner core, suggesting that a small amount of light element(s) may be needed to increase the V_P to match the inner core. Different conclusions for the composition of the inner core are made based on the linear extrapolation of the V_P of Fe to inner core pressures. Inelastic x-ray scattering [Fiquet et al., 2001] and shock-wave experiments [Brown and McQueen, 1986] suggest that the inner core has a higher V_P than that of Fe, while NRIXS experiments on Fe to 153 GPa suggest that the inner core may contain 10 wt% of heavy elements such as Ni. Precise measurements under extreme pressures and temperatures are essential to address the slight difference in the extrapolation.

[11] The average Debye sound velocity of Fe_{0.85}Si_{0.15} alloy at 55 GPa, derived from the PDOS spectrum, is $V_D = 4.59 (\pm 0.02)$ km/s (x-ray beam parallel to compression axis)

¹ Auxiliary material is available at ftp://ftp.agu.org/apend/gl/2003GL018405.

and $V_D = 4.48 (\pm 0.02)$ km/s (x-ray beam perpendicular to compression axis). The difference in the sound velocity between two orientations is only 2%, suggesting that no significant anisotropy of the sound velocity in the hcp phase. See online supplementary materials¹ for details.

[12] The bulk sound velocity of the outer core appears to be 3% higher than that of pure liquid Fe [Anderson and Ahrens, 1994]. Therefore, if silicon is the dominant light element in the core, Fe-Si alloys should have higher bulk sound velocity than that of Fe under core conditions. As shown in Figure 3, substitution of Si in hcp-Fe increases the V_P and V_S at high pressures at a given density. We note that the increase in V_P and V_S of $\text{Fe}_{0.85}\text{Si}_{0.15}$ is mainly contributed from the density decrease of adding Si in Fe, because differences in K_S and G of $\text{Fe}_{0.85}\text{Si}_{0.15}$ and Fe are small when plotted against pressure (See Supplementary Figure 1 for details¹).

[13] The fractionation of light element(s) in the core and their exclusion relative to the inner core have been used to explain compositional buoyancy for convection and generation of the magnetic field [Buffet, 2000]. Since the substitution of Si in Fe has a large effect on the crystal structure [Lin et al., 2002a] and can increase the sound velocity, the alloying effects of light elements on the physical properties of liquid Fe such as viscosity would also affect the convection and fractionation of the core, with important implication for the geodynamo [Buffet, 2000]. There are other potential major light elements in the core [Poirier, 1994; Hemley and Mao, 2001]. *In situ* x-ray diffraction studies on Fe-S liquid under high pressures and high temperatures have shown that sulfur strongly modifies the local structure of liquid Fe, and addition of sulfur in liquid Fe can increase the compressibility significantly [Sanloup et al., 2002]. The alloying effects of oxygen, sulfur, and hydrogen on the elastic, vibrational, and thermodynamic properties should also be studied in the future. This new generation of *in situ* x-ray spectroscopic studies of Fe light-element alloys will enable us to better evaluate proposed light elements in the core.

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