1 Revision 1

2	Sound Velocities of Iron-Nickel (Fe ₉₀ Ni ₁₀) Alloy up to 8 GPa and 773 K: The Effect of
3	Nickel on the Elastic Properties of bcc-Iron at High <i>P-T</i>
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14 Abstract

15 Sound velocities of iron and iron-based alloys at high pressure and high temperature are crucial 16 for understanding the composition and structure of Earth's and other telluric planetary cores. In 17 this study, we performed ultrasonic interferometric measurements of both compressional $(V_{\rm P})$ 18 and shear (Vs) velocities on a polycrystalline body-centered-cubic (bcc)-Fe90Ni10 up to 8 GPa 19 and 773 K. The elastic moduli and their pressure and temperature derivatives are derived from 20 least square fits to third-order finite strain equations, yielding $K_{s0} = 154.2(8)$ GPa, $G_0 = 73.2(2)$ GPa, $K_{s0}' = 4.6(2)$, $G_0' = 1.5(1)$, $\partial K_s / \partial T = -0.028(1)$ GPa/K, and $\partial G / \partial T = -0.023(1)$ GPa/K. A 21 22 comparison with literature data on bcc-Fe suggests that nickel not only decreases both P and S 23 wave velocities but also weakens the temperature effects on the elastic moduli of Fe-Ni alloys. 24 Key words: Fe-Ni alloy; sound velocity; high pressure and high temperature; ultrasonic

25 interferometry

26 **1. Introduction**

27 Understanding the nature of Earth's core, which is the least accessible region of the Earth, is one 28 of the most challenging tasks in geophysical research. Seismic waves can travel inside the Earth 29 and serve as a powerful tool to probe the physical properties of Earth's interior, such as the 30 density, compressional (P) and shear (S) wave velocities depth profiles; see for example the 31 Preliminary Reference Earth Model (Dziewonski and Anderson 1981). Comparing seismic 32 results with lab-based mineral physics investigations, as well as other evidence from 33 geochemical and cosmochemical studies, it has been widely accepted that Earth's core is 34 composed of iron alloyed with approximately 10 wt.% nickel and several percent of light 35 elements (such as Si, O, H, S, C, etc.) (e.g., Birch 1952, 1964; Li and Fei 2014; Mcdonough and 36 Sun 1995). However, direct studies on the behavior and elasticity properties of iron alloys at high 37 pressure and high temperature are still scarce.

38 Iron-nickel alloys can exist in several crystallographic structures: body-centered-cubic (bcc) 39 structure (α phase), face-centered cubic (fcc) structure (γ phase), and hexagonal close-packed 40 (hcp) structure (ϵ phase), etc., depending on the pressure (P) and temperature (T) conditions and 41 the nickel concentration (Fig. 1). At ambient conditions, iron crystallizes in bcc structure while 42 nickel prefers the fcc structure; when the nickel concentration exceeds ~20 wt.%, Fe-Ni alloys 43 will gradually transform from bcc to fcc structure. However, there is no conclusive consensus on 44 the phase diagram of Fe-Ni systems at high pressure and high temperature (e.g., Dubrovinsky et 45 al. 2007; Kuwayama et al. 2008; Mao et al. 1990; Sakai et al. 2011; Tateno et al. 2012; Tateno et 46 al. 2010). While there are several experimental and theoretic predictions arguing that the bcc 47 structure could be the stable phase (e.g., Dubrovinsky et al. 2007; Vocadlo et al. 2003) at Earth's 48 core conditions, these predictions were not supported by later experiments (e.g., Sakai et al. 2011;

Tateno et al. 2012; Tateno et al. 2010). The more recent calculations by Stixrude (2012) demonstrate a wide stability field of hcp Fe to 23 Mbar (2,300 GPa) and 19,000 K, supporting the later high *P-T* experiments. With the complexity of alloying with light elements, the phase diagram is even more controversial. Thus, more information about the physical and chemical properties (such as, density, sound velocity, bulk modulus, shear modulus, anisotropy, etc.) of the different phases of the Fe-Ni alloys are needed to further constrain the composition and structure of the Earth's core.

Sound velocities of pure iron (Fe) have been experimentally accessed by ultrasonic 56 57 interferometry (UI), inelastic X-ray scattering (IXS), nuclear resonant inelastic X-ray scattering (NRIXS), and laser pulses (LP), etc.] at room temperature (e.g., Chigarev et al. 2008; Decremps 58 59 et al. 2014; Figuet et al. 2001; Gleason et al. 2013; Mao et al. 1998; Murphy et al. 2013) and 60 high temperature (e.g., Antonangeli et al. 2012; Lin et al. 2005; Liu et al. 2014; Mao et al. 2012; 61 Ohtani et al. 2013; Shibazaki et al. 2016). In contrast, experimental studies on the sound velocity 62 of iron-nickel (Fe-Ni) alloys are still limited (Kantor et al. 2007; Lin et al. 2003; Morrison et al. 63 2019; Wakamatsu et al. 2018), especially for the shear properties under simultaneous high 64 pressure and high temperature conditions.

In the present study, we have carried out ultrasonic interferometric (UI) measurements on a polycrystalline bcc-Fe90Ni10 sample at simultaneous pressure and temperature conditions. Compared to other sound velocity measurement techniques, UI in large volume apparatus embeds the advantages of stable and uniform heating of sample and direct measurement of both P and S wave velocities simultaneously. We applied a third-order finite strain approach for data analysis; the resultant compressional and shear velocities as well as the bulk and shear moduli

for bcc-Fe90Ni10 are compared with those for pure iron to evaluate the effects of nickel content on
the elastic properties of Fe-Ni alloys.

73 **2.** Experimental methods

The polycrystalline sample of Fe₉₀Ni₁₀ (10 wt.% Nickel) was a cylindrical disk cut from a rod purchased from Princeton Scientific Cooperation. Before the ultrasonic measurements, the sample was annealed at 3 GPa, 773 K. Scanning electron microscope (SEM) analysis was conducted on the recovered sample and the results (**Fig. 2**) indicated that the sample was homogenous with an average grain size less than 1 µm. There was no detectable oxygen observed in the Energy-dispersive X-ray spectroscopy (EDS), suggesting that no oxidation reactions occurred during the high temperature annealing process.

To optimize the acoustic signals in the ultrasonic measurement, both sides of the sample were polished using diamond lapping film to 1 μ m. The final dimensions of the polished sample were 0.930(2) mm in length and 2.010(2) mm in diameter, with a bulk density of 7.95(3) g/cm³, as obtained by the Archimedes' method.

85 High pressure and high temperature ultrasonic measurements were performed to about 8 GPa, 86 773 K in a 2000-ton uniaxial split-cylinder apparatus (USCA-2000) in the High-Pressure Lab at 87 Stony Brook University. A sketch of the 14/8 cell assembly used in this study is shown in Fig. 3. A dual mode LiNbO3 transducer (10° Y-cut) was used to generate and receive both the 88 89 compressional wave and shear wave simultaneously (50 MHz resonant frequency for P waves 90 and 30 MHz for S waves). A dense alumina rod was placed on the top of the sample and served 91 as the acoustic buffer rod. Due to the low yield strength of NaCl at high temperatures, a disk of 92 NaCl was placed at the back of the sample to provide a pseudo-hydrostatic environment during

93 the experiment (Li et al. 2001). The high temperature environment was generated by a graphite 94 heater and monitored by W/Re5%-W/Re26% type-C thermocouples. The thermocouple junction 95 was placed at a location that mirrors the center of the sample position relative to the center of the 96 high-pressure cell. Even though they were not directly in contact with each other, the 97 thermocouple reading is believed to closely represent the sample temperatures at high pressure. 98 The temperature measurement uncertainty in current experiment is approximately ± 10 K. P and 99 S wave travel times were acquired using the transfer function technique and analyzed using the 100 pulse echo overlap (PEO) method by overlapping the buffer rod and sample echoes (Fig. 4). 101 Details about the transfer function technique for data acquisition and processing have been 102 discussed elsewhere (Li et al. 2002; Li et al. 2004). Cell pressures were calculated from the shear 103 wave travel times of the alumina buffer rod using the pressure scale at high temperature by 104 equation:

105
$$P = 242.5(9) \times \left(1 - t_{S_bf} / t_{S_0 bf}\right) + 0.01099(5) \times (T - T_0)$$
(1.)

where *P* is cell pressure, $t_{S_{bf}}$ is the *S* wave travel time of the buffer rod, and $t_{S0_{bf}}$ is the *S* wave travel time at ambient conditions (for further details of the use of alumina as a pressure marker, see Wang et al. 2015). The details of the experimental data on buffer rod are listed in supplementary **Table S1**. The pressure uncertainty is estimated to be around ± 0.2 GPa in current study.

The experimental *P*-*T* path is shown in the **Fig. 1**, superimposed with the previously determined phase diagram from the diamond anvil cell (DAC) experiments (Huang et al. 1988). The sample was first compressed at room temperature to a maximum pressure of \sim 8 GPa, followed by heating to a peak temperature of 773 K to release the deviatoric stress in the cell, then the 115 ultrasonic data were collected at 100 K intervals along cooling paths to room temperature while 116 the sample was under nearly hydrostatic environment (Li et al. 2001). Multiple heating and 117 cooling cycles were performed during decompression to provide a dense coverage of 118 experimental data in *P-T* space. The P and S wave travel times were obtained at 35 and 27 MHz, 119 respectively, in this study, to maximize the signal-to-noise ratio.

120 **3. Data analyses**

After the experiment, the sample length and diameter were 0.926(2) mm and 2.010(5) mm respectively, indicating that, within 0.4% uncertainty, the sample can be considered to have undergone elastic compression under pseudo-hydrostatic conditions during the entire course of the experiment. As indicated by the P and S wave signals obtained at 7.6 GPa and 776 K in **Fig.** 4, the reflections from the front (buffer rod/sample) and rear (sample/backing) surfaces are highly distinguishable from the background, providing a reliable measurements of travel times with 0.1-0.6% in precision.

The travel time results at all experimental conditions from this study are summarized in **Table 1**. As shown in previous studies, velocities (V_P and V_S), and elastic moduli (K_S and G) as well as their pressure and temperature derivatives (K_S , G, K_S' , G', $\partial K_S / \partial T$, and $\partial G / \partial T$) can be obtained by a third-order finite strain approach (Davies and Dziewonski 1975; Li and Zhang 2005).

First, because the sample has undergone nearly hydrostatic deformation during cooling along decompression the experiment, it is reasonable to assume that density (ρ), volume (V), and length (*l*) have the following relationships:

135
$$\frac{\rho}{\rho_0} = \frac{V_0}{V} = \left(\frac{l_0}{l}\right)^3 \tag{2.}$$

The elastic properties at high pressure and temperature can be calculated through the sound

136

velocities $V_{(P,S)} = \frac{2l}{2t_{(P,S)}}$ and densities ρ by the relationships $K_S = \rho(V_P^2 - \frac{4}{3}V_S^2)$ and $G = \rho V_S^2$ 137 138 for the bulk and shear modulus, respectively. Under adiabatic compression, the finite strain 139 equations are expressed as the following: $\rho V_P^2 = (1 - 2\varepsilon)^{\frac{5}{2}} (L_1 + L_2 \varepsilon)$ 140 (3.) $\rho V_{S}^{2} = (1 - 2\varepsilon)^{\frac{5}{2}} (M_{1} + M_{2}\varepsilon)$ 141 (4.) $K_{S(0,T)} = L_1 - \frac{4}{3}M_1$ 142 (5.) $G_{(0,T)} = M_1$ 143 (6.) $K_{S(0,T)}' = \frac{5L_1 - L_2}{3K_{S(0,T)}} - \frac{4G_{(0,T)}'}{3}$ 144 (7.) $G_{(0,T)}' = \frac{5M_1 - M_2}{3K_{s(0,T)}}$ (8.) 145 146 where the subscript (P,T) indicates values at the pressure P and temperature T, and the Eulerian strain $\varepsilon = \frac{1}{2} \left[1 - \left(\frac{\rho_{(P,T)}}{\rho_{(0,T_{foot})}} \right)^{2/3} \right]$ (The *T_{foot}* here refers to the foot temperature of an adiabat at 147 148 ambient pressure and T refers to the temperature along this adiabat at pressure P). All 149 temperatures reached in the entire experiment are assumed to be raised along separate adiabats 150 from different foot temperatures T_{foot} . Thus, the adiabatic foot temperature for each data point as

151 well as the corresponding density and elastic properties at ambient pressure and T_{foot} can be 152 extracted through the following equations:

153
$$\left(\frac{\partial T}{\partial P}\right)_{S} = \frac{\gamma T}{K_{S}}$$
(9.)

154
$$\rho_{(0,T_{foot})} = \rho_{(0,T_0)} e^{-\int \alpha dT}$$
(10.)

155
$$K_{S(0,T_{foot})} = K_{S(0,T_0)} + \left(T_{foot} - T_0\right) \left(\frac{\partial K_S}{\partial T}\right)_P$$
(11.)

156
$$G_{(0,T_{foot})} = G_{(0,T_0)} + (T_{foot} - T_0) \left(\frac{\partial G}{\partial T}\right)_P$$
(12.)

157
$$K'_{SS(0,T_{foot})} = K'_{SS(0,T_0)} + \left(T_{foot} - T_0\right) \left(\frac{\partial^2 K_S}{\partial P \partial T}\right)_P + \left(\frac{\partial K_S}{\partial T}\right)_P \frac{\gamma T}{K_S}$$
(13.)

158
$$G'_{S(0,T_{foot})} = G'_{S(0,T_0)} + \left(T_{foot} - T_0\right) \left(\frac{\partial^2 G}{\partial P \partial T}\right)_P + \left(\frac{\partial G}{\partial T}\right)_P \frac{\gamma T}{K_S}$$
(14.)

159
$$P = -3K_{S(0,T_{foot})}(1-2\varepsilon)^{5/2} \left(1 + \frac{3}{2}(4-K'_{SS(0,T_{foot})})\varepsilon\right)\varepsilon$$
(15.)

160 The sample lengths, as well as the thermoelastic properties Ks, G, Ks', G', $\partial Ks/\partial T$, $\partial G/\partial T$ at 161 ambient conditions, were refined using a least-square fit by minimizing the difference between the observed compressional and shear velocities $(V_{(P,S)} = \frac{2l}{2t_{(P,S)}})$ and pressures from Eq.(1) with 162 163 those calculated by finite strain theory [Eqs. (3), (4), and (15)]. More details about the data 164 analysis procedures can be found elsewhere (Li and Zhang 2005). In the P-T range of the current experiment, the thermal expansivity α was assumed to be a constant value of 4.67×10⁻⁵ (Zhang 165 166 and Guyot 1999); the Grüneisen parameter γ was constrained by the assumption of $\rho\gamma$ = constant 167 with $\gamma_0 = 1.65$ (Quareni and Mulargia 1988); cross derivatives $(\partial^2 K_s / \partial P \partial T)_P$ and $(\partial^2 G / \partial P \partial T)_P$ were assumed to be zero in the current P-T range. The minimization usually takes only a few 168 169 iterations to achieve convergence, and the results for the elastic properties are shown in **Table 2**.

170 **4. Results and discussion**

171 According to Fig. 1, some of our experimental data were collected close to the bcc-fcc boundary 172 or within the stability filed of the fcc phase of Fe90Ni10 as suggested by DAC experiments from 173 Huang et al. (1988). However, a recent electrical resistivity measurement in the large volume 174 press with a similar experimental setup as current study suggested the bcc-to-fcc phase transition 175 of Fe90Ni10 would not occur until ~900 K at the pressure range of 4.5 GPa and 8 GPa (Pommier 176 2020). A close examination of the recorded waveforms as well as the subsequent analysis of P 177 and S wave travel times did not suggest a phase transition to fcc phase in our P-T range. This 178 was further tested by performing a separate fit without the data at 773 K. As indicated by the 179 results shown in Table 2, within the uncertainty, the inclusion of the data at 773 K has an 180 insignificant effect on the fitting results and can be reliably treated as the representative values 181 for the bcc phase.

182 The compressional and shear wave velocities data obtained in this study are compared in Fig. 5 183 with those from ultrasonic measurements (Shibazaki et al. 2016) and an IXS study on bcc-Fe 184 (Liu et al. 2014), as well as data from NRIXS studies on both bcc-Fe and bcc-Fe₉₁Ni₀₉ (Morrison 185 et al. 2019). At room temperature, the velocities of both P and S waves for bcc-Fe₉₀Ni₁₀ are 186 consistently lower than pure Fe from Shibazaki et al. (2016) by 5% and 6%, respectively, which 187 is in good agreement with the ~6% velocity depression observed in NRIXS studies on Fe-Ni 188 alloys with 0 and 9 at.% (which corresponding to ~ 10 wt.%) nickel (Morrison et al. 2019). 189 However, the absolute values for both P and S waves from NRIXS are systematically lower than 190 those from other techniques (UI, IXS), which could be attributed to the fact that NRIXS is based 191 on the Debye model to analyze the data instead of measuring the sound velocity directly. 192 Comparing to those for bcc-Fe from Shibazaki et al. (2016), VP of bcc-Fe90Ni10 from current

study exhibits a slower rate of increase with pressure [$\sim 5.1 \times 10^{-2}$ km/s/GPa versus (*vs.*) 6.9×10^{-2} km/s/GPa for Fe₉₀Ni₁₀ and Fe, respectively] while *V*_S increases at a relatively similar rate ($\sim 2.1 \times 10^{-2}$ km/s/GPa *vs.* 2.0×10^{-2} km/s/GPa for Fe₉₀Ni₁₀ and Fe, respectively).

196 With increasing temperature, both V_P and V_S decrease within the entire P-T range of the current 197 experiment with a larger reduction in $V_{\rm S}$ than $V_{\rm P}$. For example, at ~3 GPa, the depressions in $V_{\rm P}$ 198 and Vs from 300 K to 800 K are 4%, 7% for Fe₉₀Ni₁₀ and 6%, 8% for pure Fe, respectively. The 199 compressional velocity (V_P) decrease from 300 to 700 K reported by Liu et al. (2014) is about 200 5%, which is larger than the 4% for bcc-Fe₉₀Ni₁₀ observed in current study. In addition, nonlinear 201 elastic anomalies indicative of a magnetic transition at high temperature (e.g., Dever 1972) were 202 not observed in the current study, which could possibly be explained by the limited temperature 203 range (300-773 K).

204 The adiabatic bulk modulus (K_s) and shear modulus (G) calculated in current study are plotted in 205 Fig. 6 as a function of pressure and temperature. Table 2 is a comparison of the thermoelastic 206 properties of Fe and Fe-Ni alloys obtained from this study and previous experimental studies. 207 Note in this table that our study reports for the first time the temperature dependences of the 208 elastic bulk and shear moduli ($\partial K_s / \partial T$ and $\partial G / \partial T$) of bcc-Fe₉₀Ni₁₀. Comparing with previous 209 ultrasonic studies listed in Table 2, the bulk and shear moduli of bcc-Fe90Ni10 at ambient 210 conditions [$K_{S0} = 154.2(8)$ GPa and $G_0 = 73.2(2)$ GPa] are lower than those values of bcc-Fe (K_{S0} = 165-168 GPa and G_0 = 78-82 GPa) by approximately 7% and 9%, respectively (Adams et al. 211 212 2006; Dever 1972; Isaak and Masuda 1995; Leese and Lord Jr 1968; Shibazaki et al. 2016). The 213 effect of nickel content on bulk modulus observed in this study is consistent with previous

suggestions based on pressure-volume (*P-V*) measurements in DAC (Morrison et al. 2018;
Takahashi et al. 1968).

It is also worthwhile to note that, comparing with pure bcc-Fe (Shibazaki et al. (2016). bcc-216 217 Fe90Ni10 exhibits a weaker pressure dependence of Ks than bcc-Fe (Fig. 6), which can be 218 quantified by the pressure derivative K_{S} ' [4.6(2) for bcc-Fe₉₀Ni₁₀ vs. 6.75(33) for pure Fe]; 219 meanwhile for the shear modulus, bcc-Fe₉₀Ni₁₀ and bcc-Fe show close agreement with each 220 other in their pressure derivatives $[G_{\theta'} = 1.5(1)$ vs. 1.66(14), respectively]. These comparisons 221 are believed to reveal primarily the intrinsic difference resulted from nickel substitution in the 222 alloy; the different pressure calibration method used in the current experiments (alumina pressure 223 gauge) and those of Shibazaki et al. (2016) [equation of state (EOS) of MgO + hBN] may also contribute, but are not considered to be an appreciable effect. Future investigations on Fe-Ni 224 225 alloys with different Ni contents using either of the pressure calibration method could help to 226 further address this issue.

227 Besides the pressure dependence, we also investigated the effect of 10 wt.% nickel content in our 228 sample on the temperature dependence of both bulk and shear moduli. For pure bcc-Fe, high 229 temperature ultrasonic measurements have been conducted at ambient pressure (e.g., Adams et al. 230 2006; Dever 1972; Isaak and Masuda 1995; Leese and Lord Jr 1968) and high pressure 231 (Shibazaki et al. 2016), the reported temperature dependence ranges from -0.029 GPa/K \sim -0.046 232 GPa/K for the bulk modulus ($\partial K_{so}/\partial T$) and -0.015 GPa/K ~ -0.034 GPa/K for the shear modulus $(\partial G_0/\partial T)$. Our results of $\partial K_{S0}/\partial T = -0.028(1)$ GPa/K and $\partial G_0/\partial T = -0.023(1)$ GPa/K for bcc-233 234 Fe₉₀Ni₁₀ are only marginally consistent with the lowest values reported for bcc-Fe, indicating that

10 wt.% nickel alloying with Fe can weakly affect the temperature dependence of both bulk andshear moduli.

237 The current adiabatic value of $\partial K_{so}/\partial T = -0.028(1)$ GPa/K can be converted to its isothermal 238 counterpart using the differentiated form of the thermodynamic identity $K_T = K_S/(1 + \alpha_V T)$, yielding $\partial K_{T0}/\partial T = -0.038(1)$ GPa/K. Two pressure-volume-temperature (*P-V-T*) investigations 239 240 have reported $\partial K_{T0}/\partial T$ on bcc-Fe based on X-ray diffraction (XRD) studies and the results are 241 largely discrepant. While Huang et al. (1987) reported a relatively small temperature dependence 242 $\left[\frac{\partial K_{T0}}{\partial T}\right] = -0.010(16)$ GPa/K], Zhang and Guyot (1999) provided a much larger value $\left[\frac{\partial K_{T0}}{\partial T}\right]$ 243 = -0.049(6) GPa/K], which is more consistent with the current ultrasonic results. To the authors' 244 best knowledge, no P-V-T investigation on bcc-Fe-Ni alloy has yet been reported to provide a 245 direct comparison with the current result.

246 **5. Implications**

247 Due to the limited coverage in pressure and temperature, our experimental results of velocities 248 are not directly applicable to the Earth's core. We discuss possible implications for other phases, such as hcp-Fe-Ni systems, by investigating how the elastic properties are affected by nickel at 249 250 high pressure and temperature. We found that the effect of nickel content on P and S wave 251 velocities observed on bcc phase in this study is roughly consistent with the previously reported 252 results on hcp Fe-Ni alloys (Lin et al. 2003; Morrison et al. 2019; Wakamatsu et al. 2018). This 253 nickel effect could lead to a velocity decrease as large as $\Delta V_P = 0.8$ km/s at inner core boundary 254 (ICB) for hcp phase, as calculated by Ohtani et al. (2013), suggesting that nickel content plays as 255 an important factor when we modelling the velocity structure of Earth's core to place constraints 256 on its composition. From our measurements, we observed $(\partial V_P / \partial T)_\rho = -0.18(2) \text{ km/(s} \cdot 10^3 \text{ K})$ for 257 bcc-Fe₉₀Ni₁₀ at a constant density in current *P*-*T* range. In comparison, the $(\partial V_P / \partial T)_\rho$ for bcc-Fe 258 varies from -0.33(4) km/(s \cdot 10³K) to -0.37(3) km/(s \cdot 10³K) by UI (Shibazaki et al. 2016) and IXS 259 (Liu et al. 2014) measurements, respectively, indicating the nickel content can also reduce the 260 effect of temperature on the $V_{\rm P}$ - ρ relationship. This implies that the use of temperature 261 derivatives of Fe would produce an upper bound or overestimated value of velocity decrease 262 $(\Delta V_{\rm P})$ at Earth's core conditions. Furthermore, we also observed a slightly smaller temperature 263 effect of shear velocity in bcc-Fe₉₀Ni₁₀ [$(\partial V_s/\partial T)_{\rho} = -0.28(2)$ km/(s·10³K)] than bcc-Fe 264 $[(\partial V_S/\partial T)_{\rho} = -0.39(3) \text{ km/(s} \cdot 10^3 \text{ K})]$. The low value of $(\partial V_S/\partial T)_{\rho}$ would introduce even larger V_S 265 of hcp-Fe-Ni than previous estimations, which would require a more significant pre-melting 266 effects (Martorell et al. 2013) or other mechanisms to account for the discrepancy of shear waves 267 with the seismological observations. Thus, the decrease in the temperature effect induced by 268 nickel alloving needs to be further evaluated in other structures of Fe-Ni allovs in an expanded 269 *P-T* range: a better and more precise understanding of the Earth's core should take the effect of 270 nickel into consideration instead of just ignoring it. Future acoustic measurements of both $V_{\rm P}$ and 271 $V_{\rm S}$ of various Fe-Ni-light elements alloys and compounds at simultaneous high P-T conditions 272 are also needed to provide a more comprehensive understanding of the composition and thermal 273 structure of Earth's and planetary cores.

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 Chemistry of Minerals, 26(3), 206-211.

405 Table 1 Experimental (<i>P</i> , <i>I</i> , $2t_P$, $2t_S$) and calculated (Length, ρ , V_P , V_S , K_S , <i>G</i>) data of bo	$cc-Fe_{90}N1_{10}$
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Р	Т	$2t_{\rm P}$	$2t_{\rm S}$	Length	ρ	$V_{\rm P}$	$V_{\rm S}$	Ks	G
(GPa)	(K)	(µs)	(µs)	(mm)	(g/cm^3)	(km/s)	(km/s)	(GPa)	(GPa)
6.2	323	0.3080(2)	0.5816(28)	0.9148	8.246	5.94(6)	3.15(3)	182.2(33)	81.6(11)
7.6	776	0.3188(4)	0.6188(18)	0.9174	8.176	5.76(6)	2.97(3)	175.0(30)	71.9(8)
7.4	667	0.3150(4)	0.6060(4)	0.9165	8.200	5.82(6)	3.02(3)	177.6(30)	75.0(8)
7.1	570	0.3124(4)	0.5968(8)	0.9160	8.212	5.86(6)	3.07(3)	179.2(31)	77.4(8)
6.7	472	0.3104(2)	0.5868(22)	0.9155	8.228	5.90(6)	3.12(3)	179.5(32)	80.1(10)
6.1	328	0.3080(4)	0.5810(28)	0.9149	8.243	5.94(6)	3.15(3)	181.9(34)	81.8(11)
5.6	322	0.3092(4)	0.5828(22)	0.9157	8.220	5.92(6)	3.14(3)	180.2(33)	81.2(10)
6.9	785	0.3210(12)	0.6208(16)	0.9188	8.140	5.72(6)	2.96(3)	171.6(35)	71.3(8)
6.8	674	0.3172(6)	0.6096(8)	0.9177	8.167	5.79(6)	3.01(3)	174.7(31)	74.0(8)
6.6	576	0.3146(8)	0.5990(10)	0.9170	8.186	5.83(6)	3.06(3)	175.9(33)	76.7(8)
6.2	470	0.3120(2)	0.5900(10)	0.9165	8.201	5.87(6)	3.11(3)	177.5(31)	79.1(8)
5.6	329	0.3098(2)	0.5826(28)	0.9158	8.219	5.91(6)	3.14(3)	179.0(33)	81.2(11)
4.3	309	0.3140(4)	0.5864(12)	0.9178	8.165	5.85(6)	3.13(3)	172.4(31)	80.0(9)
5.6	782	0.3256(2)	0.6244(6)	0.9213	8.073	5.66(6)	2.95(3)	164.8(28)	70.3(7)
5.4	661	0.3214(2)	0.6130(4)	0.9201	8.103	5.73(6)	3.00(3)	168.3(29)	73.0(7)
5.2	573	0.3192(2)	0.6050(2)	0.9195	8.121	5.76(6)	3.04(3)	169.5(29)	75.0(8)
4.9	468	0.3172(2)	0.5984(2)	0.9188	8.139	5.79(6)	3.07(3)	170.8(29)	76.7(8)
4.3	316	0.3150(2)	0.5878(10)	0.9181	8.158	5.83(6)	3.12(3)	171.0(30)	79.6(8)
2.6	310	0.3206(4)	0.6010(18)	0.9211	8.077	5.75(6)	3.07(3)	165.5(30)	75.9(9)
3.1	779	0.3336(2)	0.6406(8)	0.9260	7.950	5.55(6)	2.89(3)	156.4(26)	66.4(7)
2.9	673	0.3300(2)	0.6268(20)	0.9251	7.974	5.61(6)	2.95(3)	158.0(28)	69.5(8)
2.8	571	0.3266(4)	0.6188(26)	0.9240	8.002	5.66(6)	2.99(3)	161.1(29)	71.4(9)
2.7	474	0.3244(4)	0.6134(38)	0.9229	8.030	5.69(6)	3.01(3)	163.0(31)	72.7(12)
2.3	318	0.3218(2)	0.6028(14)	0.9217	8.062	5.73(6)	3.06(3)	164.0(29)	75.4(8)
3.2	776	0.3334(2)	0.6352(16)	0.9259	7.952	5.55(6)	2.92(3)	155.2(27)	67.6(8)
3.0	674	0.3302(2)	0.6244(4)	0.9249	7.978	5.60(6)	2.96(3)	157.0(27)	70.0(7)
2.8	571	0.3270(2)	0.6188(22)	0.9239	8.003	5.65(6)	2.99(3)	160.4(28)	71.4(9)
2.8	473	0.3246(2)	0.6114(4)	0.9229	8.031	5.69(6)	3.02(3)	162.1(28)	73.2(7)
2.5	343	0.3226(2)	0.6050(10)	0.9218	8.060	5.71(6)	3.05(3)	163.4(29)	74.8(8)
Note: The uncertainty of length calculated in this study is approximately $\pm 1\%$.									

407 **Table 2** Comparison of thermoelastic properties of bcc-Fe and bcc-Fe-Ni alloys

												·	i	i
Reference		P range	T range	K _{S0}	$\partial K_{s0}/\partial P$	$\partial K_{s0}/\partial T$	G ₀	$\partial G_0 / \partial P$	$\partial G_0 / \partial T$	K _{T0}	$\partial K_{T0} / \partial P$	$\partial K_{T0}/\partial T$	EOS	Notes
		(GPa)	(K)	(GPa)		(GPa/K)	(GPa)		(GPa/K)	(GPa)		(GPa/K)		
This study	Fe Ni	~8	~773	154.2(8)	4.6(2)	-0.028(1)	73.2(2)	1.5(1)	-0.023(1)	-	-	-	3rd Finite strain	Ultrasonic, adiabatic
This study	109014110		~673	153.8(7)	4.7(2)	-0.027(2)	72.7(2)	1.6(1)	-0.022(1)	-	-	-		
Shibazaki et al. (2016)	Fe	~6.3	~800	163.2(15)	6.75(33)	-0.038(3)	81.4(6)	1.66(14)	-0.029	-	-	-	Polynomial	Ultrasonic, adiabatic
Adams et al. (2006)	Fe	0	~500	166.2	-	-0.029	81.5 ^a	-	-0.025	-	-	-	-	Ultrasonic, adiabatic
Isaak and Masuda (1995)	Fe	0	~800	165.7	-	-0.046	82.0 ^a	-	-0.034	-	-	-	-	Ultrasonic, adiabatic
Dever (1972)	Fe	0	~773	167.8	-	-0.035	82.0 ^a	-	-0.029	-	-	-	-	Ultrasonic, adiabatic
Leese and Lord (1968)	Fe	0	~773	168.7	-	-0.041	77.9 ^a	-	-0.015	-	-	-	-	Ultrasonic, adiabatic
Zhang and Guyot (1999)	Fe	~9	~773	-	-	-	-	-	-	155(2)	5.3 ^b	-0.049(6)	3rd Birch Murnaghan	XRD, isothermal
Huang et al. (1987)	Fe	~12	~723	-	-	-	-	-	-	171(8)	4 ^b	-0.010(16)	Birch Murnaghan	XRD, isothermal
	Fe	~15	300	-	-	-	-	-	-	162(5)	5.5(8)	-		
Takahashi et al. (1968)	Fe95Ni5	~16	300	-	-	-	-	-	-	155(10)	4.2(8)	-	Murnaghan	XRD, isothermal
	Fe90Ni10	~17	300	-	-	-	-	-	-	155(10)	5.7(8)	-]	
Morrison et al. (2018)	Fe91Ni09	~15	300	-	-	-	-	-	-	146.8(31)	6.39(64)	-	3rd Birch Murnaghan	XRD, isothermal
Notes: ^a : Voigt-Reuss-Hill average; ^b : fixed value.														

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410	Figure 1 Phase diagram of Fe-Ni alloy system at high <i>P-T</i> based on the data of Huang et al.
411	(1988). Solid dots indicate the experimental $P-T$ conditions where the ultrasonic data were
412	acquired in this study.
413	
414	Figure 2 Scanning electron microscope image of sample after high temperature annealing.
415	
416	Figure 3 Sketch of the cell assembly used in current study for ultrasonic measurement.
417	
418	Figure 4 Signal example of (a) P wave and (b) S wave obtained at 7.6 GPa and 776 K.
419	
420	Figure 5 Compressional (V_P) and shear (V_S) wave velocities as a function of pressure and
421	temperature. Solid lines are the finite strain fitted curves from this study. Temperature
422	information are color coded and shown in legend.
423	
424	Figure 6 Bulk and shear modulus as a function of pressure and temperature. Solid lines are the
425	finite strain fitted curves from this study. Dashed lines are calculated from Shibazaki et al.

426 (2016). Temperature information are color coded and shown in legend.













