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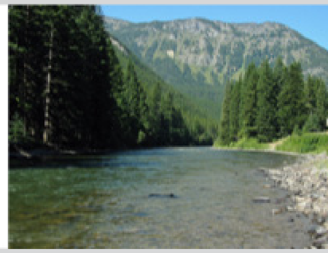
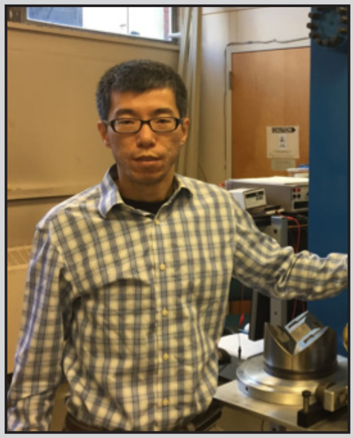
BIG SKY MONTANA



Newsletter February 2019

Some New Faculty Appointments within the COMPRES Community

Alisha Clark
Assistant Professor, Fall 2019
Geological Sciences, University of Colorado Boulder



Zhicheng Jing
Associate Professor, July 2018
SUSTech Southern University of Science and Technology

Megan Duncan
Assistant Professor, Fall 2019
Virginia Tech Geosciences

Recent COMPRES Workshop on "Nuclear Resonant Inelastic X-ray Scattering and Data Analysis"

SciPhon

PHOENIX
PHOnon Excitation by Nuclear Inelastic X-ray scattering

This workshop was held on November 2-5, 2018, at the Advanced Photon Source, Argonne National Lab. It was organized by Wenli Bi, Ercan Alp, and Jay Bass. Guest speakers included John Tse (Saskatchewan), Wolfgang Sturhahn (Caltech), Jennifer Jackson (Caltech), Anat Shahar (Geophysical Lab), Nicholas Dauphas (Chicago), Justin Hu (Chicago), and Jiyong Zhao (ANL). This two-and-half-day workshop was held to promote the application of the state-of-the-art Nuclear Resonant Scattering (NRS) techniques for characterizing the properties of materials under high P-T conditions of planetary interiors. The workshop was designed to train current and potential scientific users in nuclear resonant inelastic x-ray scattering and data analysis using PHOENIX and SciPhon. Nuclear Resonant Inelastic X-ray Scattering (NRIXS) provides information on vibrational and elastic properties, such as the phonon density of states, sound velocities, and isotope fractionation. NRIXS technique has become a powerful tool to understand the lattice and thermo-dynamics of Fe-bearing planetary materials in extreme pressure temperature conditions.

Some Recently Published COMPRES Supported Science Highlights (I)

American Mineralogist, Volume 103, pages 1516–1519, 2018

LETTER

Making tissintite: Mimicking meteorites in the multi-anvil

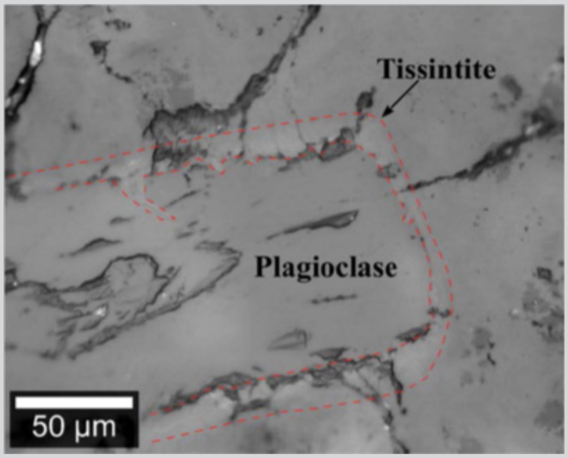
MELINDA J. RUCKS[1,*], MATTHEW L. WHITAKER[1,2], TIMOTHY D. GLOTCH[1], JOHN B. PARISE[1,2], STEVEN J. JARET[1], TRISTAN CATALANO[1], AND M. DARBY DYAR[3]

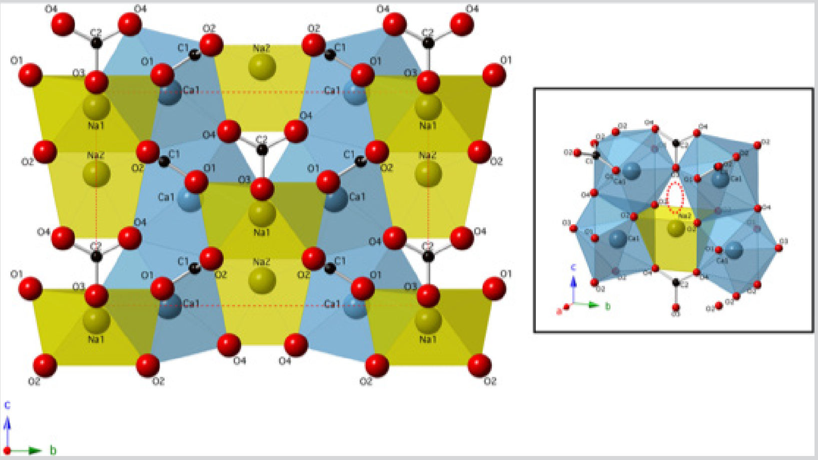
[1]Department of Geosciences, Stony Brook University, Stony Brook, New York 11794-2100, U.S.A.
[2]Mineral Physics Institute, Stony Brook University, Stony Brook, New York 11794-2100, U.S.A.
[3]Department of Astronomy, Mount Holyoke College, South Hadley, Massachusetts 01075, U.S.A.

ABSTRACT

Tissintite is a shock-induced, Ca-rich mineral, isostructural to jadeite, observed in several meteorite samples such as the martian shergottite Tissint. It may form within a "Goldilocks Zone," indicating a potential to provide strict constraints on peak pressure and temperature conditions experienced during impact. Here we present the first laboratory synthesis of tissintite, which was synthesized using a large volume multi-anvil apparatus at conditions ranging from 6–8.5 GPa and 1000–1350 °C. For these experiments, we utilized a novel heating protocol in which we reached impact-relevant temperatures within 1 s and in doing so approximated the temperature-time conditions in a post-shock melt. We have established that heating for impact-relevant timescales is not sufficient to completely transform crystalline labradorite to tissintite at these pressures. Our findings suggest that tissintite forms from amorphous plagioclase during decompression.

Keywords: Tissintite, high-pressure, high-temperature, shock, multi-anvil





Journal of Geophysical Research: Solid Earth

RESEARCH ARTICLE
10.1029/2018JB015846

High-Pressure/Temperature Behavior of the Alkali/Calcium Carbonate Shortite ($Na_2Ca_2(CO_3)_3$): Implications for Carbon Sequestration in Earth's Transition Zone

Cara E. Vennari[1], Christine M. Beavers[1,2], and Quentin Williams[1]

[1]Department of Earth and Planetary Sciences, University of California Santa Cruz, Santa Cruz, CA, USA, [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Key Points:
- Three phase transitions are observed in shortite at high pressure and high pressure/temperatures
- Evidence for dimerization of the carbonate ions in shortite-II, providing constraints on carbon bonding configurations in the deep earth
- High pressure and temperature polymorphism in shortite implies that equimolar sodium/calcium carbonates are stabilized at depth

Supporting Information:
- Supporting Information S1
- Data Set S1

Correspondence to:
C. E. Vennari,
cvennari@ucsc.edu

Citation:
Vennari, C. E., Beavers, C. M., & Williams, Q. (2018). High-pressure/temperature behavior of the alkali/calcium carbonate Shortite ($Na_2Ca_2(CO_3)_3$): Implications for carbon sequestration in Earth's transition zone. *Journal of Geophysical Research: Solid Earth, 123*, 6574–6591. https://doi.org/10.1029/2018JB015846

Abstract The behavior of shortite ($Na_2Ca_2(CO_3)_3$) has been probed using synchrotron-based single crystal X-ray diffraction and Raman spectroscopy at high pressures and following laser heating to illuminate carbon retention within the deep earth, and phase equilibria of alkali/calcium carbonate-rich systems. Above 15 GPa, a transition to the shortite-II structure occurs at 300 K. This phase is novel as it involves a large distortion of the carbonates, with an onset of 3 + 1 coordination and near-dimerization of carbonate groups. Above 22 GPa, shortite-II amorphizes. Samples laser heated at pressures between 12 and 30 GPa crystallize in a new structure, shortite-III. Below 12 GPa, this phase appears to decompose into a mixture of shortite, nyerereite ($Na_2Ca(CO_3)_2$), and aragonite ($CaCO_3$) in accord with prior phase equilibria results. The high-pressure behavior of nyerereite using Raman spectroscopy was also investigated to 25 GPa. The structural response of shortite to pressure is modulated by the sodium cations in the structure; hence, the behavior of alkali-rich carbonates within kimberlitic systems at depth is likely dependent on the bonding and local geometry of alkali cations. Our results show that complex, dense high-pressure structures are generated in the shortite system, and phase equilibria of the protoliths of carbonatites and kimberlites at deep upper mantle and transition zone pressures will involve intermediate alkali-calcium carbonate phases, including the high-pressure phases of shortite. Moreover, 3 + 1 coordination of carbon is observed at far lower pressures than other systems: this coordination could become important in complex carbonates and possibly liquids at substantially shallower depths than previously anticipated.

Journal of Geophysical Research: Solid Earth

RESEARCH ARTICLE
10.1002/2017JB015169

Phase Transitions in Orthoenstatite and Subduction Zone Dynamics: Effects of Water and Transition Metal Ions

Jingui Xu[1,2,3], Dongzhou Zhang[2], Dawei Fan[1], Jin S. Zhang[4], Yi Hu[2], Xinzhuan Guo[5], Przemyslaw Dera[2], and Wenge Zhou[1]

[1]Key Laboratory of High Temperature and High Pressure Study of the Earth's Interior, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang, China, [2]Hawaii Institute of Geophysics and Planetology, School of Ocean and Earth Science and Technology, University of Hawaii at Manoa, Honolulu, HI, USA, [3]University of Chinese Academy of Sciences, Beijing, China, [4]Institute of Meteoritics, Department of Earth and Planetary Sciences, University of New Mexico, Albuquerque, NM, USA, [5]State Key Laboratory of Geological Processes and Mineral Resources, China University of Geoscience, Wuhan, China

Key Points:
- Single-crystal X-ray diffraction experiments are carried out on hydrous Mg end-member and Ni-bearing orthoenstatite(oEn) to 30 GPa and 700 K
- Several hundred ppm of water has negligible effects on the phase transition and bulk modulus of oEn but promotes the thermal expansion
- Ni^{2+} strongly influences the phase transition of oEn and causes a different high-pressure transition (β-opx→β-opxII) than that in Fe-oEn

Supporting Information:
- Supporting Information S1
- Table S1
- Table S2
- Table S3
- Table S4

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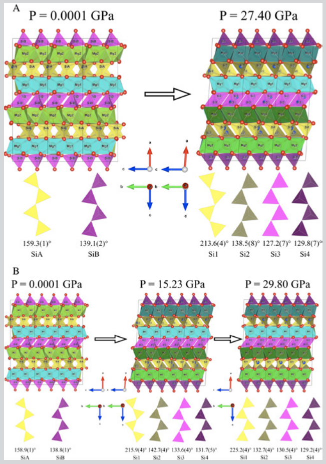
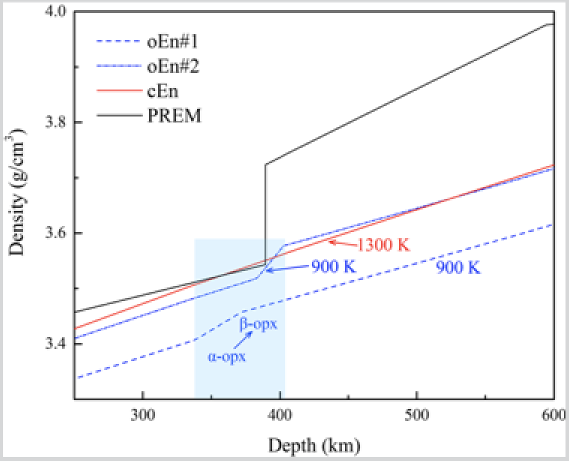
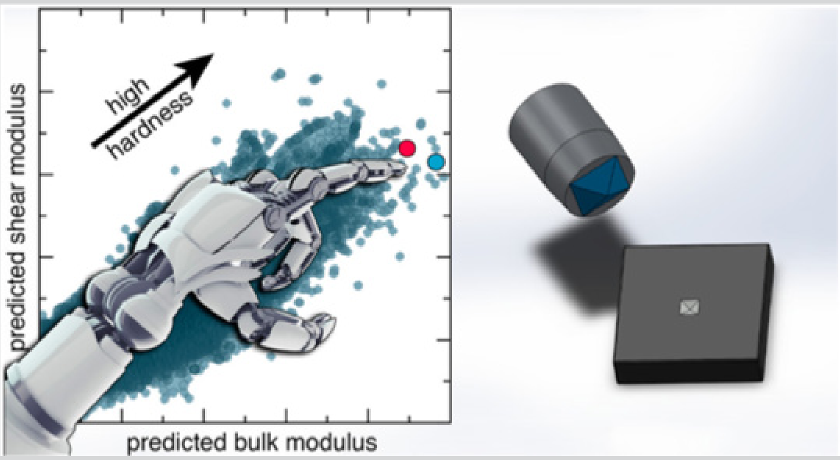
pdera@hawaii.edu

Citation:
Xu, J., Zhang, D., Fan, D., Zhang, J. S., Hu, Y., Guo, X., et al. (2018). Phase transitions in orthoenstatite and subduction zone dynamics: Effects of water and

Abstract Synchrotron-based high-pressure and temperature single-crystal X-ray diffraction experiments were conducted on two hydrous orthoenstatite samples (oEn#1: $Mg_{1.004}Si_{0.998}O_3$, ~619 ppm water; oEn#2: $Mg_{0.947}Ni_{0.053}Si_{0.998}O_3$, ~696 ppm water) to ~34 GPa and 700 K, using resistively heated diamond anvil cells. The α-opx (*Pbca* space group)→β-opx ($P2_1/c$ space group) phase transition of oEn#1 occurs at 12.90(2) GPa, and the β-opx phase persists to 34.25(1) GPa. The α-β transition of oEn#2 occurs at 13.50(1) GPa, and a new isosymmetric β-opx→β-opxII transition takes place at 29.80(4) GPa. The β-opxII phase is preserved down to 24.53(3) GPa during decompression. The transition to the monoclinic β-opxII phase is interpreted as a result of incorporation of Ni^{2+} into the orthoenstatite structure. Fitting the third-order Birch-Murnaghan thermal equation of state to the single-crystal P-V-T data yields the thermoelastic parameters of the α- and β-opx phases for both orthoenstatite samples. This study is the first attempt to determine the thermal equation of state of the β-opx phase. Our results suggest that several hundred ppm of water has negligible effects on the bulk modulus of orthoenstatite but notably enhances the thermal expansion. The potential effects of metastable orthoenstatite on subduction zone dynamics are discussed, and the possible contributions of displacive phase transitions to enhancement of the transformational faulting mechanism of the deep-focus earthquakes in subducted slabs are considered. The presence of metastable orthoenstatite within cold slabs could promote slab stagnation above the 660-km discontinuity.







JACS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Article

Cite This: J. Am. Chem. Soc. 2018, 140, 9844–9853

pubs.acs.org/JACS

Machine Learning Directed Search for Ultraincompressible, Superhard Materials

Aria Mansouri Tehrani,[†,⊥] Anton O. Oliynyk,[†,⊥] Marcus Parry,[‡] Zeshan Rizvi,[†] Samantha Couper,[§] Feng Lin,[§] Lowell Miyagi,[§] Taylor D. Sparks,[‡] and Jakoah Brgoch[*,†]

[†]Department of Chemistry, University of Houston, Houston, Texas 77204, United States
[‡]Department of Materials Science and Engineering, University of Utah, Salt Lake City, Utah 84112, United States
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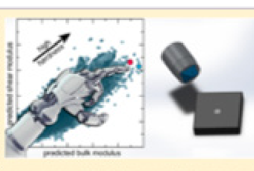
Supporting Information

ABSTRACT: In the pursuit of materials with exceptional mechanical properties, a machine-learning model is developed to direct the synthetic efforts toward compounds with high hardness by predicting the elastic moduli as a proxy. This approach screens 118 287 compounds compiled in crystal structure databases for the materials with the highest bulk and shear moduli determined by support vector machine regression. Following these models, a ternary rhenium tungsten carbide and a quaternary molybdenum tungsten borocarbide are selected and synthesized at ambient pressure. High-pressure diamond anvil cell measurements corroborate the machine-learning prediction of the bulk modulus with less than 10% error, as well as confirm the ultraincompressible nature of both compounds. Subsequent Vickers microhardness measurements reveal that each compound also has an extremely high hardness exceeding the superhard threshold of 40 GPa at low loads (0.49 N). These results show the effectiveness of materials development through state-of-the-art machine-learning techniques by identifying functional inorganic materials.



Some Recently Published COMPRES Supported Science Highlights (II)

nature COMMUNICATIONS

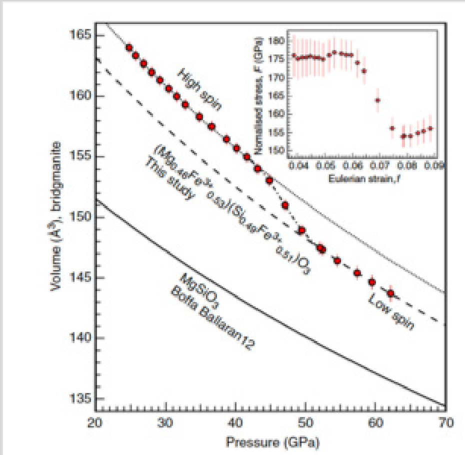
ARTICLE

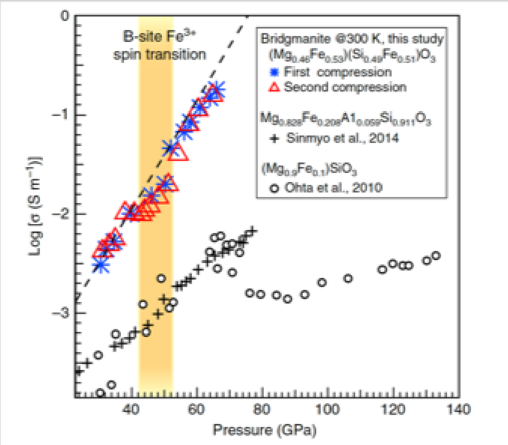
DOI: 10.1038/s41467-018-03671-5 OPEN

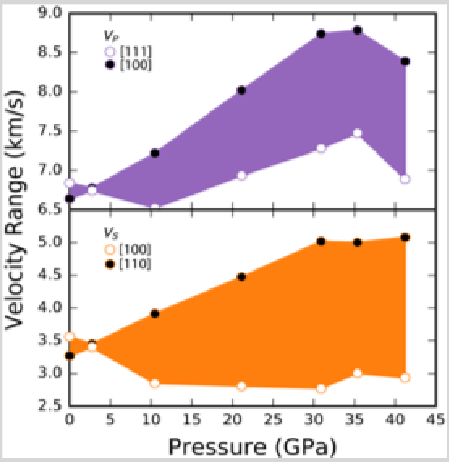
Valence and spin states of iron are invisible in Earth's lower mantle

Jiachao Liu[1], Susannah M. Dorfman[1], Feng Zhu[2], Jie Li[2], Yonggang Wang[3], Dongzhou Zhang[4], Yuming Xiao[5], Wenli Bi[6,7] & E. Ercan Alp[6]

Heterogeneity in Earth's mantle is a record of chemical and dynamic processes over Earth's history. The geophysical signatures of heterogeneity can only be interpreted with quantitative constraints on effects of major elements such as iron on physical properties including density, compressibility, and electrical conductivity. However, deconvolution of the effects of multiple valence and spin states of iron in bridgmanite (Bdg), the most abundant mineral in the lower mantle, has been challenging. Here we show through a study of a ferric-iron-only $(Mg_{0.46}Fe^{3+}_{0.53})(Si_{0.49}Fe^{3+}_{0.51})O_3$ Bdg that Fe^{3+} in the octahedral site undergoes a spin transition between 43 and 53 GPa at 300 K. The resolved effects of the spin transition on density, bulk sound velocity, and electrical conductivity are smaller than previous estimations, consistent with the smooth depth profiles from geophysical observations. For likely mantle compositions, the valence state of iron has minor effects on density and sound velocities relative to major cation composition.







Journal of Geophysical Research: Solid Earth

RESEARCH ARTICLE

10.1029/2017JB015349

Strongly Anisotropic Magnesiowüstite in Earth's Lower Mantle

Gregory J. Finkelstein[1,2], Jennifer M. Jackson[1], Ayman Said[3], Ahmet Alatas[3], Bogdan M. Leu[3,4], Wolfgang Sturhahn[1], and Thomas S. Toellner[3]

[1]Division of Geological and Planetary Sciences, Caltech, Pasadena, CA, USA, [2]Now at Hawai'i Institute of Geophysics and Planetology, University of Haw[...]lu, HI, USA, [3]Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA, [4]Now at Department of Physics, Miami University, Oxford, OH, USA

Key Points:

- Magnesiowüstite is proposed as a major contributor to the seismic anisotropy detected at the bottom of the mantle
- High-energy resolution inelastic X-ray scattering experiments conducted on magnesiowüstite single crystals at high pressure indicate that its shear anisotropy strongly increases with pressure
- At lower-mantle pressures, the shear anisotropy of magnesiowüstite may be as much as a factor of 2 to 3 higher than postperovskite

Supporting Information:

- Supporting Information S1

Correspondence to:
G. J. Finkelstein and J. M. Jackson,
gjfinkel@hawaii.edu;

Abstract The juxtaposition of a liquid iron-dominant alloy against a mixture of silicate and oxide minerals at Earth's core-mantle boundary is associated with a wide range of complex seismological features. One category of observed structures is ultralow-velocity zones, which are thought to correspond to either aggregates of partially molten material or solid, iron-enriched assemblages. We measured the phonon dispersion relations of (Mg,Fe) O magnesiowüstite containing 76 mol % FeO, a candidate ultralow-velocity zone phase, at high pressures using high-energy resolution inelastic X-ray scattering. From these measurements, we find that magnesiowüstite becomes strongly elastically anisotropic with increasing pressure, potentially contributing to a significant proportion of seismic anisotropy detected near the base of the mantle.

Geochemistry, Geophysics, Geosystems

RESEARCH ARTICLE

10.1002/2017GC007168

High-Pressure Geophysical Properties of *Fcc* Phase FeH_X

E. C. Thompson[1], A. H. Davis[1], W. Bi[2,3], J. Zhao[3], E. E. Alp[3], D. Zhang[4], E. Greenberg[5], V. B. Prakapenka[5], and A. J. Campbell[1]

[1]Department of the Geophysical Sciences, University of Chicago, Chicago, IL, USA, [2]Department of Geology, University of Illinois, Urbana, IL, USA, [3]Argonne National Laboratory, Advanced Photon Source, Argonne, IL, USA, [4]Hawaii Institute of Geophysics & Planetology, University of Hawaii Manoa, Honolulu, HI, USA, [5]Center for Advanced Radiation Sources, University of Chicago, Argonne, IL, USA

Key Points:

- X-ray diffraction and nuclear resonant inelastic X-ray scattering were performed on *fcc* FeH_x to determine densities and sound velocities to 82 GPa
- The Earth's outer core may contain up to 0.8–1.3 wt % hydrogen based on matching the density and velocities of variable stoichiometry iron hydrides to PREM
- The hydrogen content of Earth's core is highly dependent on the influence of temperature on the Birch's law relationship in iron alloys

Supporting Information:

- Supporting Information S1

Correspondence to:
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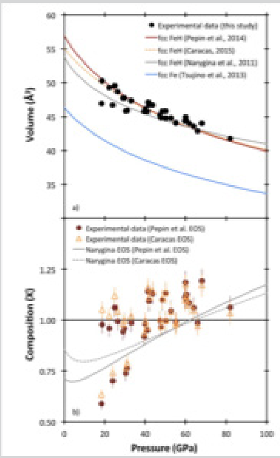
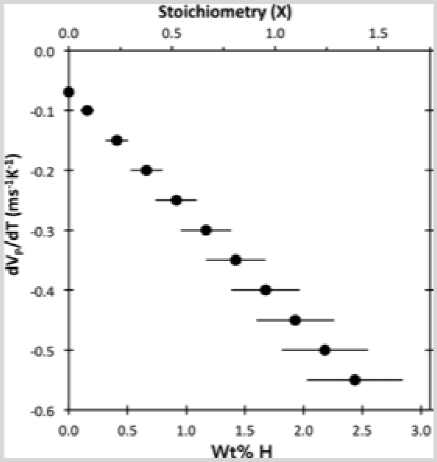
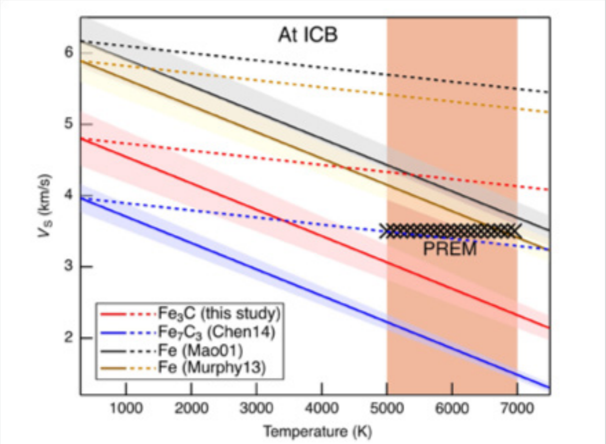
ecthompson@uchicago.edu

Citation:
Thompson, E. C., Davis, A. H., Bi, W., Zhao, J., Alp, E. E., Zhang, D., . . . Campbell, A. J. (2018). High-pressure

Abstract Face centered cubic (*fcc*) FeH_x was synthesized at pressures of 18–68 GPa and temperatures exceeding 1,500 K. Thermally quenched samples were evaluated using synchrotron X-ray diffraction (XRD) and nuclear resonant inelastic X-ray scattering (NRIXS) to determine sample composition and sound velocities to 82 GPa. To aid in the interpretation of nonideal ($X \neq 1$) stoichiometries, two equations of state for *fcc* FeH_x were developed, combining an empirical equation of state for iron with two distinct synthetic compression curves for interstitial hydrogen. Matching the density deficit of the Earth's core using these equations of state requires 0.8–1.1 wt % hydrogen at the core-mantle boundary and 0.2–0.3 wt % hydrogen at the interface of the inner and outer cores. Furthermore, a comparison of Preliminary Reference Earth Model (PREM) to a Birch's law extrapolation of our experimental results suggests that an iron alloy containing ~0.8–1.3 wt % hydrogen could reproduce both the density and compressional velocity (V_P) of the Earth's outer core.







Contents lists available at ScienceDirect

Earth and Planetary Science Letters

www.elsevier.com/locate/epsl

Experimental constraints on the sound velocities of cementite Fe_3C to core pressures

Bin Chen[a,*], Xiaojing Lai[a,b], Jie Li[c], Jiachao Liu[c], Jiyong Zhao[d], Wenli Bi[d], E. Ercan Alp[d], Michael Y. Hu[d], Yuming Xiao[e]

[a] Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa, Honolulu, HI, USA
[b] Department of Geology and Geophysics, University of Hawaii at Manoa, Honolulu, HI, USA
[c] Department of Earth and Environmental Sciences, University of Michigan, Ann Arbor, MI, USA
[d] Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA
[e] HPCAT, Geophysical Laboratory, Carnegie Institution of Washington, Argonne, IL, USA

ARTICLE INFO

Article history:
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inner core
magnetic transition
Poisson's ratio
compressional-wave velocity
shear-wave velocity

ABSTRACT

Sound velocities of cementite Fe_3C have been measured up to 1.5 Mbar and at 300 K in a diamond anvil cell using the nuclear resonant inelastic X-ray scattering (NRIXS) technique. From the partial phonon density of states (pDOS) and equation of state (EOS) of Fe_3C, we derived its elastic parameters including shear modulus, compressional (V_P) and shear-wave (V_S) velocities to core pressures. A pressure-induced spin-pairing transition in the powdered Fe_3C sample was found to occur gradually between 10 and 50 GPa by the X-ray Emission Spectroscopy (XES) measurements. Following the completion of the spin-pairing transition, the V_P and V_S of low-spin Fe_3C increased with pressure at a markedly lower rate than its high-spin counterpart. Our results suggest that the incorporation of carbon in solid iron to form iron carbide phases, Fe_3C and Fe_7C_3, could effectively lower the V_S but respectively raise the Poisson's ratio by 0.05 and 0.07 to approach the seismically observed values for the Earth's inner core. The comparison with the preliminary reference Earth model (PREM) implies that an inner core composition containing iron and its carbon-rich alloys can satisfactorily explain the observed seismic properties of the inner core.

Congratulations to Christine Beavers

Congratulations to Christine Beavers on her new position as Principal Beamline Scientist at Diamond Light Source in Oxfordshire, UK. Christine was a COMPRES Beamline Scientist at the ALS 12.2.2 from 2013-2018. We will miss you Christine, but we hope you can still attend the annual meeting!

Farewell to Shannon Clark

Shannon Clark will be leaving COMPRES and UNM at the end of February to embark on a new chapter in her life in Colorado. Shannon served as COMPRES Program Director since 2015 and has been at UNM, working with Carl Agee and the Institute of Meteoritics, for over 15 years. We also welcome to COMPRES Shannon's new successor Gloria Statom (gstatom@unm.edu).

COMPRES Annual Meeting SAVE THE DATE! August 2-5, 2019

We are pleased to announce that the 2019 COMPRES Annual Meeting will be held on August 2-5, 2019 at the Big Sky Resort, Montana, USA. http://compres.us/events/annual-meeting/2019/2019-compres-annual-meeting-general-information

Friday 8/2. Arrival day with 5 PM poster session + reception, followed by 7 PM dinner.
Saturday 8/3. Full day of meeting
Sunday 8/4. Full day of meeting
Monday 8/5. Morning meeting, noon departure.

More details on registration and program will be posted in early 2019. We anticipate offering one or more pre-meeting COMPRES supported workshops to be held on Friday 8/2, with resort check-in on Thursday 8/1. We also plan to offer a pre-meeting all-day field trip to Yellowstone National Park on Thursday 8/1, with resort check-in on Wednesday 7/31. Meeting Questions? Contact Beth Ha: beth3ha@unm.edu. See you in Montana, August 2019!

Contact: Dr. Carl Agee
COMPRES President
agee@unm.edu
505-750-7172
www.compres.us

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