Thermodynamic and Mechanical Properties of SSP Materials: Simultaneous Ultrasonic and Synchrotron X-ray Studies at High P and T

Baosheng Li
Stony Brook University

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2017 Current Participants  (DE-NA0002907)

Baosheng Li (SBU, PI)
Robert C. Liebermann (SBU, co-PI)
Nao Cai (SBU, Postdoc)
Ting Chen (SBU, Graduate Student)
Xington Qi (SBU, Graduate Student)
Siheng Wang (SBU, Graduate Student)

Former Participants now in National Labs/FFDRCs
Matthew Whitaker (Beamline Scientist, SBU/BNL)
Matthew Jacobsen (Staff Scientist, Institute for Defense Analyses (IDA))

Collaborators
Jianzhong Zhang (LANL)
Hongwu Xu (LANL)
Tony Yu (13-ID-D, GSECARS, APS/U of Chicago)
Yanbin Wang (13-ID-D, GSECARS, APS/U of Chicago)
David Welch (BNL/SBU)
Haiyan Chen (6-BM/APS, COMPRES/SBU)
Liping Wang (UNLV)
Our Objectives

- Understanding thermodynamic and mechanical properties of SSP materials under extreme conditions
  - Sound velocity and density measurements at high pressure and temperature conditions (metallic, covalent, ionic) for precise equation of state determination

- Education, Training, Technology Transfer
  - Provide training for the next generation scientists, collaborate with and transfer knowledge to national labs

- Development of Experimental Techniques
  - New techniques for material characterization and data analysis
  - Extending ultrasonic measurements to $P \sim 50$ GPa to bridge the gap between static and dynamic/shock compressions
Our Toolkit at SBU

Single Stage, Boron Epoxy Pressure Medium, mm sized Sample, P <20 GPa T<1800K (6-BM, APS/COMPRES)

Double Stage MA-8 MgO Pressure Medium P <30 GPa, T<2500K Sample 5-100 mm³ (also T25 at 13-ID-D, APS)
New Development to reach ~50 GPa

DAC, Liquid or solid Pressure Medium P to Mbar pressures sub-millimeter sample

(56-core Cluster, as well as Computing Center at SBU)
Integrated Ultrasonics+X-ray Technique in Multi-anvil, High-pressure Apparatus

- Accurate equation of state and sound velocities (10^{-3} precision)
- Characterization of stress (macroscopic and microscopic), yield strength, and rheology studies

Pressure is directly calculated using measured V and K of sample ("absolute Pressure")
Publications of 2017-2018

2. Qi, X., Y. Zou, X. Wang, T. Cheng, D. Welch, B. Li (2017) Elastic anomaly and polyamorphic transition in (La, Ce)-based bulk metallic glass under pressure, Scientific Reports 7,724, doi:10.1038/s41598-017-00737-0.
4. Du, W., D. Walker, S.M. Clark, X. Li, B. Li (2017) Microscopic strain in a grossular-pyrope solution anti-correlates with excess volume through local Mg-Ca cation arrangement, more strongly at high Ca/Mg ratio, American Mineralogist, 102, 2307-2316.

Submitted/Under Review
2. Abnormal elasticity in Fe₃O₄ (Physical Review Applied, under review)

To be submitted/In Preparation/Work-in-Progress
Sound Velocity Results for Pr, Nd, W, Hf, Ta + Three posters here: Mat-16, 17, 18
Thermoelasticity and anomalies in the pressure dependence of phonon velocities in niobium

Yongtao Zou,1,2,a) Ying Li,1 Haiyan Chen,1 David Welch,3,4 Yusheng Zhao,2
and Baosheng Li1,a)

1Mineral Physics Institute, State University of New York, Stony Brook, New York 11794, USA
2Academy for Advanced Interdisciplinary Studies, and Department of Physics, Southern University of Science and Technology, Shenzhen 518055, China
3Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA
4Department of Materials Science and Engineering, State University of New York, Stony Brook, New York 11794, USA

Science Highlights:
1. A pressure-induced softening behavior in the phonon velocities, probably owing to the topological change in the Fermi surface induced by s-d electron transfer at 4.8 GPa.

2. First direct measurements of velocities and densities at current P AND T
   $B_{S0} = 174.9(3.2)$ GPa, $G_0 = 37.1(3)$ GPa
   $\frac{dB_S}{dP} = 3.97(9)$, $\frac{dG}{dP} = 0.83(5)$
   $\frac{dB_S}{dT} = -0.064(7)$ GPa/K, $\frac{dG}{dT} = -0.012(3)$ GPa/K

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## Thermoelastic Properties of Nb (bcc)

<table>
<thead>
<tr>
<th></th>
<th>$B_0$ (GPa)</th>
<th>$G_0$ (GPa)</th>
<th>$(\partial B / \partial P)_T$</th>
<th>$(\partial G / \partial P)_T$</th>
<th>$(\partial B / \partial T)_P$ (GPa/K)</th>
<th>$(\partial G / \partial T)_P$ (GPa/K)</th>
<th>Ref.</th>
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<td>174.9(32)</td>
<td>37.1(3)</td>
<td>3.97(9)</td>
<td>0.83(5)</td>
<td>-0.064(7)</td>
<td>-0.012(3)</td>
<td>This study (Exp)</td>
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<tr>
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<td>170.2</td>
<td>34.4</td>
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<td>This study (Theory)</td>
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<tr>
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<td>174(5)</td>
<td>---</td>
<td>4</td>
<td>---</td>
<td>-0.060(8)</td>
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<td>Zou et al. $^a$</td>
</tr>
<tr>
<td>4</td>
<td>170.7</td>
<td>37.8</td>
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<td>Katahara et al. $^b$</td>
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<td>Graham et al. $^c$</td>
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<td>Kenichi and Singh$^d$</td>
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<td>3.85</td>
<td>---</td>
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<td>Koči et al. $^f$</td>
</tr>
</tbody>
</table>
SiO$_2$

Stishovite: The Strongest Oxide
Quartz: Poisson ratio ~ 0.08
Cristobalite: neg. Poisson ratio & thermal expansion

Image created by John Winter
https://serc.carleton.edu/research_education/equilibria/simplephasediagrams.html
Thermoelasticity of SiO$_2$ Coesite: (Chen et al, GRL, 2018)

- Low $dV_P/dP$
- Negative $dV_s/dP$
- Low $dK/dT$
- Very low thermal expansion
- Very low $dG/dP$
Magnetite \( \text{Fe}_3\text{O}_4 \)

\( Fd \overline{3} m \),

Tet: A site: \( \text{Fe}^{3+} \)
Oct: B site: \( \text{Fe}^{2+} \) and \( \text{Fe}^{3+} \)
Praseodymium under Pressure

Pressure-induced phase transitions from I (dhcp)→II (fcc)→III (distorted fcc, hR24)→(Pr VII, X)→IV (α-U, Cmcm)

- Pr ([Xe] 4f^25d^1 6s^2), dhcp
  - (e.g., Chesnut and Vohra, 2000; Baer et al., 2003; Dimtriev et al., PRB 2004 Velisavljevic et al., up to 179 GPa and other theoretical studies)

“…a great deal of uncertainty as to the structural behavior of Pr between 7 and 20 GPa. In particular: (i)What is the structure of the d-fcc phase of Pr between 7 and 10–12 GPa? (ii)Is there a phase transition at 10–12 GPa to another, possibly monoclinic phase?”

--Evans et al. (PRB, 2009)
Experiment P: Up to 12 GPa
In-situ pressure determination
Very reliable P wave signals but high attenuation in S wave signals
Sample length change after exp. < 0.5%

At high P:
\[ \left( \frac{L}{L_0} \right)^3 = \frac{\rho_0}{\rho} \]

OR:
\[ K_T = -V \frac{dP}{dV} \]
\[ K_S = (1 + \alpha \gamma T) K_T \]

\[ \frac{L_0}{L} = 1 + \frac{1 + \alpha \gamma T}{3 \mu_0} \int_0^P \frac{dP}{t_P^2} - \frac{4}{3} \frac{\mu_0}{t_S^2} \]

⇒ ts is obtained using previous density data
Comparison with previous data
Red lines: ultrasonic pulse transmission under high non-hydrostatic conditions
Bridgeman/opposed anvil apparatus by Boguslavakii et al. (JETP, 1985)

Softening $K_s$ results in density change $\sim 0.5\%$ relative to extrapolated Values
Ultrasonic Measurements to ~50 GPa are in Progress

Update: TJS cubes are in hands and testing experiments are underway.

Li and Liebermann (2014)

Kunimoto et al. 2016

WC anvil
Example:

Sound velocity data from previous shock wave studies on Ce to be compared with future measurements from this study.
Education, Training, and Technology Transfer

- Techniques for Ultrasonic Measurements

High pressure elasticity and thermal properties of depleted uranium

M. K. Jacobsen$^a$ and N. Velisavljevic$^b$

Shock and Detonation Physics (M-9), Los Alamos National Laboratory, Los Alamos, New Mexico 87544, USA

(Received 26 December 2015; accepted 15 April 2016; published online 29 April 2016)

Studies of the phase diagram of uranium have revealed a wealth of high pressure and temperature behaviors. However, the dependence of elasticity and thermal properties on pressure and temperature is not well established. In this study, we report on the high pressure elasticity and thermal properties of depleted uranium from 0.1 to 6 GPa and from 10 to 400 K.

Shear-driven instability in zirconium at high pressure and temperature and its relationship to phase-boundary behaviors

M. K. Jacobsen,$^1$* N. Velisavljevic,$^1$ Y. Kono,$^2$ C. Park,$^2$ and C. Kenney-Benson$^2$

$^1$Shock and Detonation Physics (M-9), Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

$^2$HPCAT, Geophysical Laboratory, Carnegie Institution of Washington, Argonne, Illinois 60439, USA

The figure shows the relationship between volume and pressure for shear-driven instability in zirconium. The reflected signal time graph illustrates the behavior at different pressures and times.
Summary of Activities and Outlook

• **Sound velocities.** Metals (transition metal, lanthanide), metal alloys, and silicates have been studied at high pressure and high temperatures using ultrasonic and X-ray studies, the full set of elasticity, $K$, $G$, $\partial K/\partial P$, $\partial G/\partial P$, $dK/dT$, $dG/dT$ contribute to those databases maintained at national labs for SSP studies.

• **Measurements to reach $P \sim 50$ GPa.** Progress have been made to establish the protocols for measurements, we plan to apply these measurements to lanthanides (Ce, Pr, Nd) to further bridge the gap between static [multi-anvil and DAC] and dynamic [shock] high-pressure experiments.

• **Education, training, and technology transfer.** Provided education and training for next generation scientists for the stewardship science program as well as technology transfer for conducting advanced experiments using X-ray/neutron source at APS/LANL.
Understanding structural origins of various properties is crucial for designing and generating new additively/3D printed materials with desired properties.
Effect of d-band Filling and Elastic Constants

4d Transition Metals
Lars Stixrude, 2001

5d Transition metals; ion-ion potential
Per Sonderlind, PRB, 1993
2016 John C. Jamieson Student Paper Award


- Ting Chen
- Xintong Qi
- Xuebing Wang

“This award is granted to a student from the Mineral and Rock Physics Focus Group community who has published the most outstanding paper in the field of high-pressure and high-temperature research in the previous year.” —AGU MRP