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

Baosheng Li
(Stony Brook University)

DOE/SSAP Symposium, Washington, DC, Feb 17-18, 2016

Participants

Baosheng Li (SBU, PI)
Robert C. Liebermann (SBU, co-PI)
Yongtao Zou (SBU Postdoc)
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Ting Chen(SBU, Graduate Student)
Xington Qi (SBU, Graduate Student)

Collaborators

Matthew Jacobsen (LANL), Jianzhong Zhang (LANL)
Tony Yu (APS/U of Chicago), Yanbin Wang (APS/U of Chicago)
David Welch (BNL/SBU), Qiang Li (BNL)
Zhiqiang Chen, (COMPRES, X17C/BNL)
Haiyan Chen (COMPRES, X17B2/BNL)

Former participants

Matthew Whitaker(now Beamline Scientist SBU/BNL)
Matthew Jacobsen (now Postdoc at LANL)

Research in Progress

(1) Sound velocity and density at high *P-T* conditions (fundamental for a wide range of scientific topics in materials)

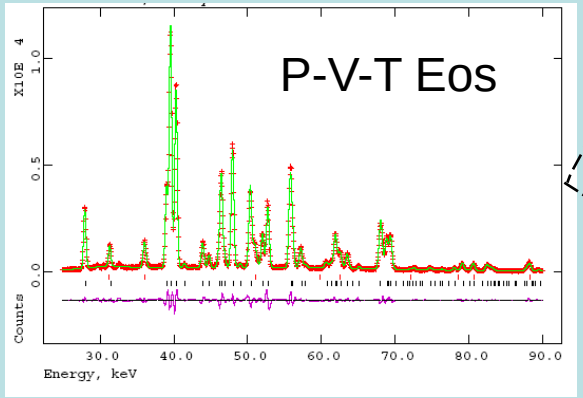
- **Thermoelasticity of Metals:** Nb, Fe, **Hf (poster by Qi et al.)**
- **Ce 4f-electron delocalization on elasticity: (La,Ce)-based metallic glass**
- **Structure, bonding, and elasticity: high pressure phase of silica (poster by T. Chen et al.)**
- Superhard and Superconducting Niobium Nitride: ε-NbN

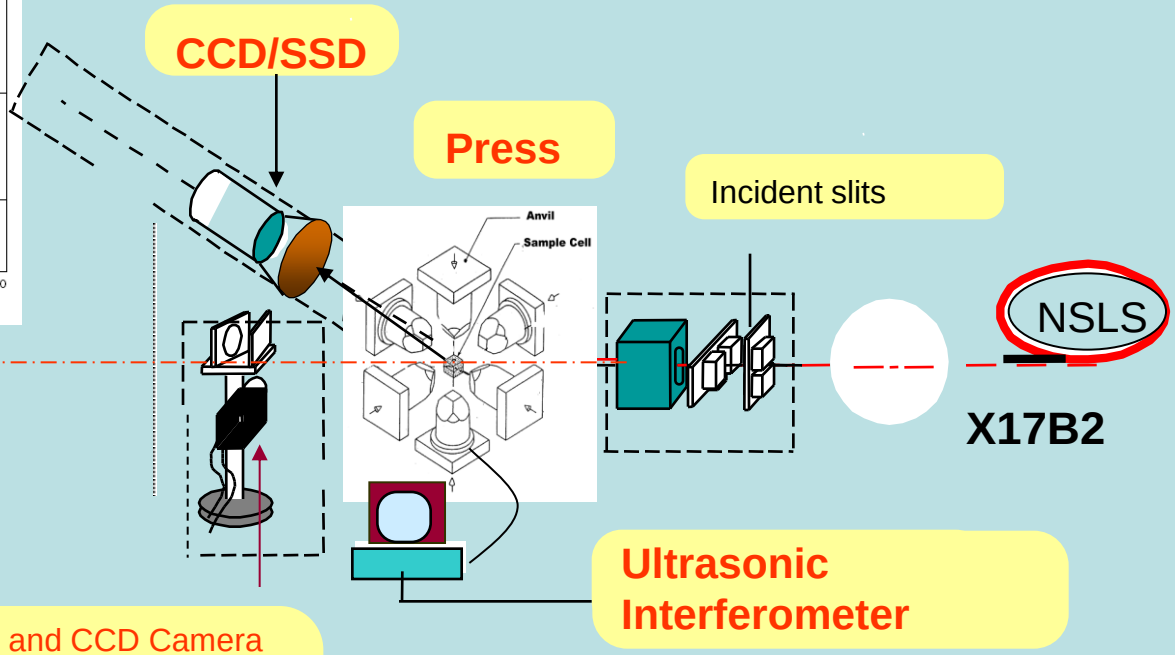
(2) New Techniques Under Development

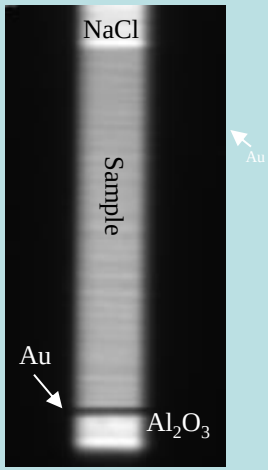
- **Macroscopic stress-strain determination under high pressure (poster by X. Wang et al.)**
- **Development of travel time pressure scale**
- Simultaneous length and velocity determination under high P-T
- Measurements to P > 30 GPa to bridge the gap between static and dynamic compressions

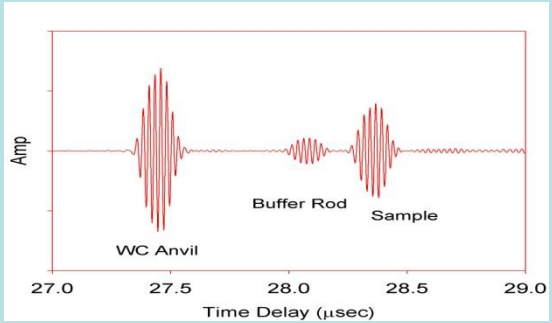
Integrated Ultrasonics+X-ray Technique in Multi-anvil, High-pressure Apparatus at NSLS

- P is directly calculated using measured V and K of sample
- Accurate equation of state results due to absolute pressure
- Characterization of macroscopic and microscopic stress, yield strength, and rheology studies



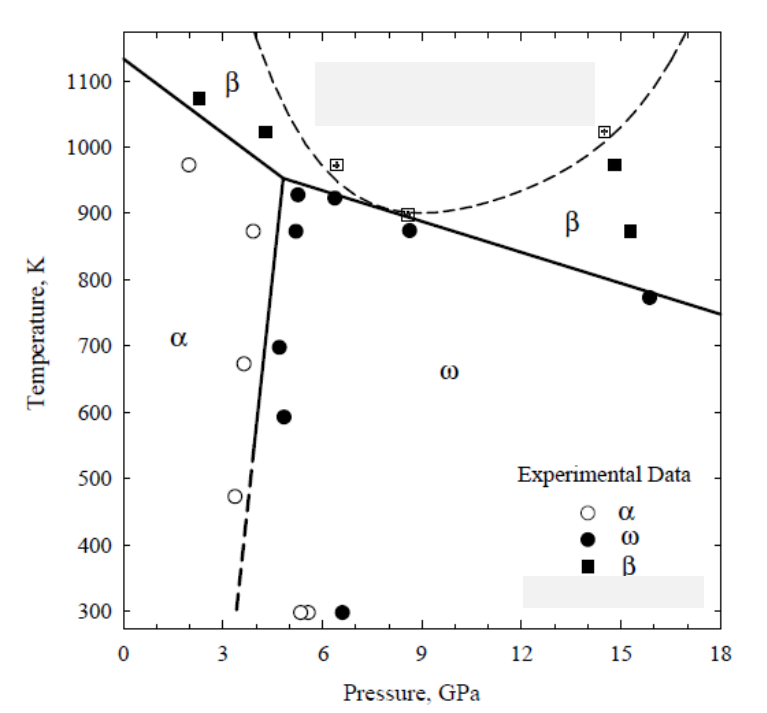






(Similar setup available also at APS)

Group IV Metals:



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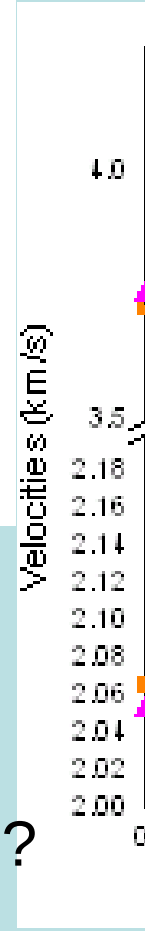
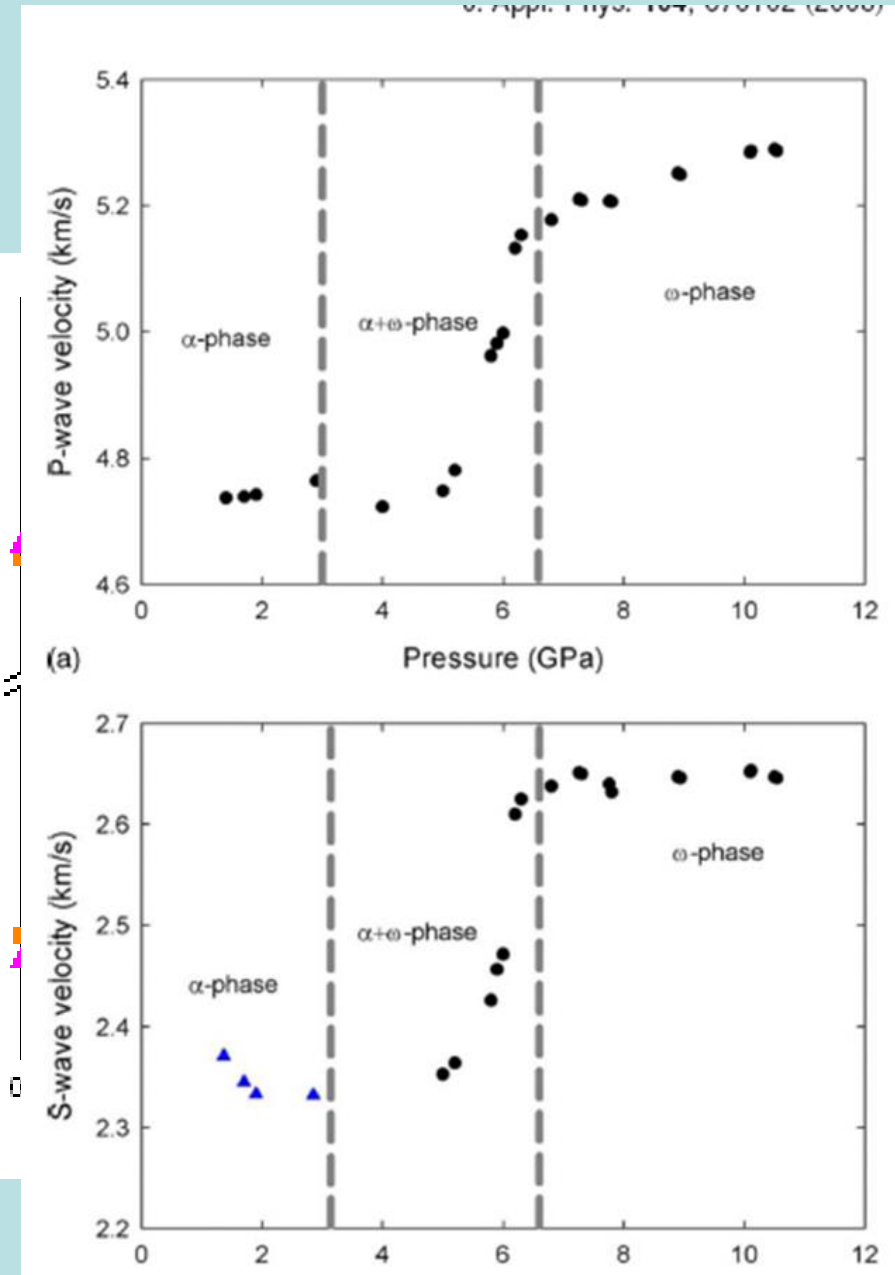




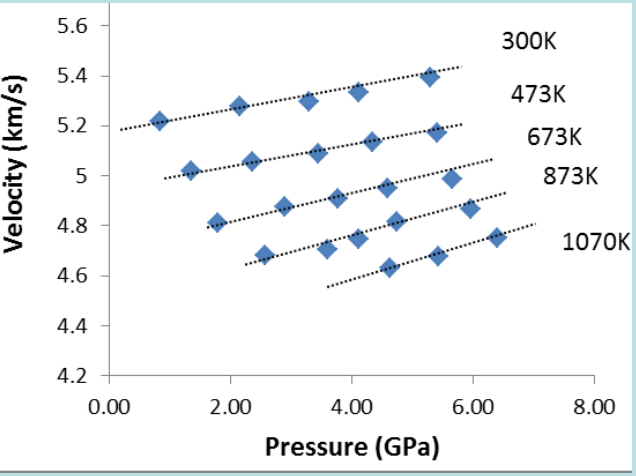
Ti and Zr: Phase transitions, Elasticity softening under pressure

See poster by X. Qi et al from Experimental and DFT studies (submitted to J. App Phy.)

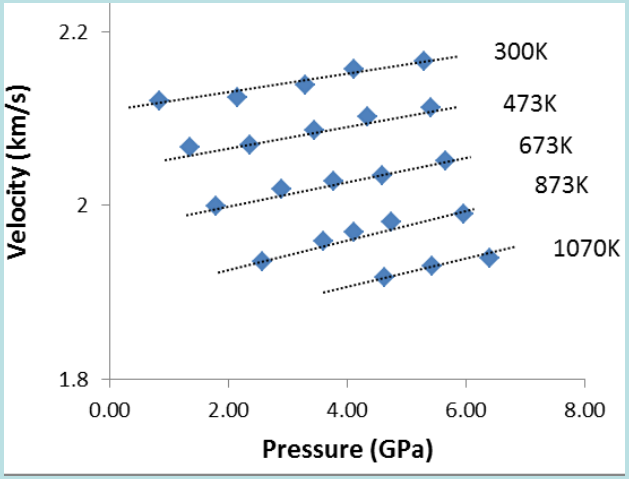
Behavior of Hf [Xe] $4f^{14}\ 5d^{2}\ 6s^{2}$?

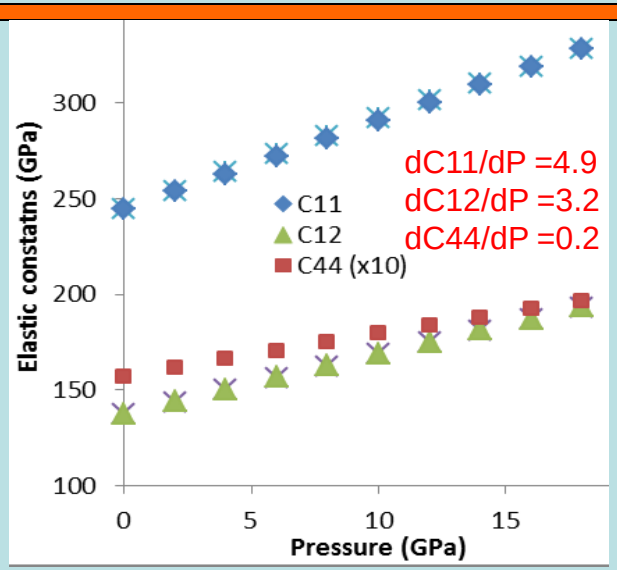
Velocity and Elastic Moduli of Nb at High P and T

P wave



S wave

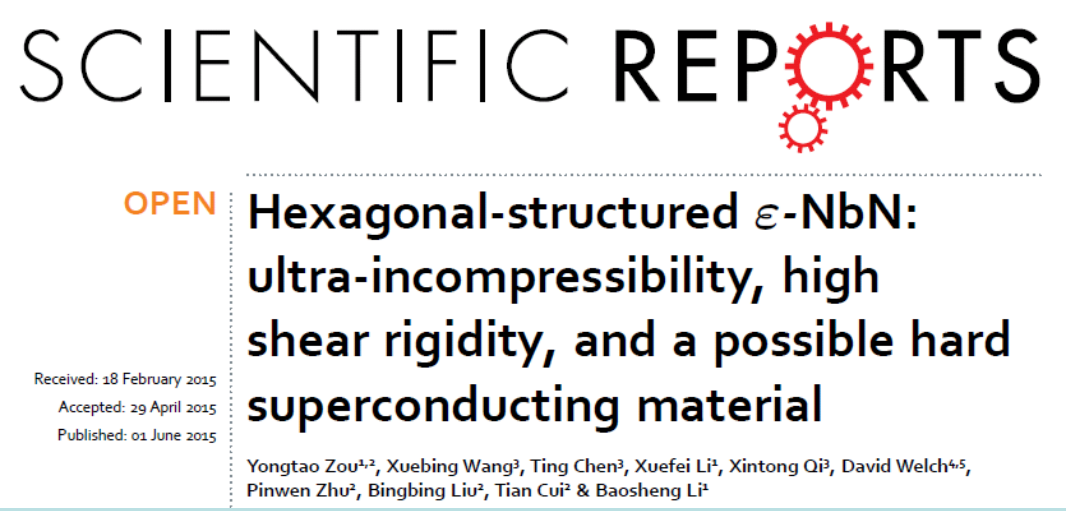




	K (GPa)	G (GPa)	dK/dP	dG/dP	dK/dT (GPa/K)	dG/dT (GPa/K)
This study	172.8(5)	37.5 (3)	4.6(2)	0.7(1)	-0.067	-0.011
Katahara (1979)	170.69		3.98	0.47		

Manuscript in preparation

Superhard and Superconducting ε–NbN (Space group: *P6$_3$/mmc*)

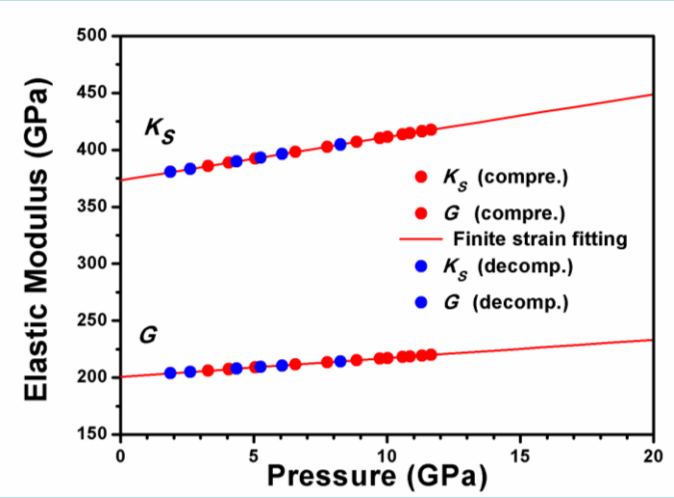

SCIENTIFIC REPORTS

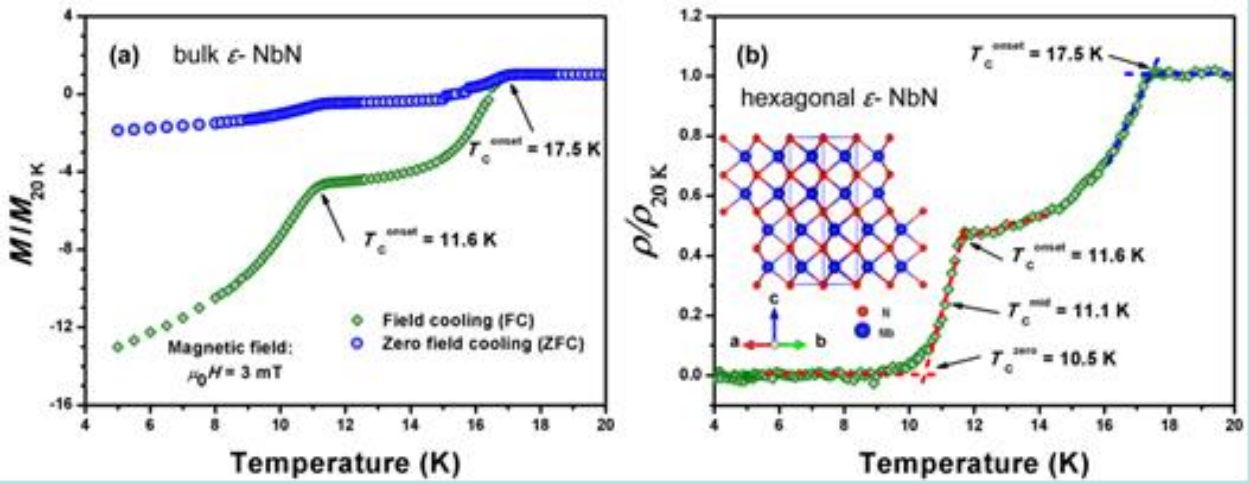
OPEN

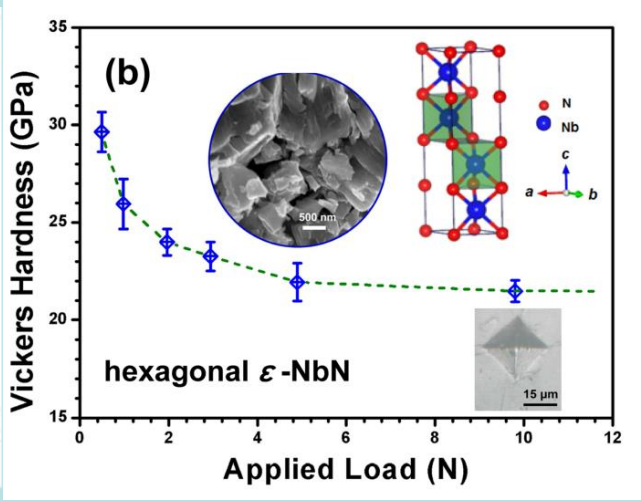
Hexagonal-structured ε-NbN: ultra-incompressibility, high shear rigidity, and a possible hard superconducting material

Received: 18 February 2015
Accepted: 29 April 2015
Published: 01 June 2015

Yongtao Zou[1,2], Xuebing Wang[3], Ting Chen[3], Xuefei Li[1], Xintong Qi[3], David Welch[4,5], Pinwen Zhu[2], Bingbing Liu[2], Tian Cui[2] & Baosheng Li[1]







Zou et al, 2016, Scientific Reports (accepted)

Journal of Physics and Chemistry of Solids 75 (2014) 1017–1023

Enhancement of thermoelectric performance with pressure in $Ce_{0.8}Fe_3CoSb_{12.1}$

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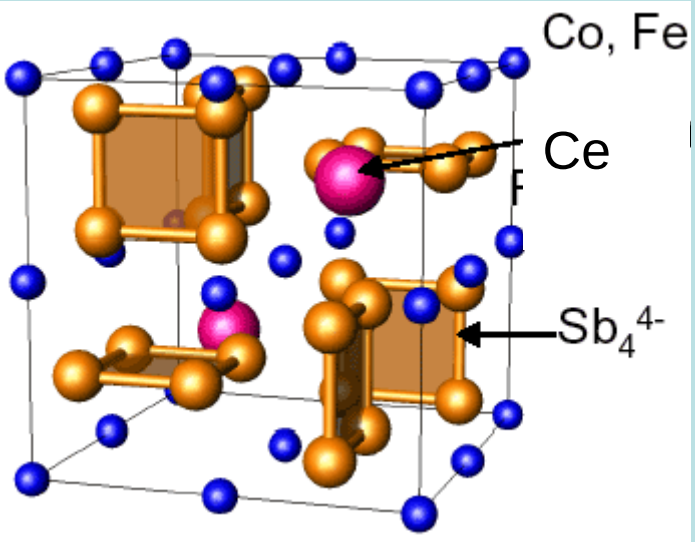
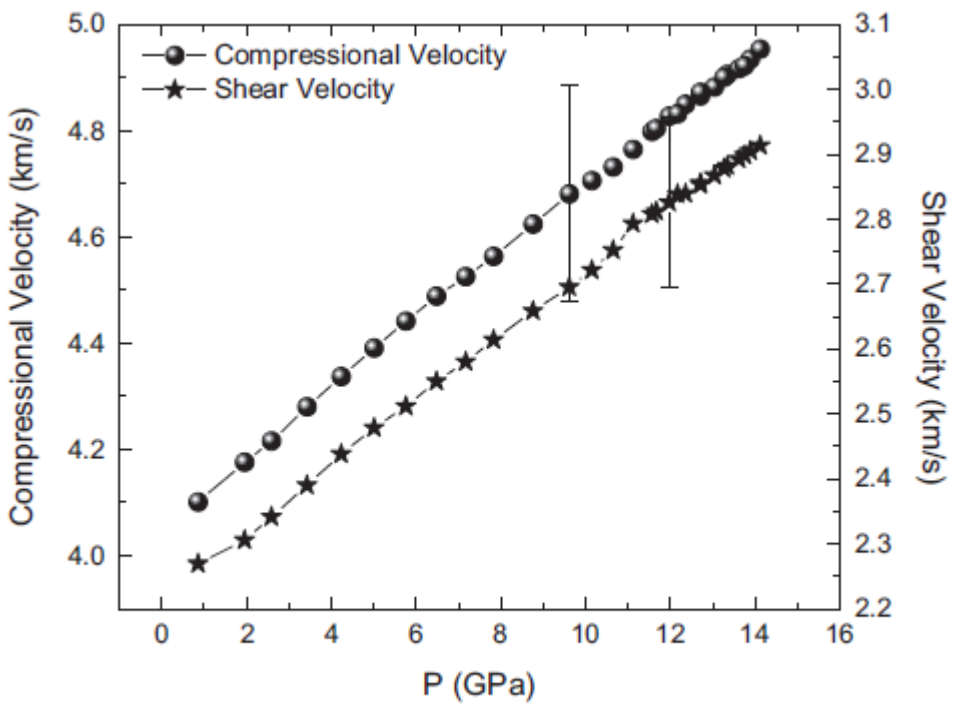
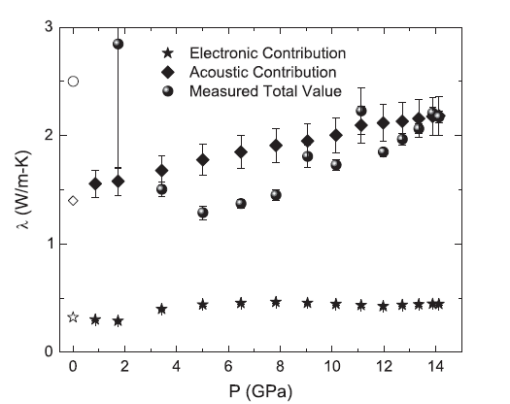
[1] Present Address: Los Alamos National Laboratory, Los Alamos NM 87544, United States.

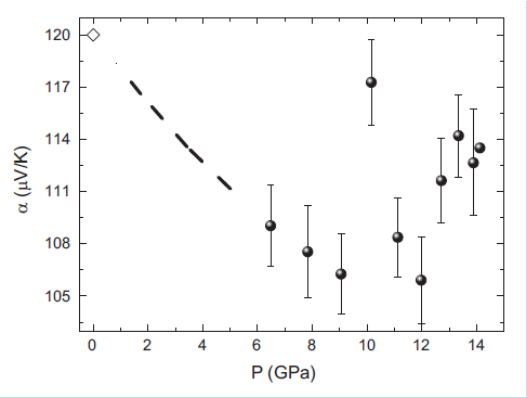




. Sound Velocity vs. Pressure for $Ce_{0.8}Fe_3CoSb_{12.1}$. In this plot, the spl

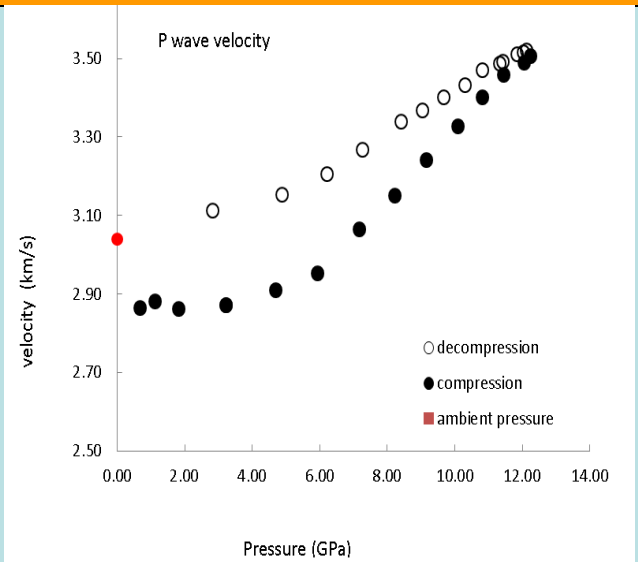


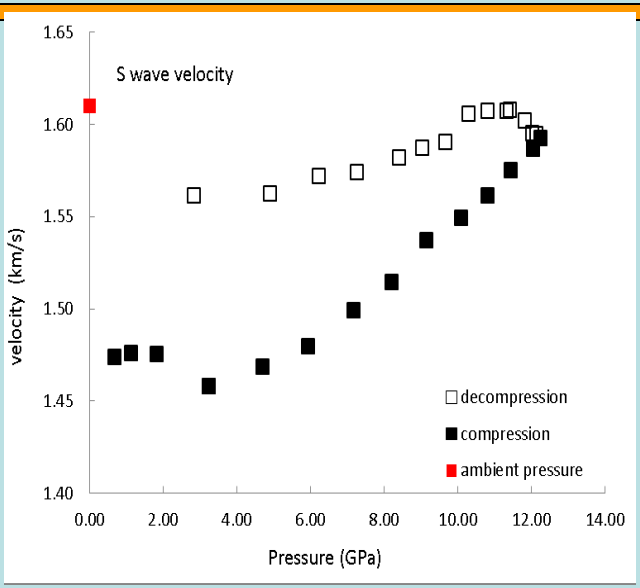
6. Thermal conductivity components vs. pressure: In this graph, the open

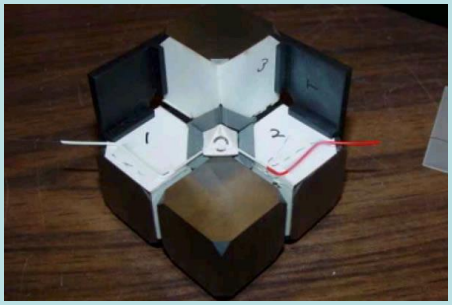


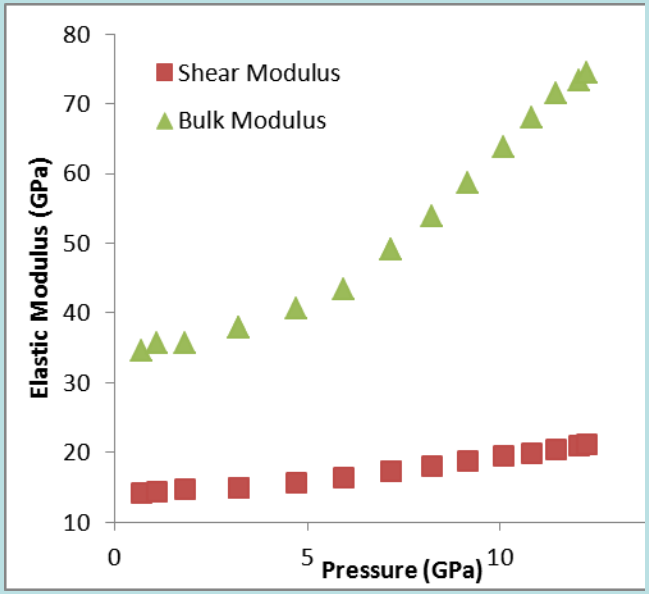
By M. Jacobsen et al., JPCS, 2014.

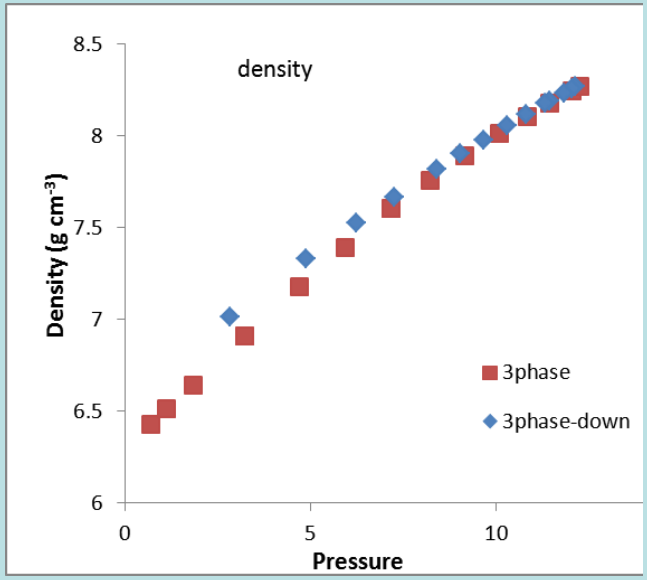
Elasticity of Metallic Glass $(La_{.5}Ce_{.5})_{64}Al_{16}Ni_5Cu_{15}$



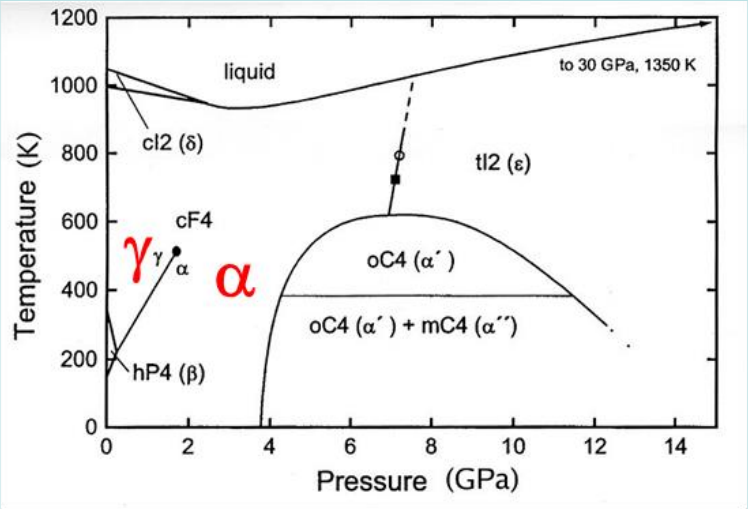


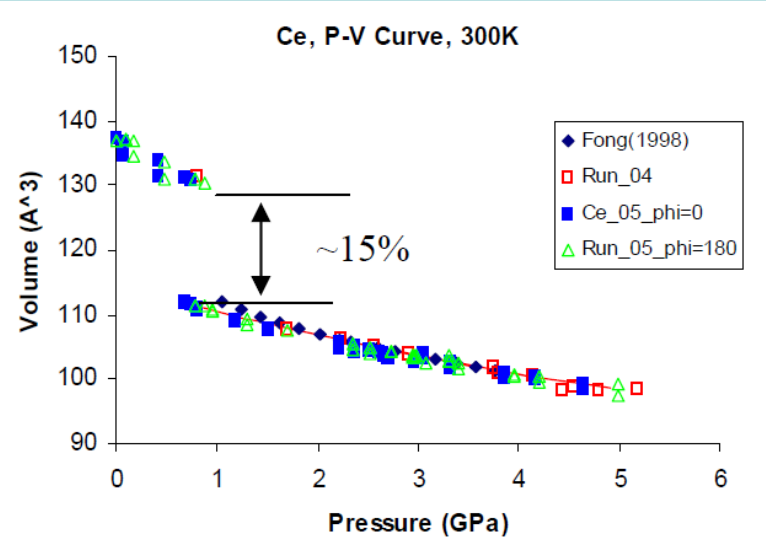






Effect of Ce 4f electron delocalization on properties





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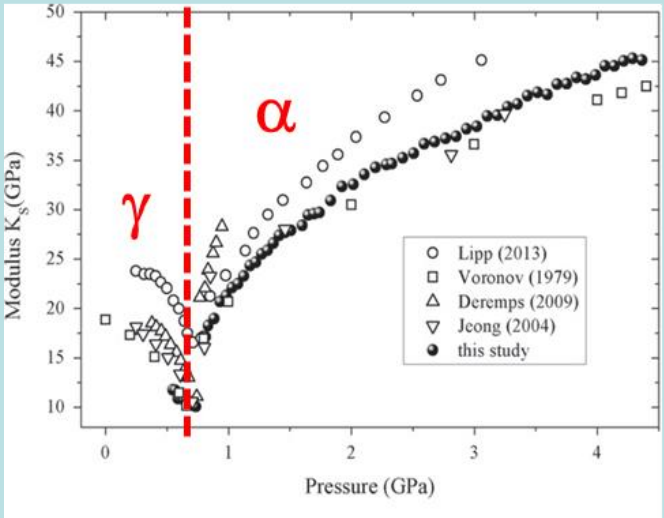
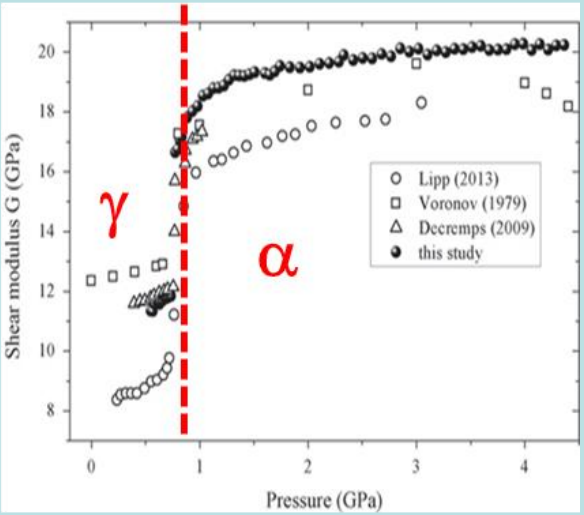
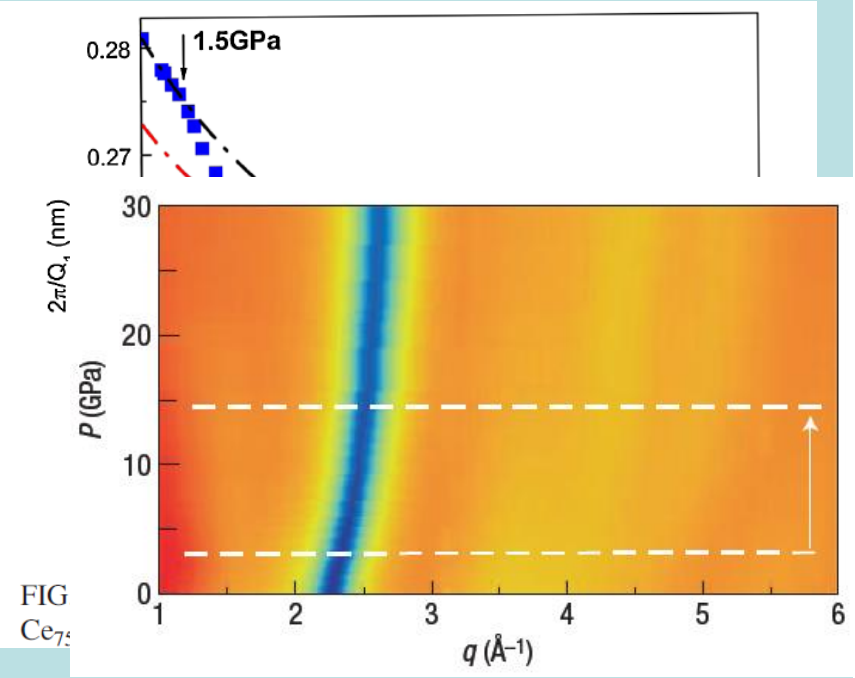


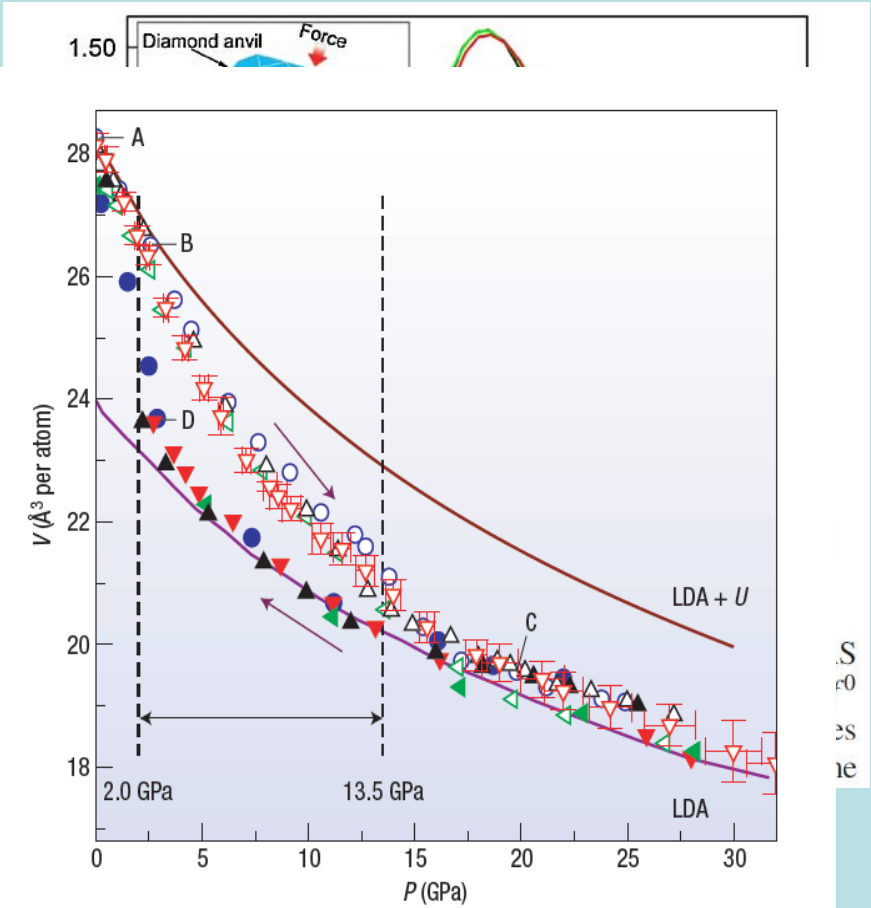


Ce metal

Wang et al., Mat. Res. Express, 2014

Pressure Induced Polyamorphism in Ce-Bulk Metallic Glass: Previous Work





Sheng et al. Nature, 2007

PRL **104,** 105702 (2010) PHYSICAL REV

Origin of Pressure-Induced Polyamo

Figure 2 Specific volume versus pressure for amorphous $Ce_{55}Al_{45}$. Four different

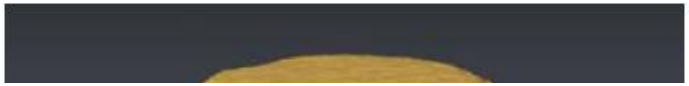
Qiao-shi Zeng,[1,2] Yang Ding,[2] Wendy L. Mao,[1,3,4,5] Wenge Yang,[2,6] Stas. V. Sinogeikin,[6] Jinfu Shu,[7] Ho-kwang Mao,[1,2,6,7] and J. Z. Jiang[1,*]

[1]*International Center for New-Structured Materials and Laboratory of New-Structured Materials, Department of Materials Science and Engineering, Zhejiang University, Hangzhou 310027, China*

[2]*HPSynC, Carnegie Institution of Washington, Argonne, Illinois 60439, USA*

Non-cubic Dependence of Volume on FSDP positon

A



C

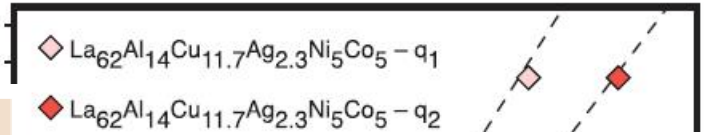
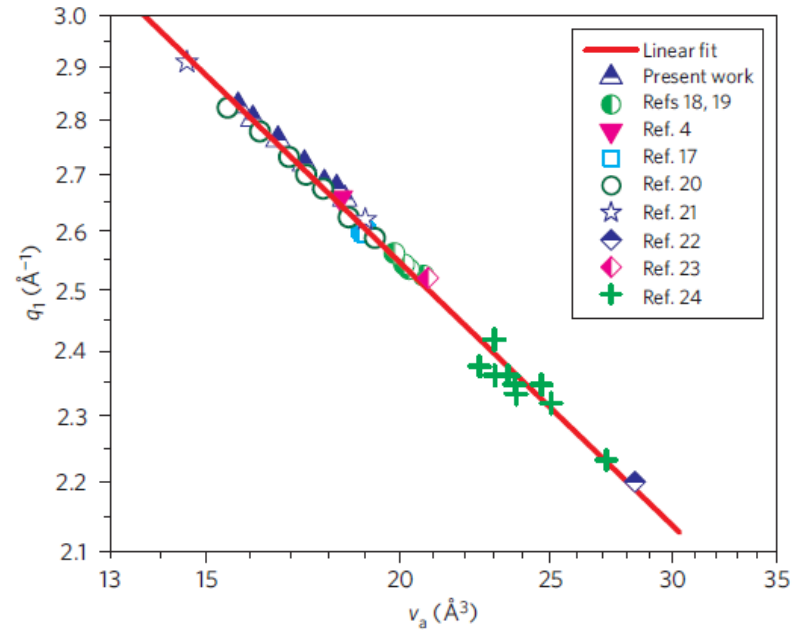


Table 1 | The FSDP position (q_1, Å^{-1}) for metallic glasses determined from neutron (labelled with an asterisk) and X-ray (labelled with a dagger) diffraction measurements.

Metallic glass	q_1	ρ	v_a	$q_1 \cdot v_a^{0.433}$	Reference
$Zr_{35.5}Cu_{64.5}$*	2.826	7.751	15.72	9.32	Present work
$Zr_{38.6}Cu_{61.4}$*	2.801	7.673	16.07	9.32	Present work
$Zr_{44.0}Cu_{56.0}$*	2.763	7.542	16.68	9.35	Present work
$Zr_{50.0}Cu_{50.0}$*	2.719	7.408	17.35	9.35	Present work
$Zr_{54.5}Cu_{45.5}$*	2.684	7.306	17.87	9.35	Present work
$Zr_{60.0}Cu_{40.0}$*	2.656	7.227	18.42	9.38	Present work
$Zr_{53.7}Cu_{28.5}Ni_{19.4}Al_{8.4}$*	2.675	6.824	18.20	9.40	Present work
$Zr_{52.5}Ti_5Cu_{17.9}Ni_{14.6}Al_{10}$*	2.658	6.629	18.30	9.36	Ref. 4
$Zr_{54.5}Ti_{7.5}Cu_{20}Ni_8Al_{10}$†	2.605	6.47	18.85	9.29	Ref. 17
$Zr_{57}Ti_5Cu_{20}Ni_8Al_{10}$†	2.602	6.54	18.92	9.29	Ref. 17
$Zr_{58}Ti_4Cu_{20}Ni_8Al_{10}$†	2.599	6.57	18.94	9.29	Ref. 17
$Zr_{59}Ti_3Cu_{20}Ni_8Al_{10}$†	2.597	6.59	19.00	9.29	Ref. 17
$Zr_{60}Ti_2Cu_{20}Ni_8Al_{10}$†	2.595	6.62	19.02	9.29	Ref. 17
$Zr_{80.0}Fe_{20.0}$†	2.524	6.75	20.71	9.38	Refs 18,19
$Zr_{76.0}Fe_{24.0}$†	2.535	6.78	20.27	9.33	Refs 18,19
$Zr_{75.0}Fe_{25.0}$†	2.543	6.80	20.12	9.33	Refs 18,19
$Zr_{73.0}Fe_{27.0}$†	2.562	6.84	19.83	9.34	Refs 18,19
$Zr_{67.0}Cu_{33.0}$†	2.588	7.07	19.27	9.32	Ref. 20
$Zr_{60.0}Cu_{40.0}$†	2.624	7.19	18.52	9.29	Ref. 20
$Zr_{54.0}Cu_{46.0}$†	2.674	7.31	17.84	9.31	Ref. 20
$Zr_{50.0}Cu_{50.0}$†	2.699	7.39	17.39	9.30	Ref. 20
$Zr_{46.0}Cu_{54.0}$†	2.731	7.47	16.96	9.30	Ref. 20
$Zr_{40.0}Cu_{60.0}$†	2.778	7.64	16.23	9.29	Ref. 20
$Zr_{34.0}Cu_{66.0}$†	2.822	7.83	15.48	9.24	Ref. 20
$Zr_{65}Ni_{35}$†	2.620	6.98	18.99	9.37	Ref. 21
$Ti_{60}Ni_{40}$*,†	2.910	5.96	14.57	9.28	Ref. 21
$La_{62}Al_{14}(Cu_{5/6}Ag_{1/6})_{14}Ni_5Co_5$†	2.20#	6.190	28.36	9.36	Ref. 22
$Mg_{65}Cu_{25}Tb_{10}$†	2.52#	3.790	20.85	9.39	Ref. 23
$Y_{55}Al_{25}Co_{20}$†	2.23#	5.802	27.18	9.32	Ref. 24
$La_{55}Al_{25}Co_{20}$†	2.32#	6.373	25.03	9.35	Ref. 24
$Pr_{55}Al_{25}Co_{20}$†	2.35#	6.584	24.68	9.42	Ref. 24
$Nd_{55}Al_{25}Co_{20}$†	2.33#	7.343	23.76	9.19	Ref. 24
$Gd_{55}Al_{25}Co_{20}$†	2.36#	7.488	23.50	9.26	Ref. 24
$Tb_{55}Al_{25}Co_{20}$†	2.35#	7.560	23.71	9.26	Ref. 24
$Dy_{55}Al_{25}Co_{20}$†	2.42#	7.888	23.00	9.41	Ref. 24
$Ho_{55}Al_{25}Co_{20}$†	2.39#	8.157	22.51	9.20	Ref. 24
$Er_{55}Al_{25}Co_{20}$†	2.36#	4.863	23.03	9.18	Ref. 24

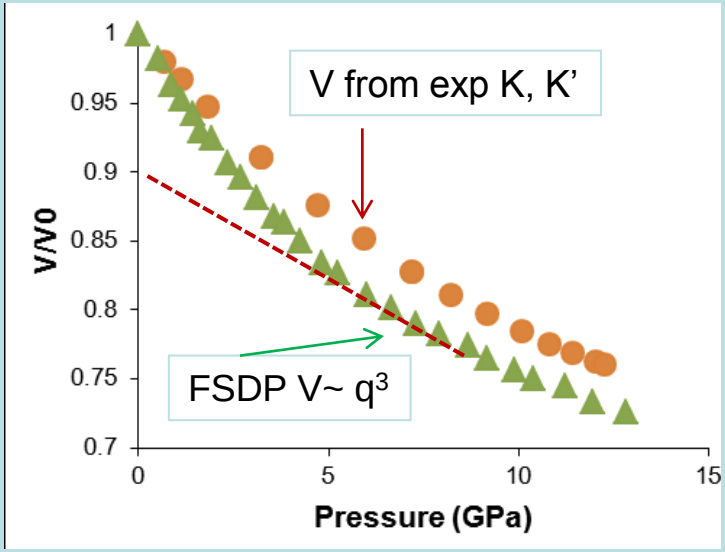


Ma et al., Nature, 2009

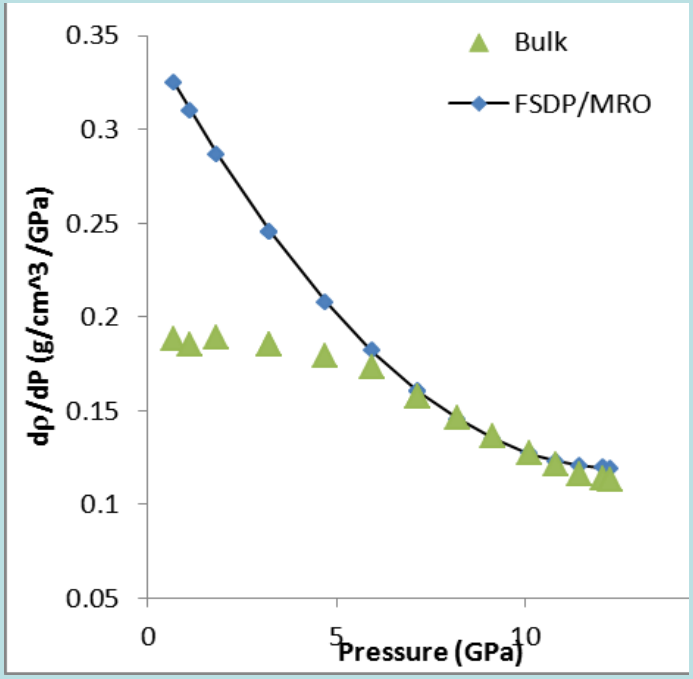
Fractal atomic-level percolation in metallic glasses

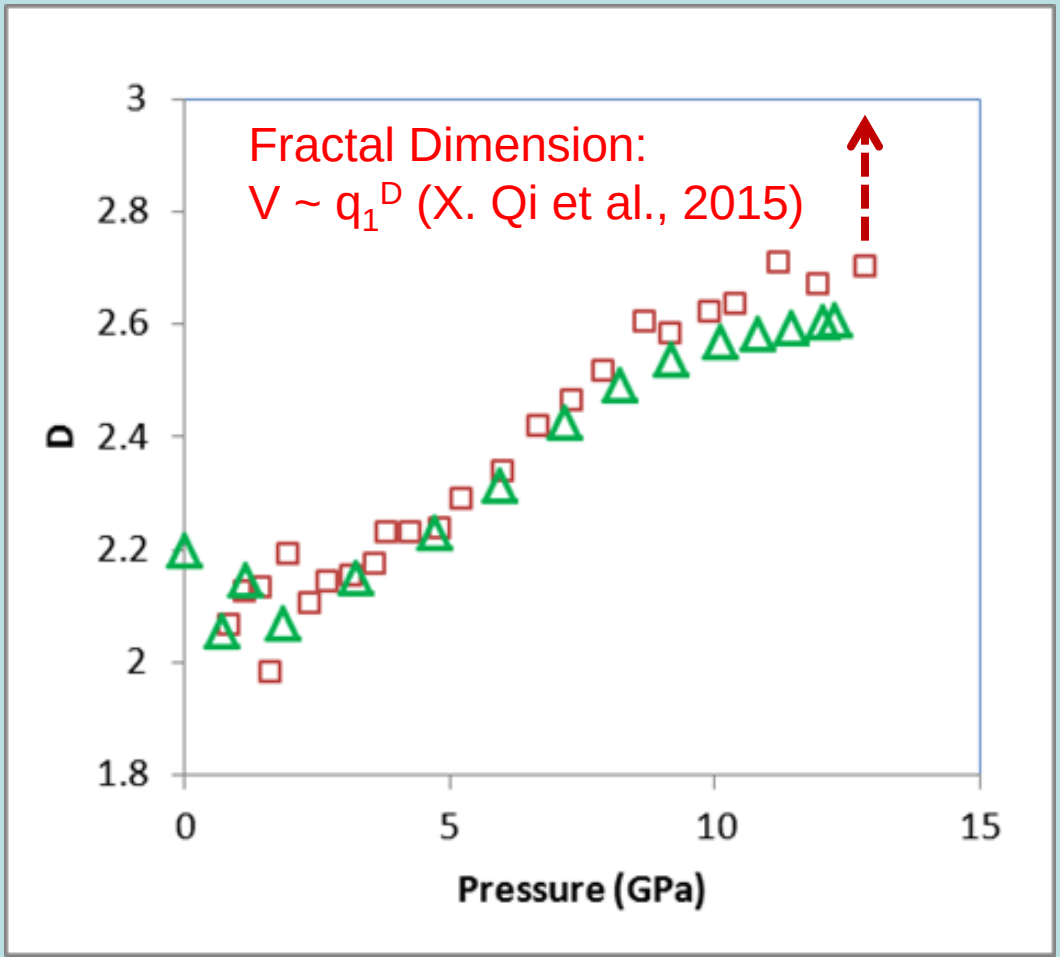
Chen et al., Science, 2015

Pressure Induced Polyamorphism in $(La_{.5}Ce_{.5})_{64}Al_{16}Ni_5Cu_{15}$

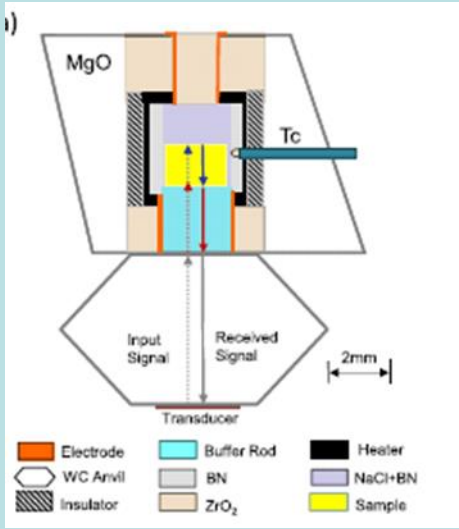


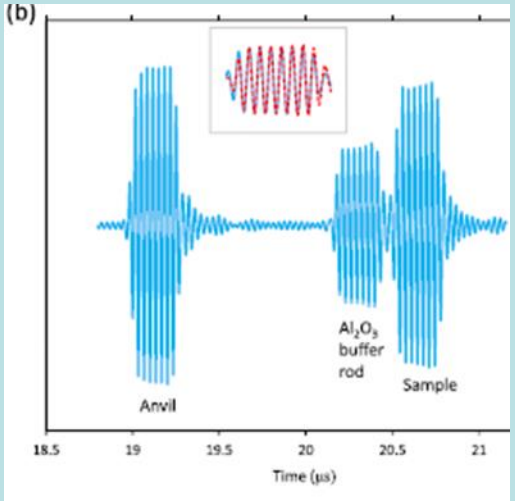
- Medium Range Order (MRO) more compressible
- At ~ 6-7 GPa, MRO and the Bulk equally compressible
- Ce 4f electron delocalization (volume collapse)





Theory for Travel Time Pressure Scale





$$V_S = \sqrt{\frac{G + 1/2\sigma}{\rho}}$$

$$L/L_0 = [L(P) + \Delta L(\sigma)]/\ L_0$$

$$t_S/t_{S0} = A + BP + CP^2$$

with $A = [(2G_0 + \sigma)/(2G_0) \times (1 + \sigma/E)]^{-1/2}$

$$B = \{1/(6K_0) \times [(2G_0 + \sigma)/(2G_0)]^{-1/2} - G'/(2G_0) \times [(2G_0 + \sigma)/(2G_0)]^{-3/2}\} \times (1 + \sigma/E)^{-1/2}$$

$$C = \{-5/(72K_0^2) \times [(2G_0 + \sigma)/(2G_0)]^{-1/2} - G'/(12K_0G_0) \times [(2G_0 + \sigma)/(2G_0)]^{-3/2} + 3G'^2/(8G_0^2) \times [(2G_0\} + \sigma)/(2G_0)^{-5/2} \times (1 + \sigma/E)^{-1/2}$$

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Acoustic travel time gauges for *in-situ* determination of pressure and temperature in multi-anvil apparatus

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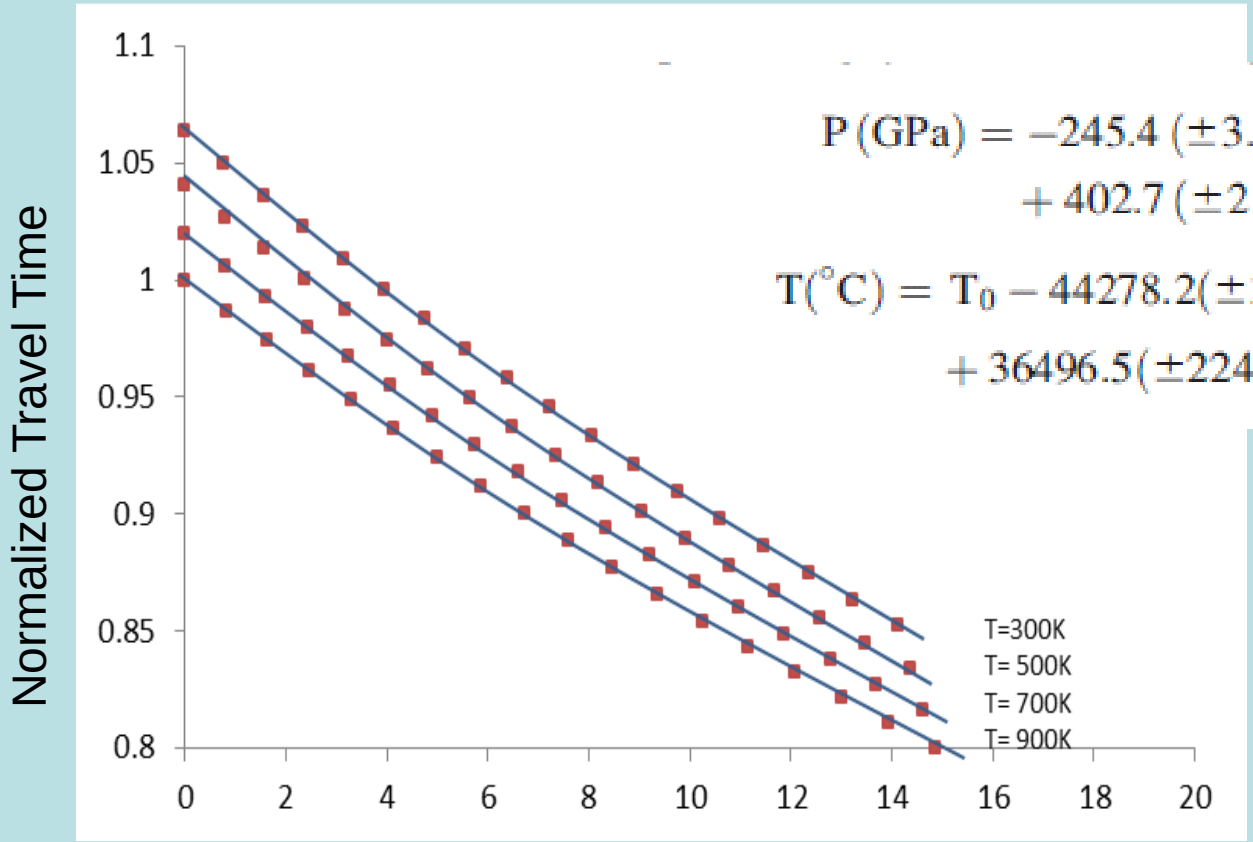
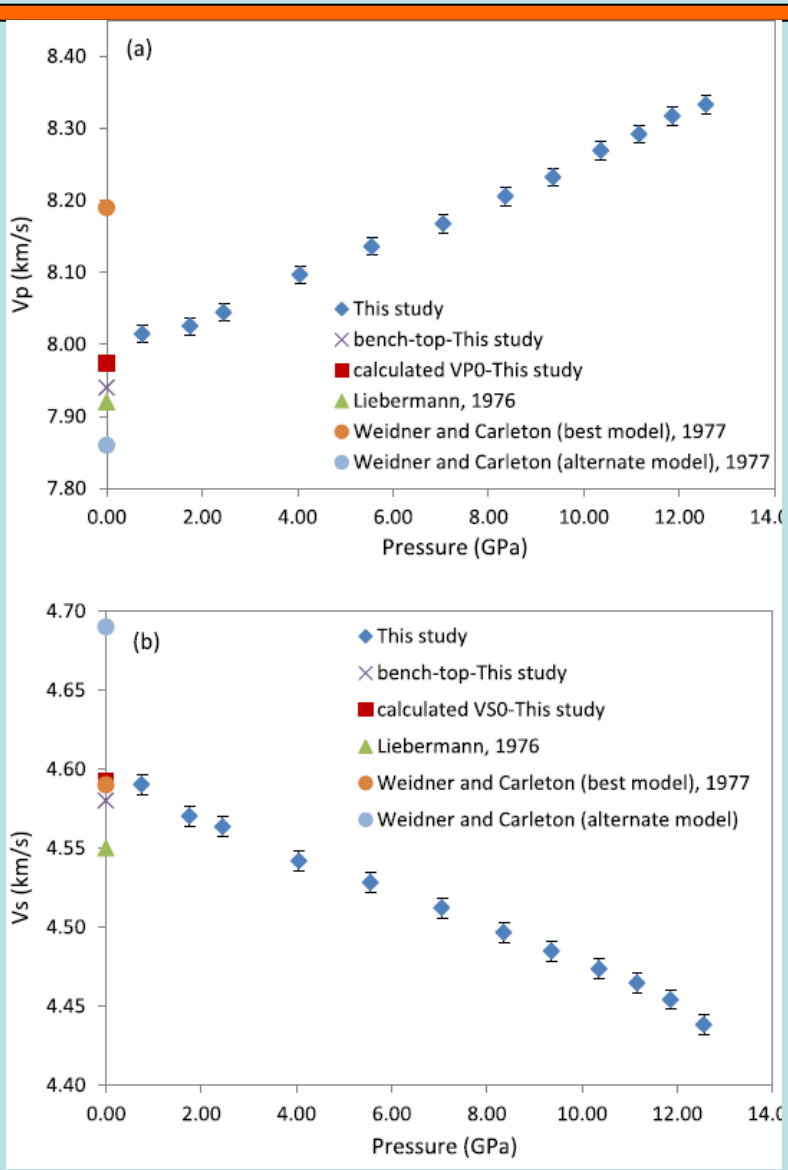


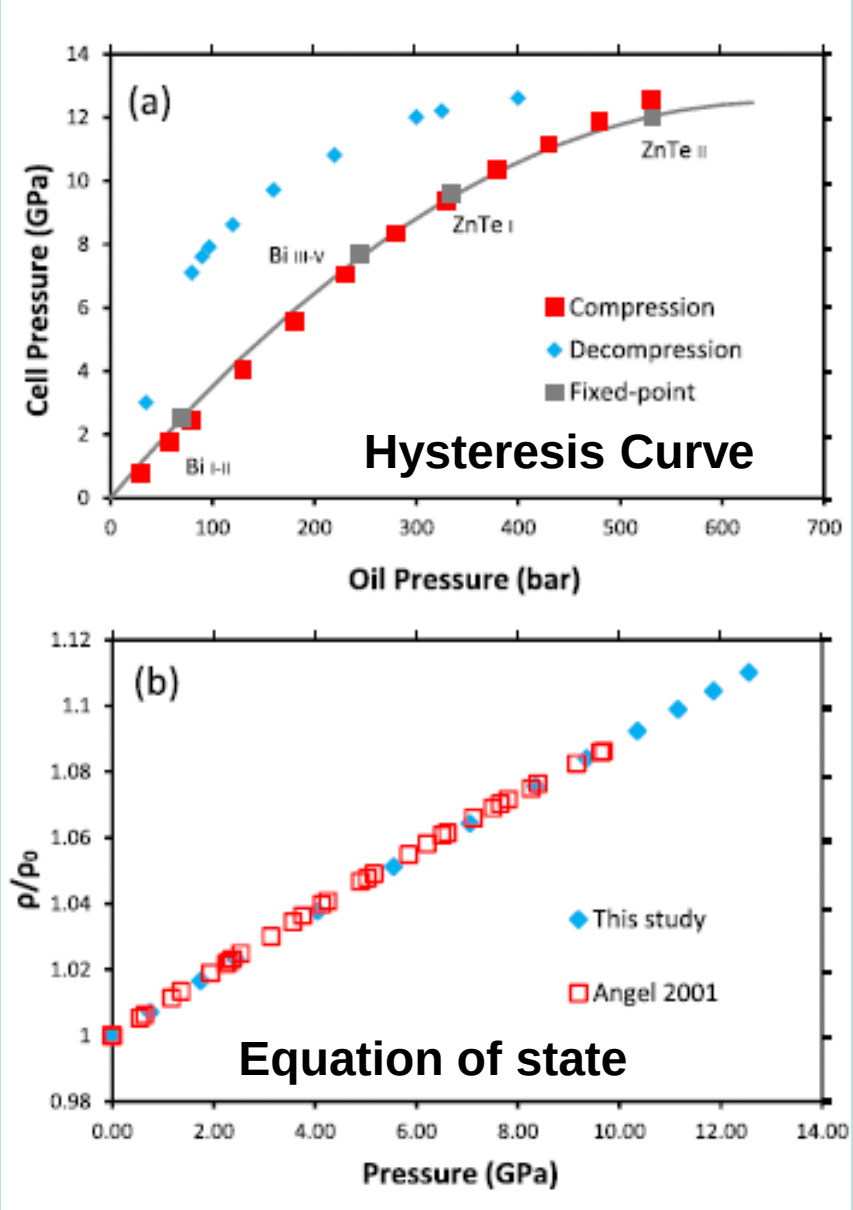
$$P\,(\mathrm{GPa}) = -245.4\,(\pm 3.4) \times (1 - t_S/t_{S0}) + 402.7\,(\pm 2.1) \times (1 - t_P/t_{P0}),$$

$$T(^\circ\mathrm{C}) = T_0 - 44278.2(\pm 353.6) \times (1 - t_S/t_{S0}) + 36496.5(\pm 224.6) \times (1 - t_P/t_{P0}).$$

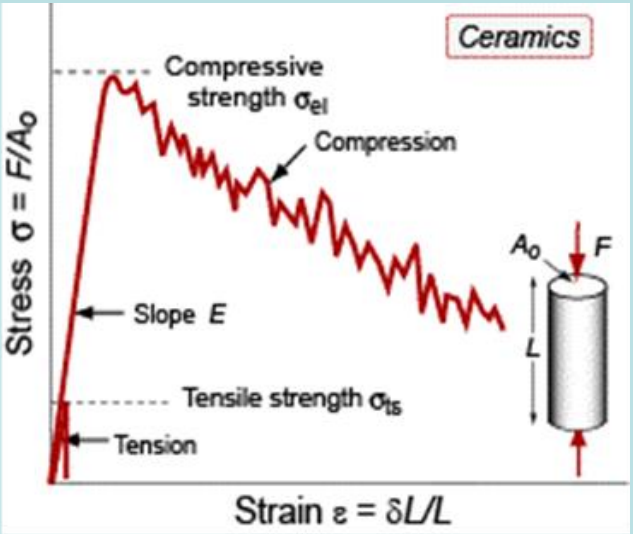
Application of the New Travel Time Pressure Scale



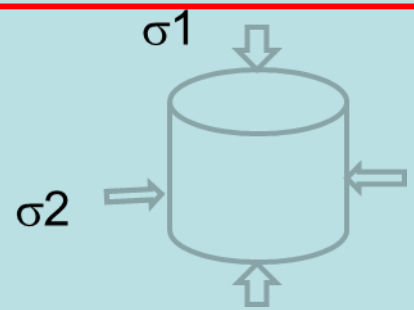
T. Chen et al., EPSL, 2015



X. Wang et al., J. App Phy., 2015

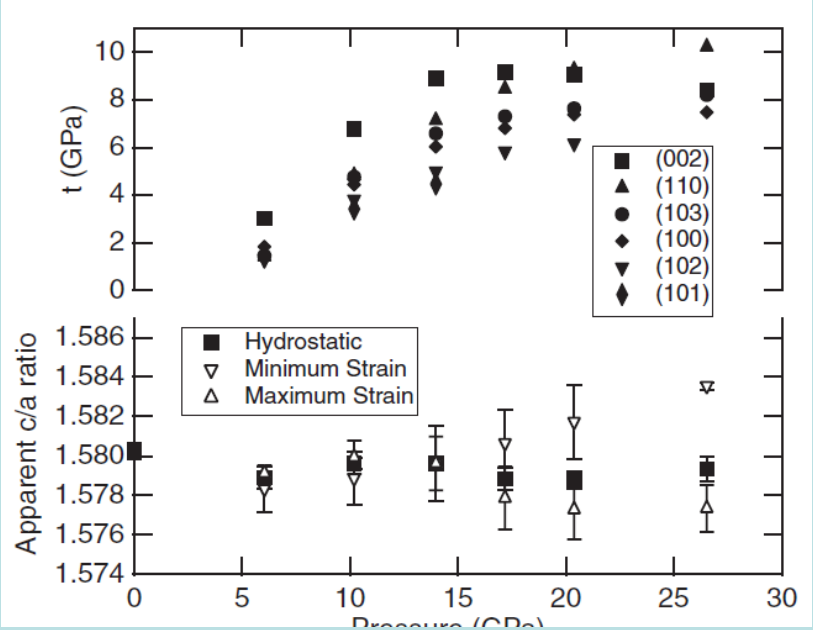


Stress States under Pressure

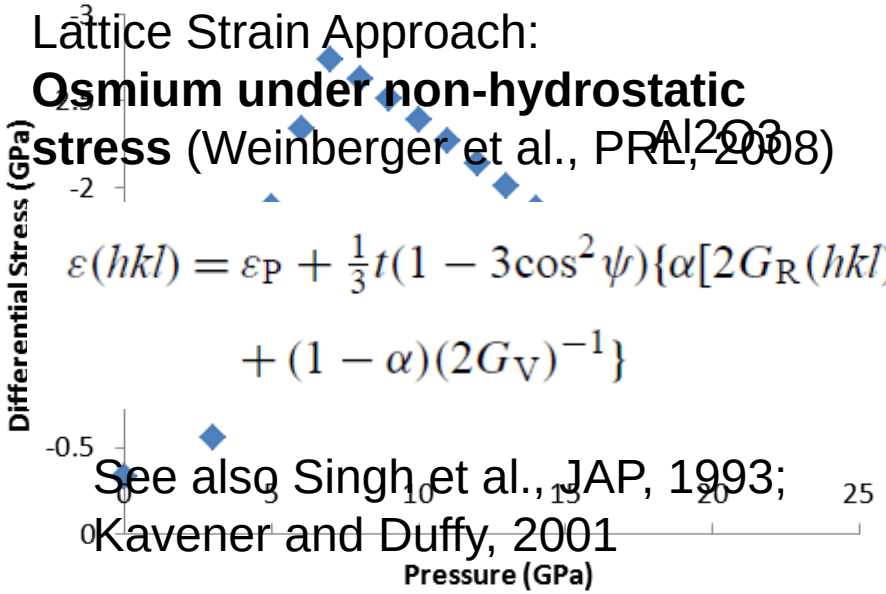


Linear Elasticity Stress-Strain Relation:
K, G from velocity measurements

$$\sigma_{ii}=(K-2G/3)(\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33})+2G\varepsilon_{ii}$$



Lattice Strain Approach:
Osmium under non-hydrostatic stress (Weinberger et al., PRL, 2008)



$$\varepsilon(hkl) = \varepsilon_P + \tfrac{1}{3}t(1-3\cos^2\psi)\{\alpha[2G_R(hkl)]^{-1} + (1-\alpha)(2G_V)^{-1}\}$$

See also Singh et al., JAP, 1993; Kavener and Duffy, 2001

Summary of Activities and Objectives

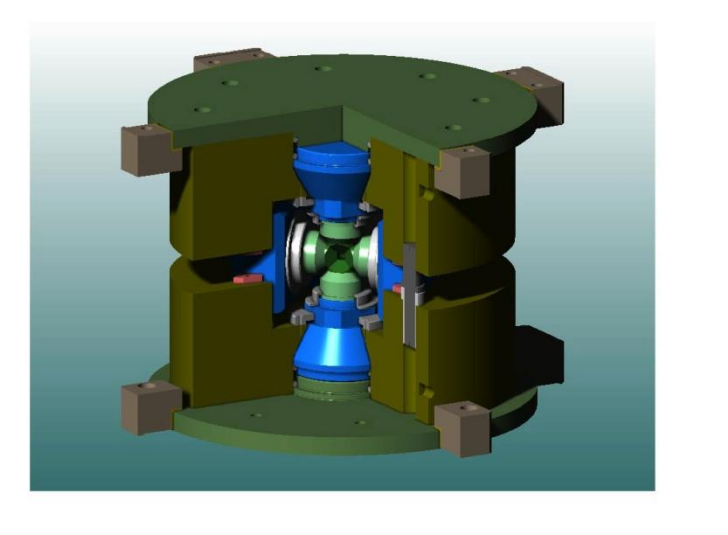
- **Sound velocities** of transition metals and alloys have been studied at high pressure and high temepratures using ultrasonic and X-ray studies, the derived elasticity, K, G, $\partial K/\partial P$, $\partial G/\partial P$, dK/dT, dG/dT contribute to those databases maintained at national labs for SSP studies. .

- **New methods** have been developed to characterize sample pressure , stress-strain, yield strength, nonlinear elasticity of materials; we will continue to improve and apply these methods to other materials.

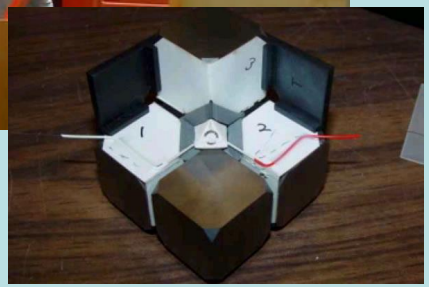
- **Measurements at higher pressures (P> 30 GPa).** We continue to apply these measurements to lanthanides (Ce, Pr, Gd, …) to bridge the gap between static [multi-anvil and DAC] and dynamic [shock] high-pressure experiments.

- **Education and training** for the 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.

Our Tools at SBU



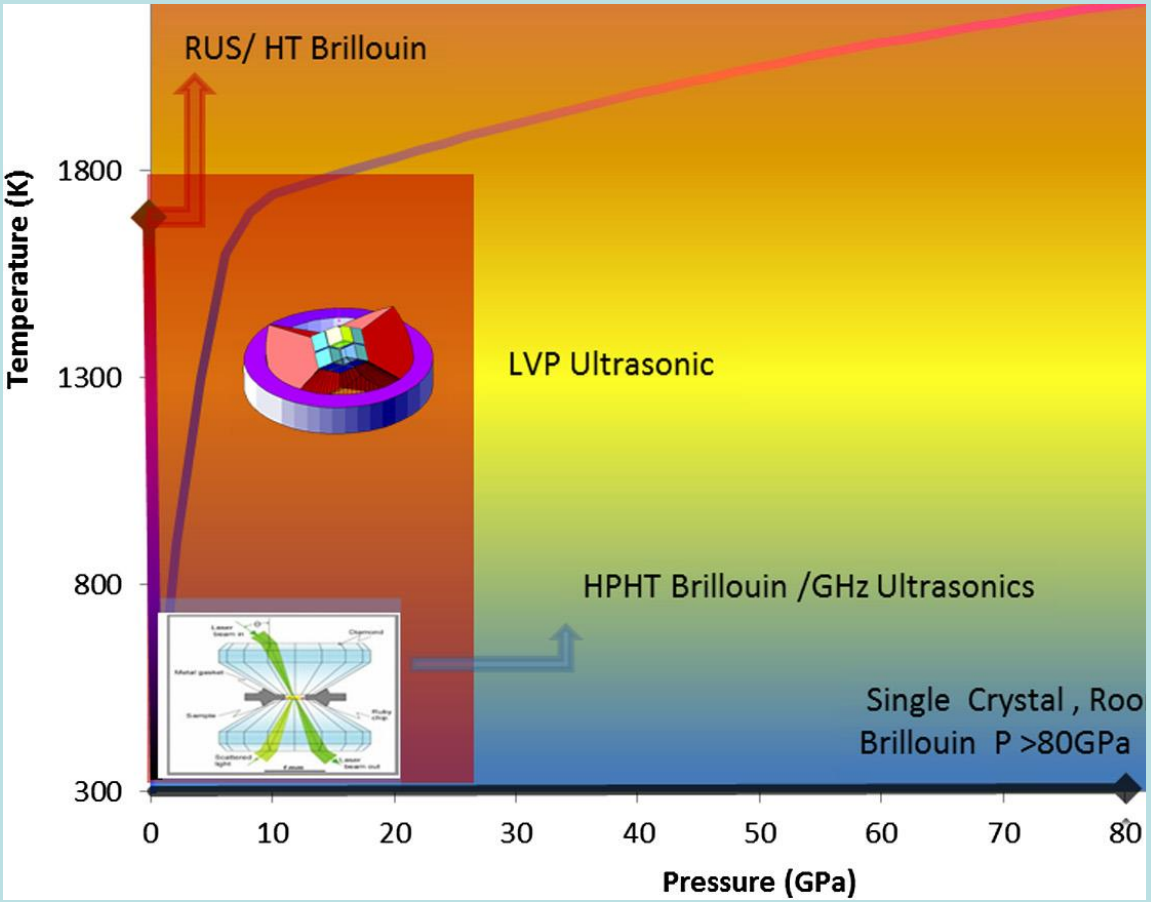
Single Stage, Boron Epoxy Pressure Medium, mm sized Sample, P <20 GPa T<1800K



Double Stage MA-8
MgO Pressure Medium
P <30 GPa, T<2500K
Sample 5-100 mm^3

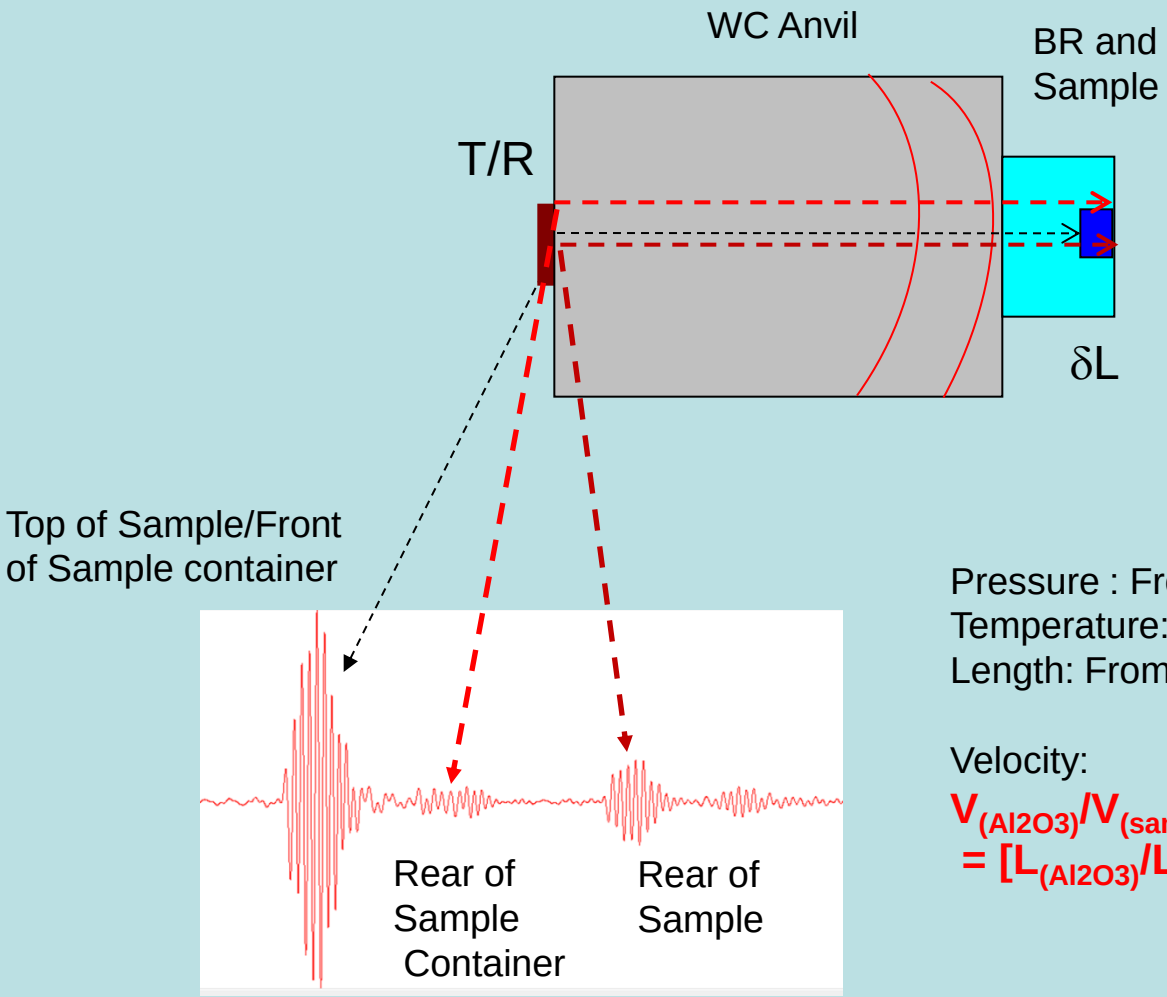
DAC, Liquid or solid
Pressure Medium
P to Mbar pressures
sub-millimeter sampl

Pressures and Temperature Range of the Current SSP Project Using LVP Ultrasonics



Review paper by Li and Liebermann (2014)

Simultaneous Pressure, Length and Travel Time Determination in Multi-Anvil High Pressure Apparatus at high P and T



Pressure : From travel time of buffer rod
Temperature: W-Re Thermocouple
Length: From Al2O3 around sample

Velocity:

$$V_{(Al2O3)}/V_{(sample)} = [L_{(Al2O3)}/L_{(Sample)}]*[(t_{(sample)}/t_{(al2o3)}]$$

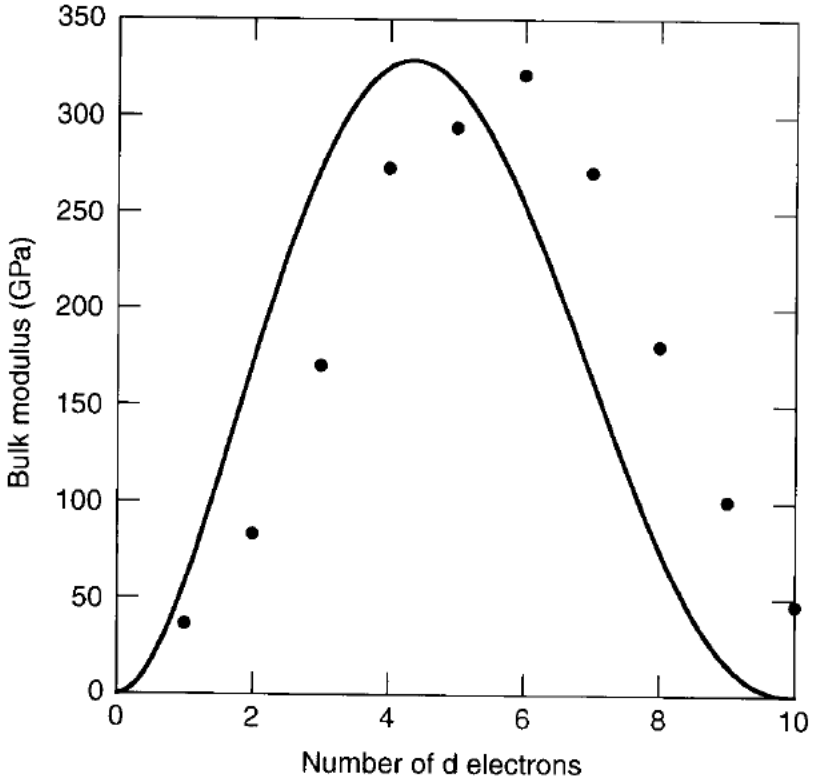


Fig. 2.5. Bulk modulus of the 4d transition metals (symbols) compared with the prediction of the second-moment Friedel model (line). All 4d transition metals are included regardless of structure because differences among structures are small compared with the effects of d-band filling.

L. Stixrude - 2001