High Pressure Science and Engineering Center (HiPSEC) at UNLV

Andrew Cornelius
UNLV Dept. Physics & Astronomy

UNLV
UNIVERSITY OF NEVADA LAS VEGAS

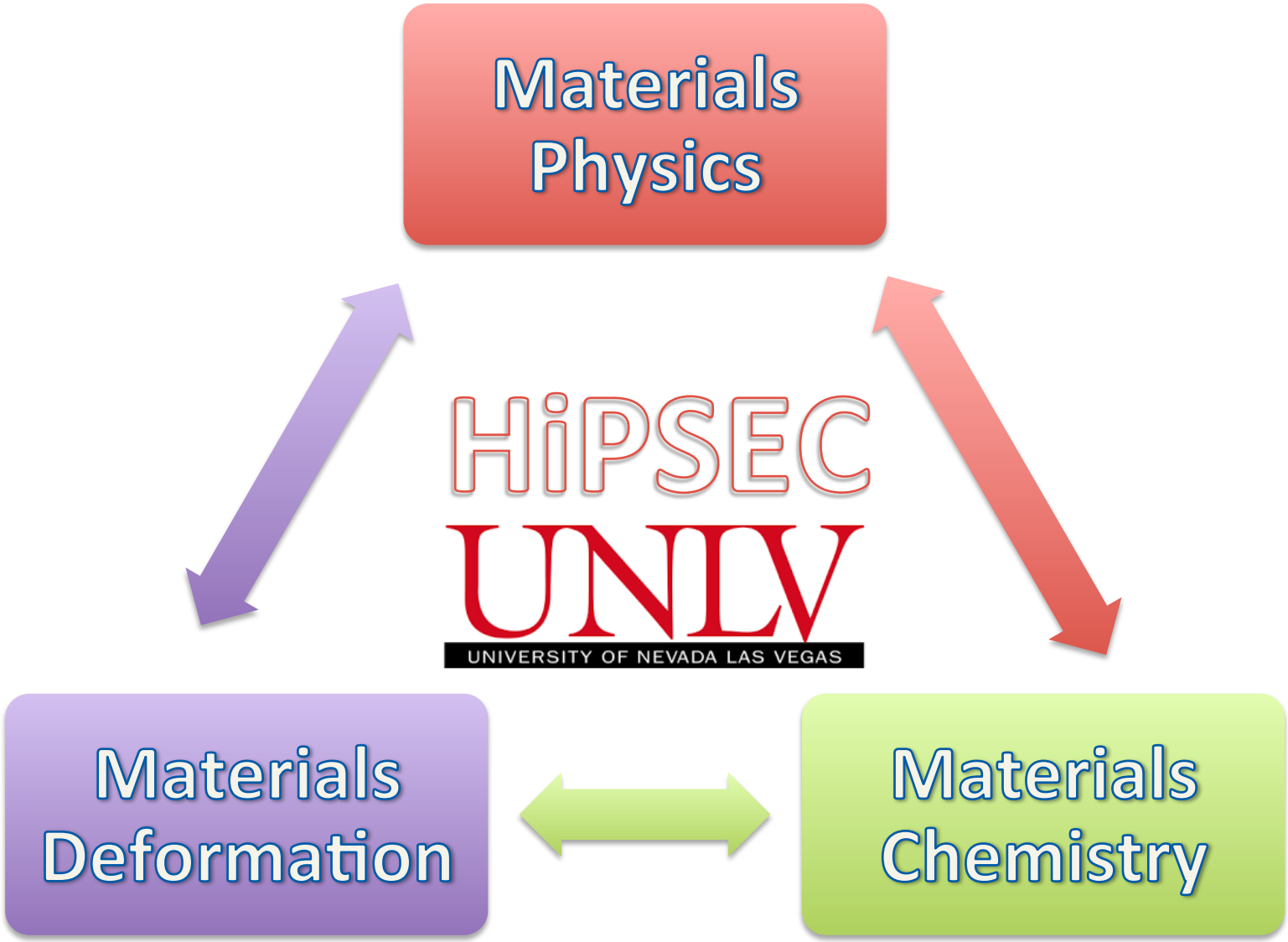
NNSA
National Nuclear Security Administration

HiPSEC, a DOE/NNSA Center of Excellence

University of Nevada, Las Vegas

https://hipsec.unlv.edu/

- HiPSEC started in 1998
  - one of ~8 SSAA Centers of Excellence
- 13 faculty - 8 postdocs
- 18 graduate students - 20+ undergraduates


Materials Physics
HiPSEC
UNLV
UNIVERSITY OF NEVADA LAS VEGAS
Materials Deformation
Materials Chemistry

Materials Physics

Changfeng Chen

Andrew Cornelius

Ravhi Kumar

Jinlong Zhu

Materials Chemistry

Paul Forster

Michael Pravica

Barbara Lavina

Ashkan Salamat

Materials Deformation

Oliver Tschauner

Pamela Burnley

Liping Wang

Qiang Zhu

New Assistant Professor of Condensed Matter Physics

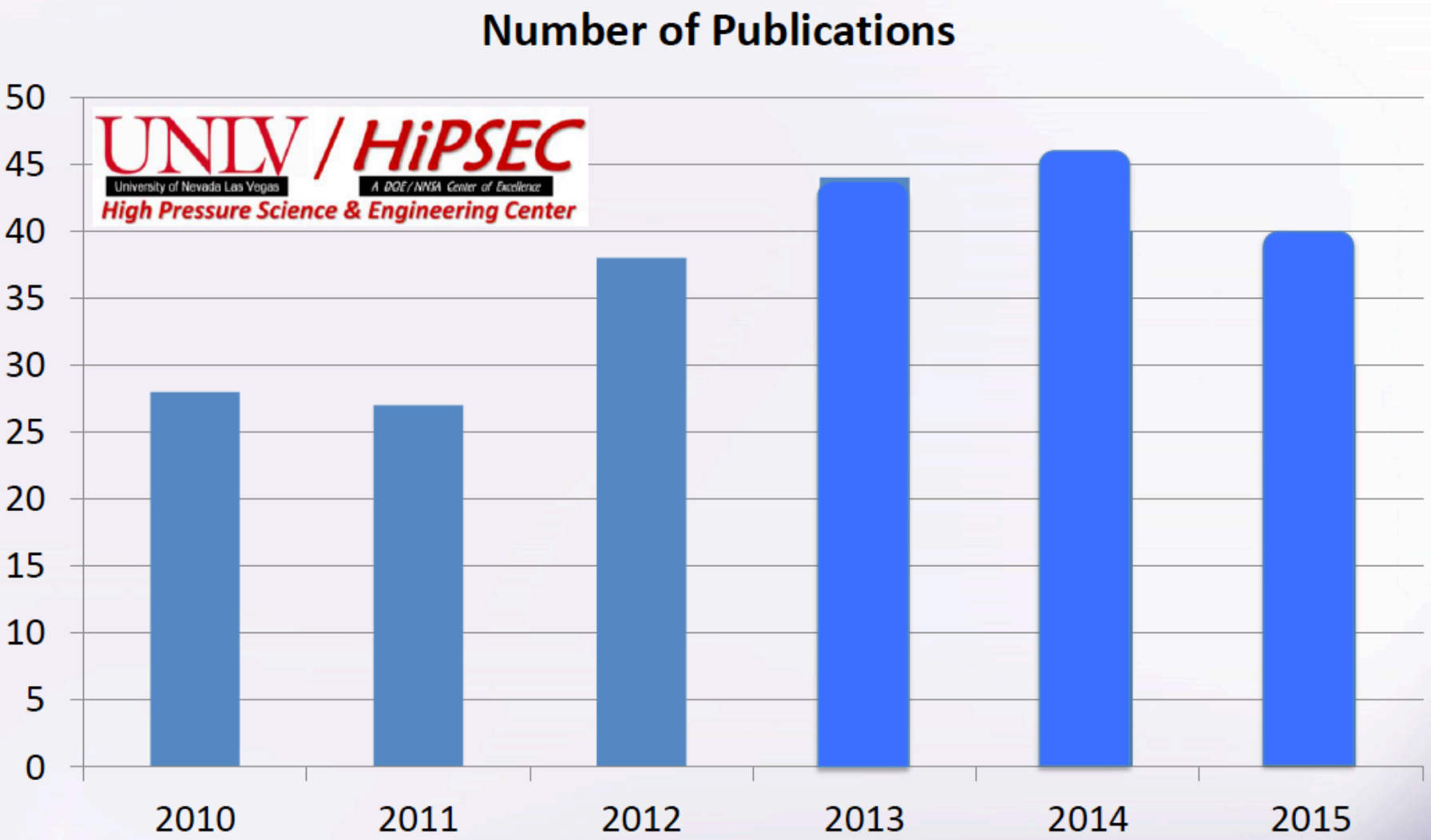
Joint NSTec-UNLV Professor of Shock Physics

Qiang Zhu (Stony Brook University)

Average Annual HiPSEC Training at HPCAT Since 2013

- 1 shift = 8 hours
- Total UNLV Beamtime ~ 100 days
- Time at HPCAT
  - Postdocs - 42 days
  - Graduate students 97 days
  - Undergraduate students 32 days

UNLV HiPSEC Publication Statistics



Materials Genome Initiative

Materials Physics

Inorganic Chemistry

Article

pubs.acs.org/IC

Effect of Pressure on Valence and Structural Properties of $YbFe_2Ge_2$ Heavy Fermion Compound—A Combined Inelastic X-ray Spectroscopy, X-ray Diffraction, and Theoretical Investigation

Ravhi S. Kumar,[*,†] Axel Svane,[§] Ganapathy Vaitheeswaran,[∥] Venkatakrishnan Kanchana,[⊥] Daniel Antonio,[†] Andrew L. Cornelius,[†] Eric D. Bauer,[‡] Yuming Xiao,[#] and Paul Chow[#]

[†]Department of Physics and Astronomy and HiPSEC, University of Nevada Las Vegas, Las Vegas, Nevada 89154, United States

[‡] Los Alamos National Laboratory, P.O. Box 1663, MS K764, Los Alamos, New Mexico 87545, United States

[§]Department of Physics and Astronomy, Aarhus University, DK-8000 Aarhus C, Denmark

[∥] Advanced Centre of Research in High Energy Materials (ACRHEM), University of Hyderabad, Gachibowli, Hyderabad – 500 046, Telengana, India

[⊥]Department of Physics, Indian Institute of Technology Hyderabad, Ordnance Factory Estate, Yeddumailaram – 502 205, Telengana, India

[#]HPCAT, Carnegie Institution of Washington and Advance Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, United States

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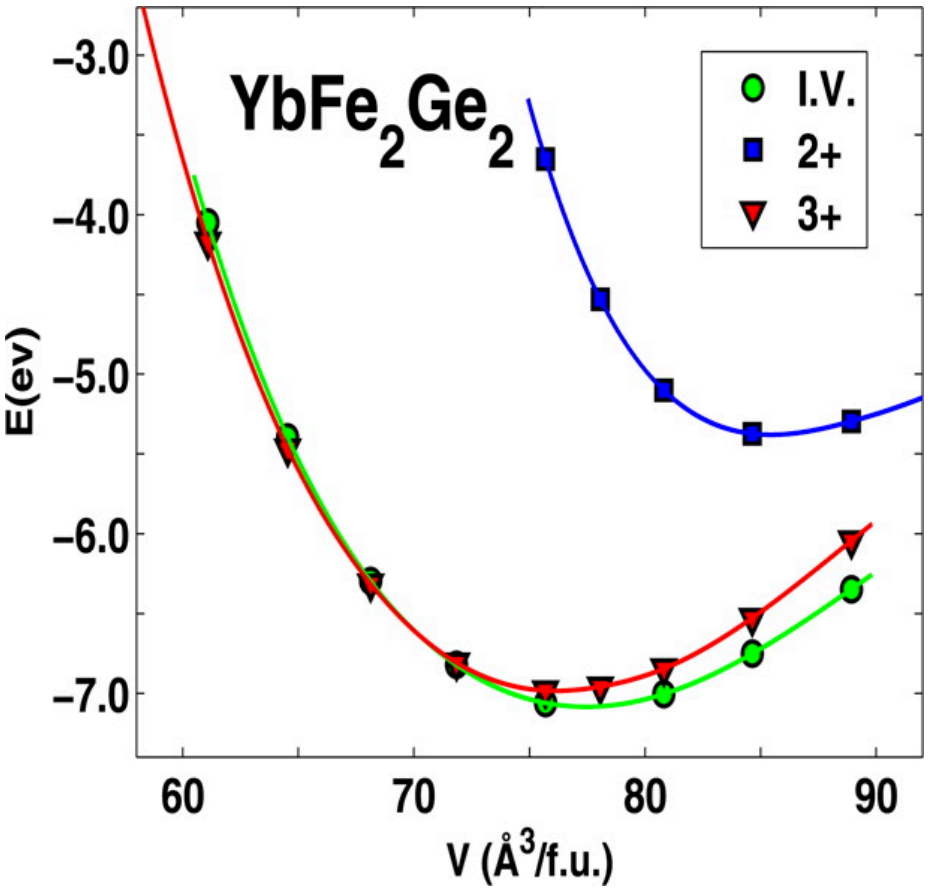
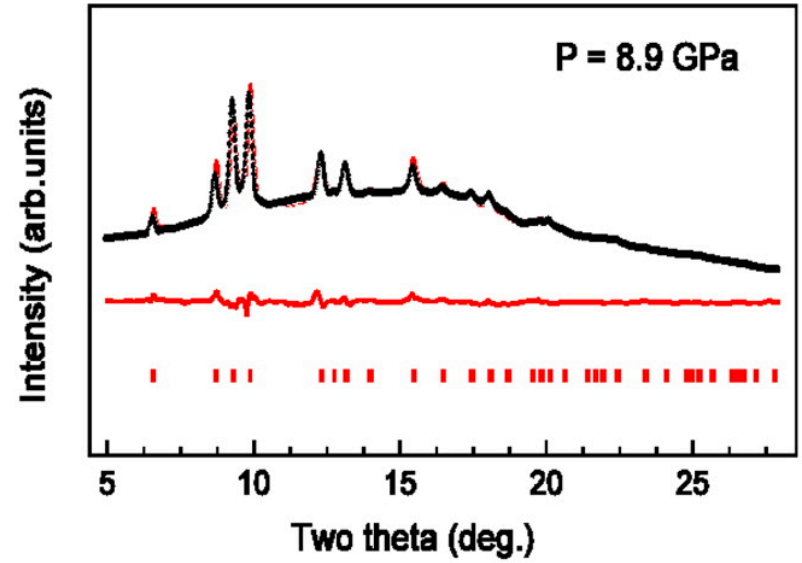
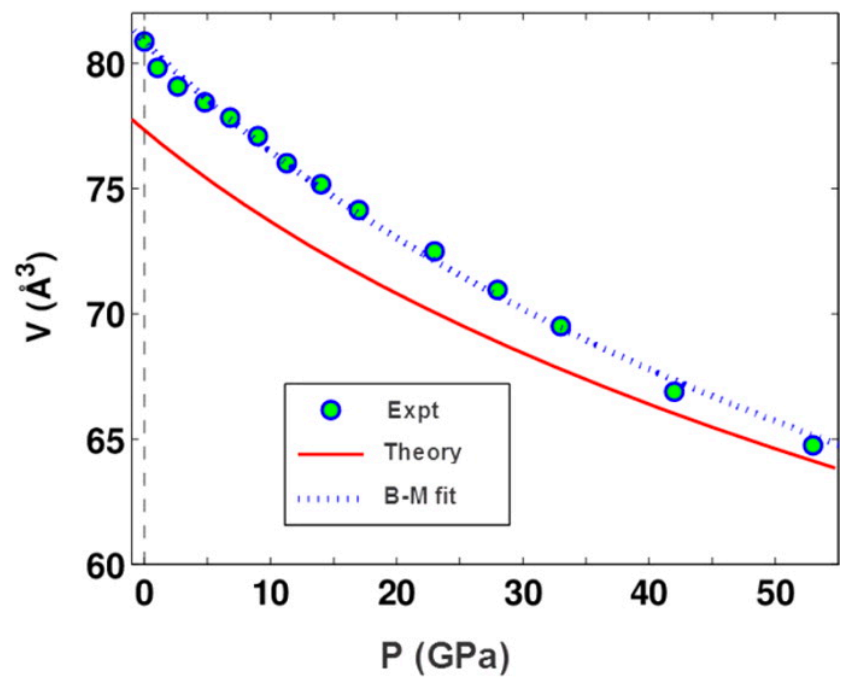
DOI: 10.1021/acs.inorgchem.5b01534
Inorg. Chem. 2015, 54, 10250−10255

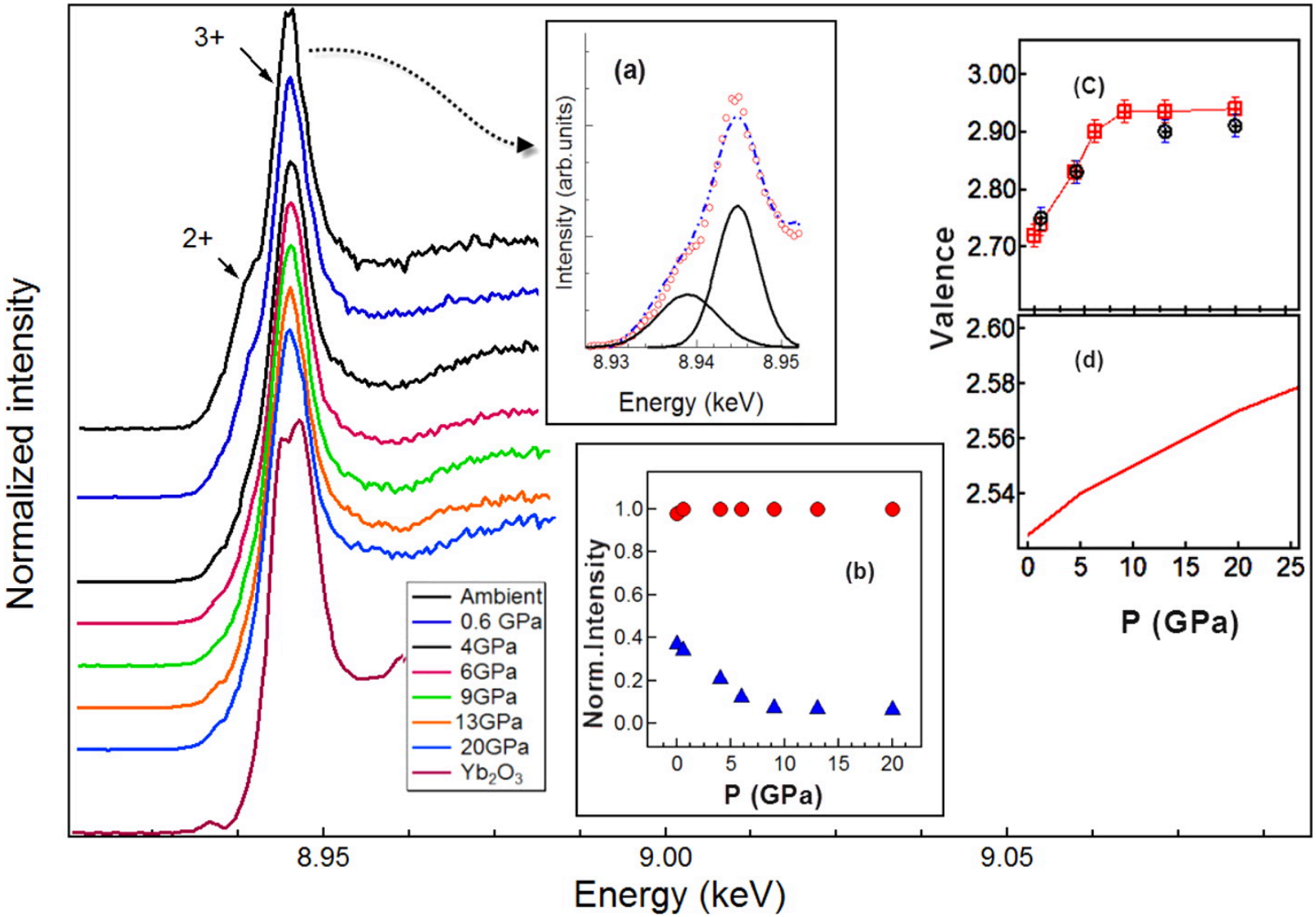
$YbFe_2Ge_2$


YbFe2Ge2
I.V.
2+
3+
E(ev)
V (Å3/f.u.)
−3.0
−4.0
−5.0
−6.0
−7.0
60
70
80
90


P = 8.9 GPa
Intensity (arb.units)
Two theta (deg.)
5
10
15
20
25


Expt
Theory
B-M fit
V (Å3)
P (GPa)
60
65
70
75
80
0
10
20
30
40
50

$YbFe_2Ge_2$


3+
2+
Normalized intensity
Energy (keV)
8.95
9.00
9.05
Ambient
0.6 GPa
4GPa
6GPa
9GPa
13GPa
20GPa
Yb2O3
(a)
Intensity (arb.units)
8.93
8.94
8.95
Energy (keV)
(b)
Norm.Intensity
P (GPa)
(C)
(d)
Valence
P (GPa)

UNLV Materials Deformation

RESEARCH ARTICLE

GEOPHYSICS

Unraveling the complexity of iron oxides at high pressure and temperature: Synthesis of Fe_5O_6

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10.1126/sciadv.1400260

Barbara Lavina[1]* and Yue Meng[2]

[1]High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Las Vegas, NV 89154–4002, USA. [2]High Pressure Collaborative Access Team, Carnegie Institution of Washington, Argonne, IL 60439–4803, USA.
*Corresponding author. E-mail: lavina@physics.unlv.edu

parable unit cell parameters, we performed multiple syntheses and purposely searched for micrometer-sized crystal grains. Therefore, our structural determination is based on the larger grains for which the diffraction effects could be isolated in the three dimensions of the reciprocal space.

observed in Fe_4O_5 (*2*). The two octahedra appear to differ significantly

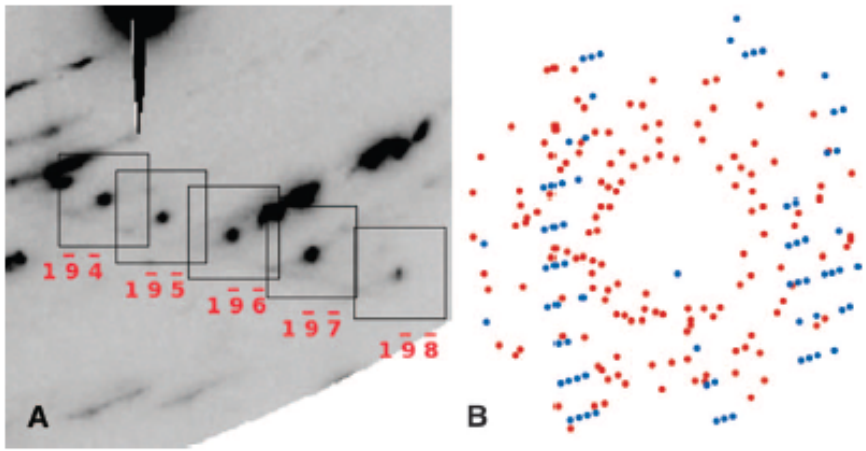


Fig. 1. Row of reflections of an Fe_5O_6 crystal in a multiphase diffraction pattern. (**A**) Detail of an x-ray diffraction pattern collected at 18 GPa, highlighting an indexed row of peaks belonging to an Fe_5O_6 crystal. (**B**) In a projection in the reciprocal space of all reflections, those belonging to the Fe_5O_6 grain are shown in blue.

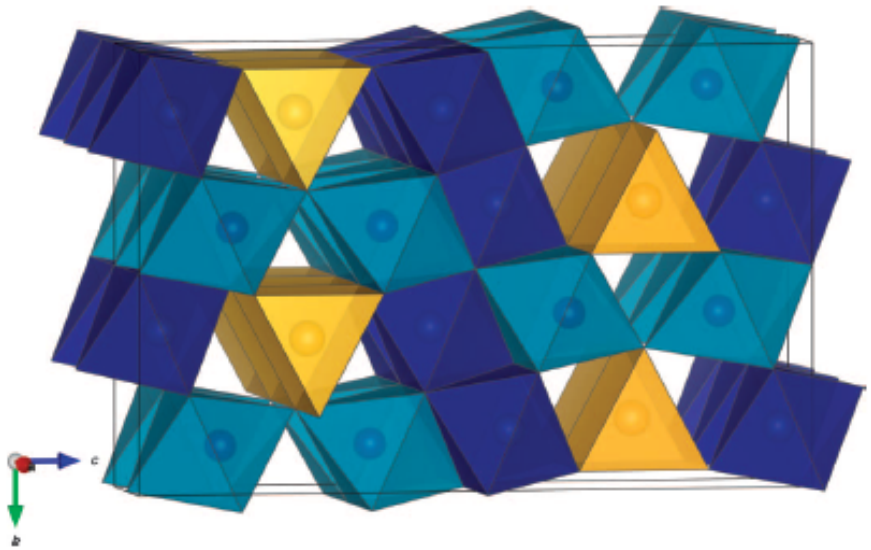


Fig. 2. The structure of Fe_5O_6. The trigonal prisms representing the coordination environment of iron in the *4c* position are shown in yellow. Layers of edge-sharing coordination octahedra of iron in the *8f* positions are shown in two shades of blue representing two non-equivalent crystallographic sites.

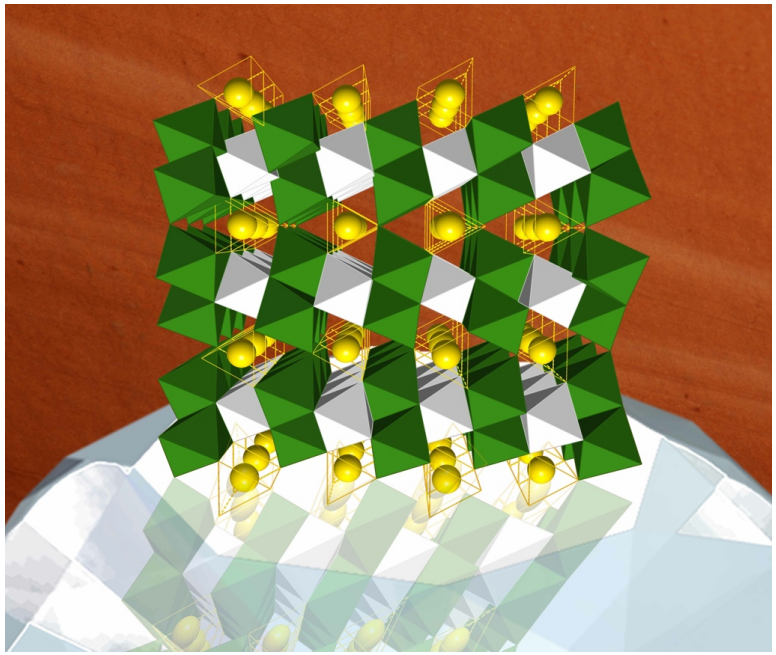
$Fe + 2Fe_2O_3 \rightarrow Fe_5O_6$ by pressurizing at 10-20 GPa and IR laser heating to 2300 K

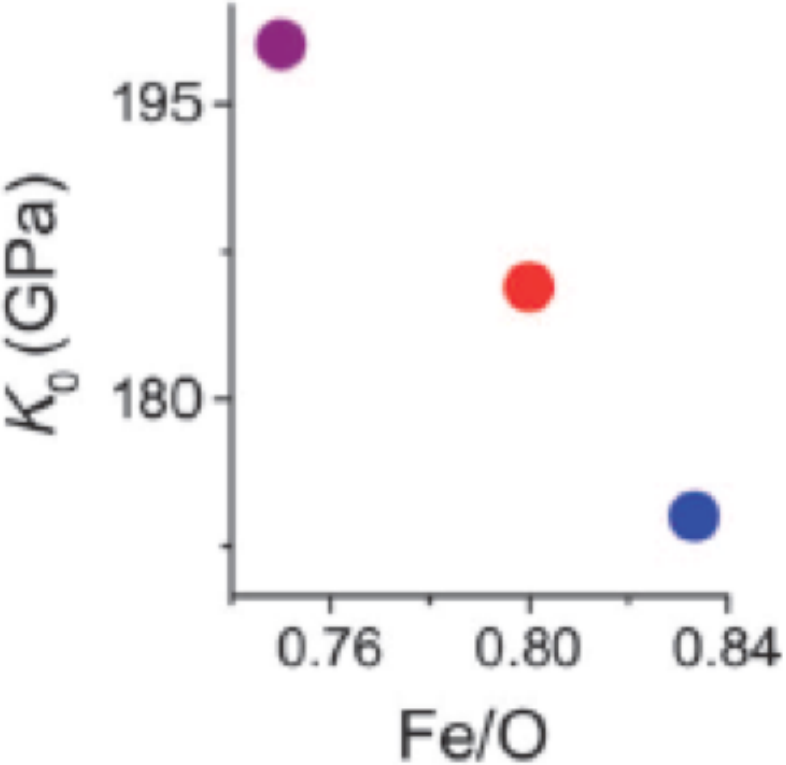
Discovery of the recoverable high-pressure iron oxide Fe_4O_5

Barbara Lavina[a,b,1], Przemyslaw Dera[c], Eunja Kim[b], Yue Meng[d], Robert T. Downs[e], Philippe F. Weck[f], Stephen R. Sutton[c], and Yusheng Zhao[a,b]

[a]High Pressure Science and Engineering Center, University of Nevada, Las Vegas, NV 89154; [b]Department of Physics and Astronomy, University of Nevada, Las Vegas, NV 89154; [c]GeoSoilEnviroCARS, Center for Advanced Radiation Sources, University of Chicago, Argonne, IL 60439; [d]High Pressure Collaborative Access Team, Carnegie Institution of Washington, Argonne, IL 60439; [e]Geosciences, University of Arizona, Tucson, AZ 85721-0077; and [f]Department of Chemistry, University of Nevada, Las Vegas, NV 89154

PNAS | **October 18, 2011** | vol. 108 | no. 42 | **17281–17285**





UNLV Materials Chemistry

Journal of Physics and Chemistry of Solids 95 (2016) 6–11

Contents lists available at ScienceDirect

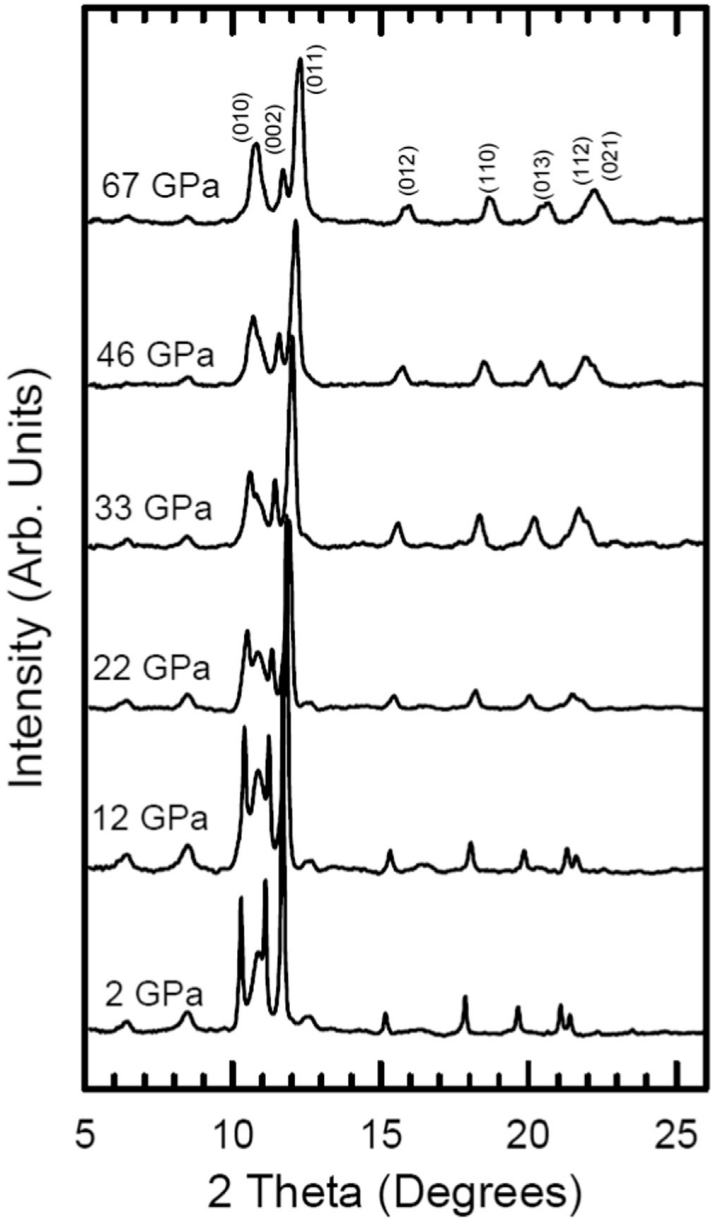
Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs

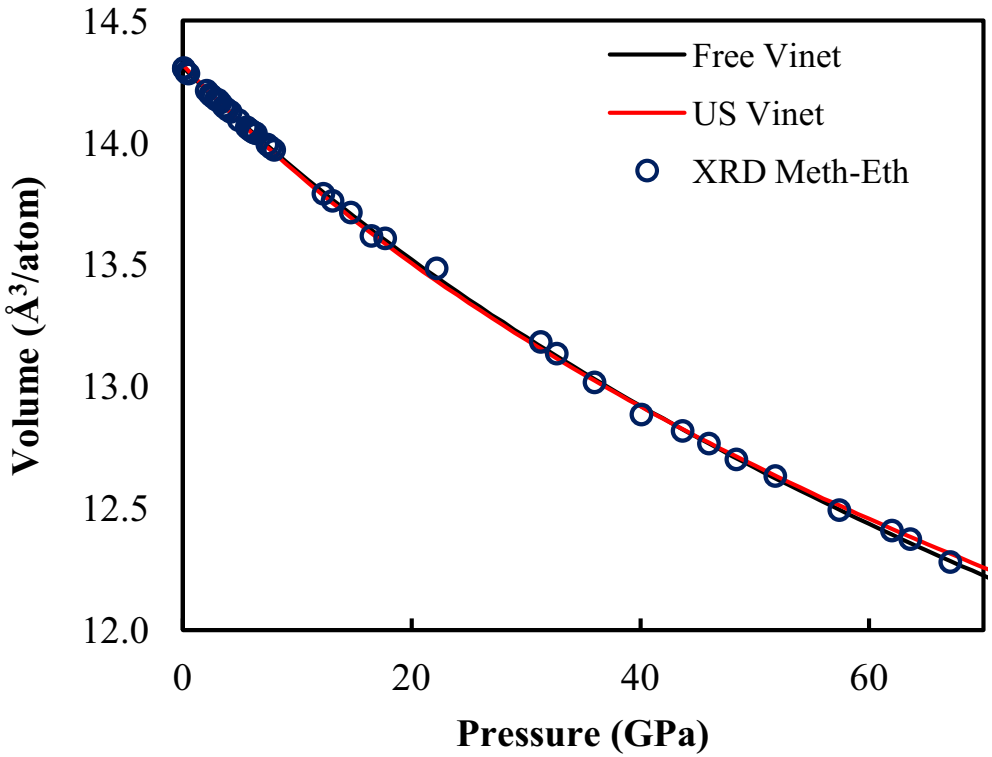
Equation of state for technetium from X-ray diffraction and first-principle calculations

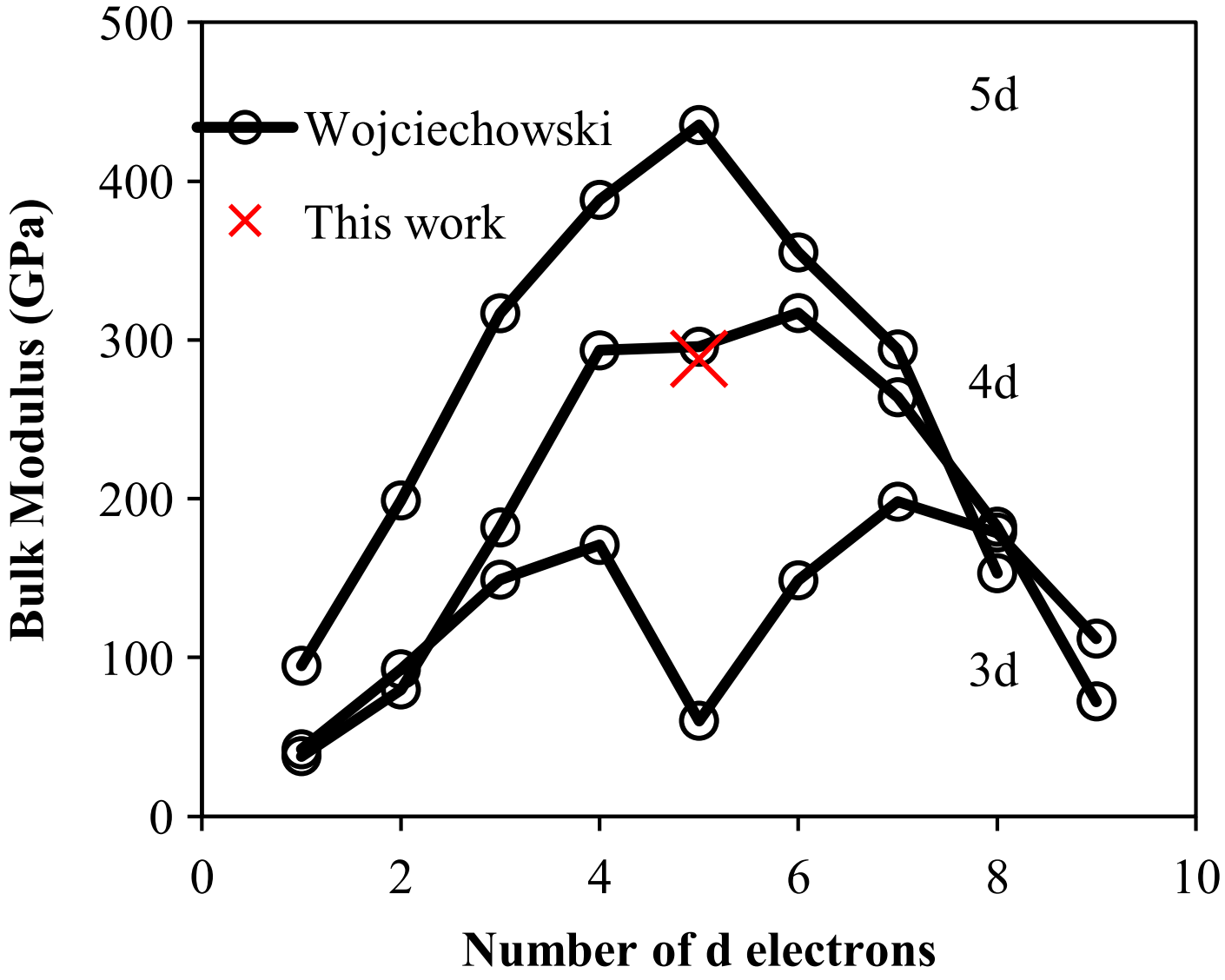
Daniel S. Mast [a,c], Eunja Kim [b], Emily M. Siska [a,c], Frederic Poineau [a], Kenneth R. Czerwinski [a], Barbara Lavina [b,c], Paul M. Forster [a,c,*]

[a] Department of Chemistry and Biochemistry, University of Nevada Las Vegas, Las Vegas 89154-4003, USA
[b] Department of Physics and Astronomy, University of Nevada Las Vegas, Las Vegas 89154-4003, USA
[c] High Pressure Science and Engineering Center, University of Nevada Las Vegas, Las Vegas 89154, USA



a) EOS of technetium




500
400
300
200
100
0
0
2
4
6
8
10
Bulk Modulus (GPa)
Number of d electrons
Wojciechowski
This work
5d
4d
3d

HiPSEC Involvement at HPCAT

Development and Student Involvement

Development at HPCAT - Cryostats

PHYSICAL REVIEW B **69**, 014515 (2004)

Anisotropic elastic properties of $CeRhIn_5$

Ravhi S. Kumar, H. Kohlmann, B. E. Light, and A. L. Cornelius
Department of Physics, University of Nevada, Las Vegas, Nevada 89154-4002, USA

V. Raghavan, T. W. Darling, and J. L. Sarrao
Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
(Received 16 May 2003; revised manuscript received 8 October 2003; published 29 January 2004)

APPLIED PHYSICS LETTERS **99**, 061913 (2011)

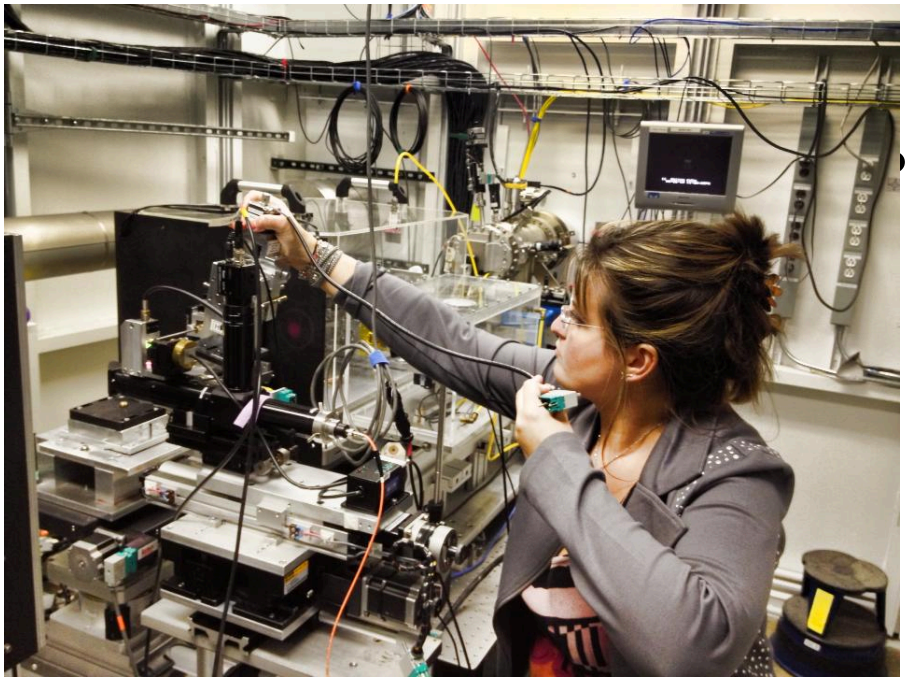
Pressure induced high spin-low spin transition in FeSe superconductor studied by x-ray emission spectroscopy and ab initio calculations

Ravhi S. Kumar,[1,a)] Yi Zhang,[1,b)] Yuming Xiao,[2] Jason Baker,[1] Andrew Cornelius,[1] Sathishkumar Veeramalai,[1] Paul Chow,[2] Changfeng Chen,[1] and Yusheng Zhao[1]
[1]*High Pressure Science and Engineering Center (HiPSEC) and Department of Physics and Astronomy, University of Nevada Las Vegas, 4505 Maryland parkway, Nevada 89154, USA*
[2]*HPCAT and Carnegie Institution of Washington, Advanced Photon Source, Argonne National Laboratory, South Cass Avenue, Argonne, Illinois 60439, USA*

(Received 12 May 2011; accepted 13 July 2011; published online 11 August 2011)

Student Involvement at HPCAT

Patricia Kalita

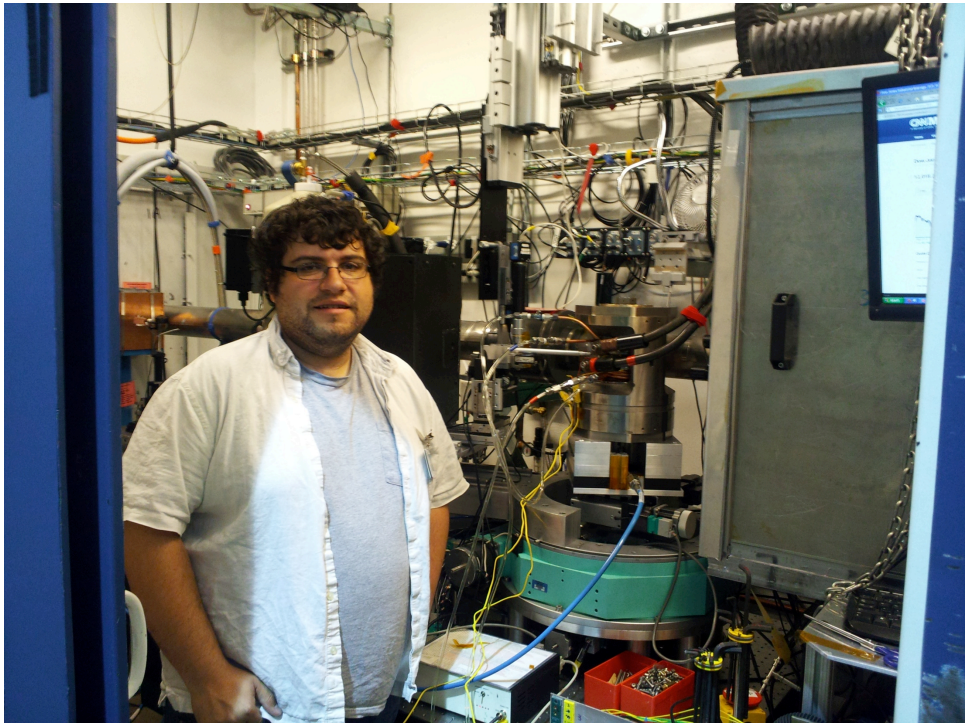


- ~100 shifts at HPCAT for MS and PhD research
- 2014-2015 Wolzinger Family Research Fellowship in Sciences for excellence in doctoral research

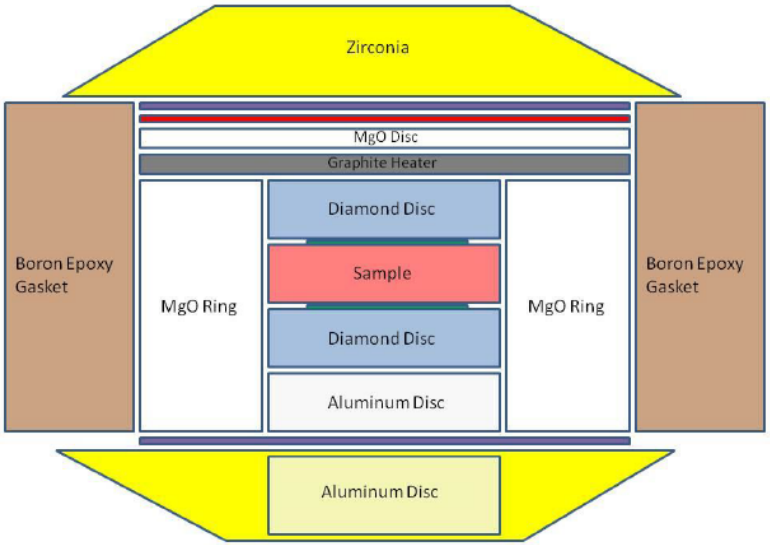
Currently a postdoc at Sandia

Jason Baker

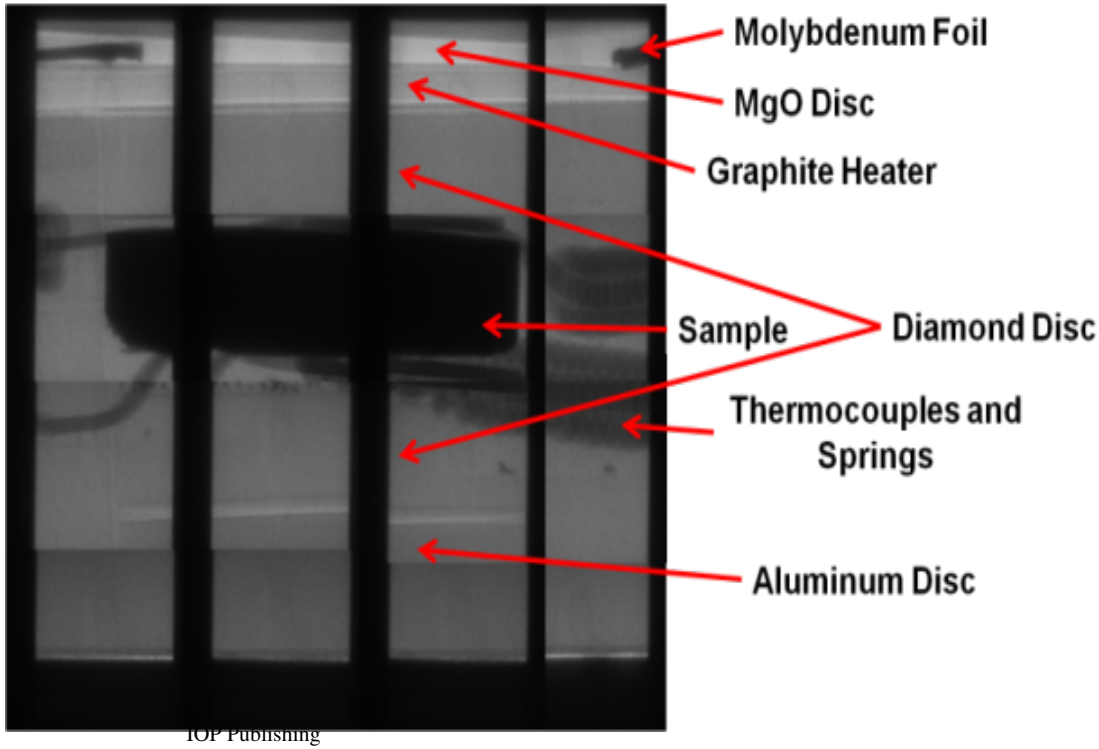
- Intimately involved in Paris-Edinburgh cell setup at BMB
- Spent 2 months at Los Alamos in 2012
- Spent 72 days at Argonne in 2013-14



Cross-section schematic of cell assembly



X-ray Radiography Image

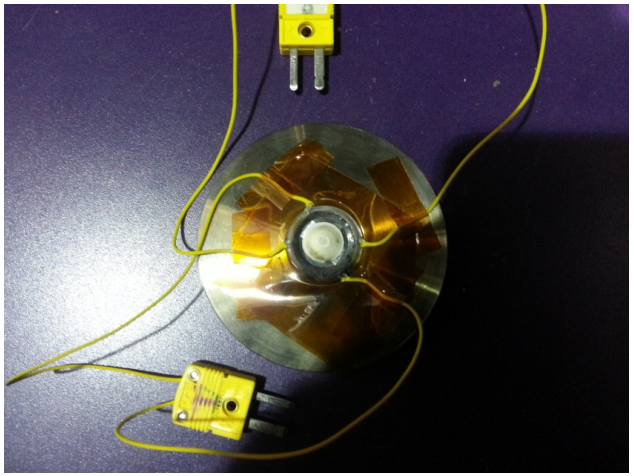


18th APS-SCCM and 24th AIRAPT IOP Publishing
Journal of Physics: Conference Series **500** (2014) 142003 doi:10.1088/1742-6596/500/14/142003

In situ x-ray diffraction, electrical resistivity and thermal measurements using a Paris-Edinburgh cell at HPCAT 16BM-B beamline

J Baker[1,2], R Kumar[1], N Velisavljevic[2], C Park[3], C Kenney-Benson[3], Y Kono[3], A Cornelius[1] and Y Zhao[1]

[1] HiPSEC, University of Nevada, Las Vegas. 4505 S. Maryland Parkway Las Vegas, NV 89154
[2] Shock and Detonation Physics Group, Los Alamos National Laboratory, Los Alamos, NM 87545
[3] HPCAT, Geophysical Laboratory, Carnegie Institution of Washington, 9700 South Cass Ave., 434E, Argonne, IL 60439, USA



Resistance/Conductivity Measurement

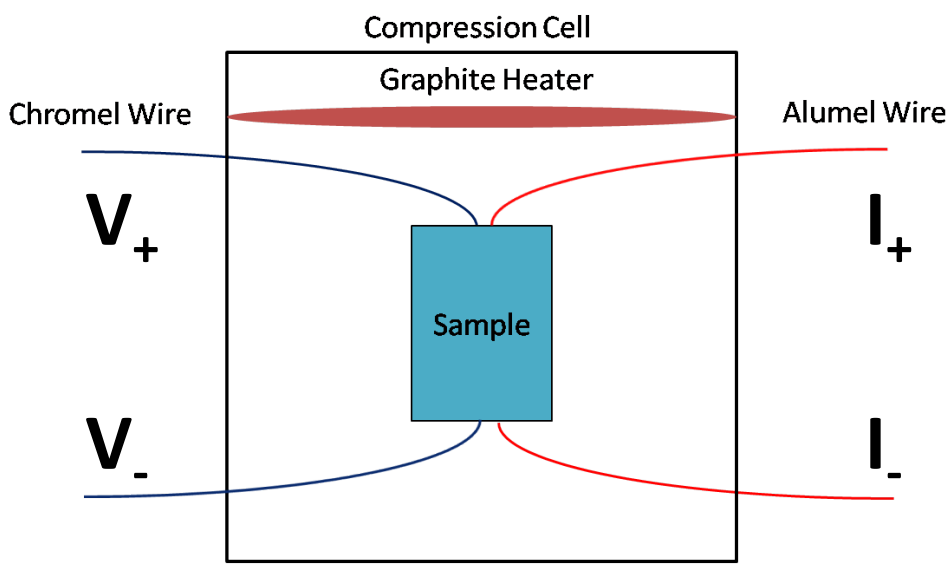
$$ZT = \frac{\alpha^2 \boxed{\sigma}}{\kappa} T$$

Electrical Resistance

$$R = \frac{V}{I}$$

Electrical Conductivity

$$\sigma = \frac{1}{\rho}$$

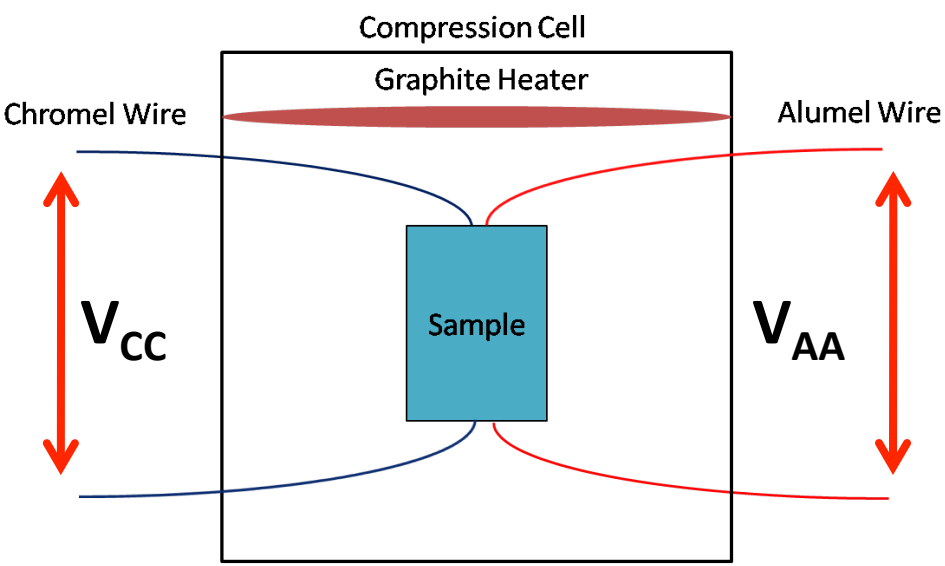


Seebeck Coefficient

$$ZT = \frac{\boxed{\alpha}^2 \sigma}{\kappa} T$$

Seebeck Coefficient

$$\alpha = \frac{\Delta V}{\Delta T}$$



Seebeck Coefficient

$$\alpha_S = \frac{\alpha_A - r\,\alpha_C}{1 - r} \quad r = \frac{\Delta V_{AA}}{\Delta V_{CC}}$$

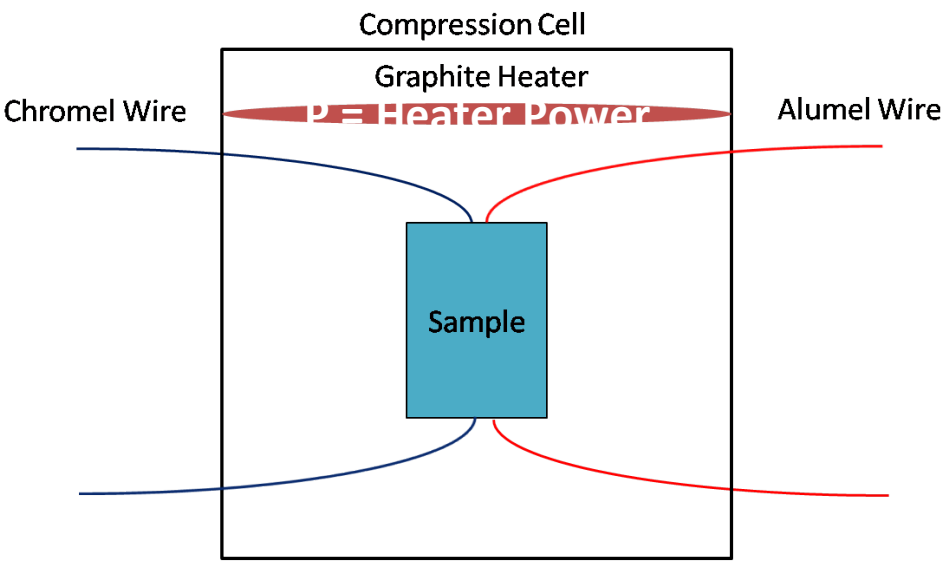
α_A = Seebeck Coefficient of Alumel
α_C = Seebeck Coefficient of Chromel

Thermal Conductivity

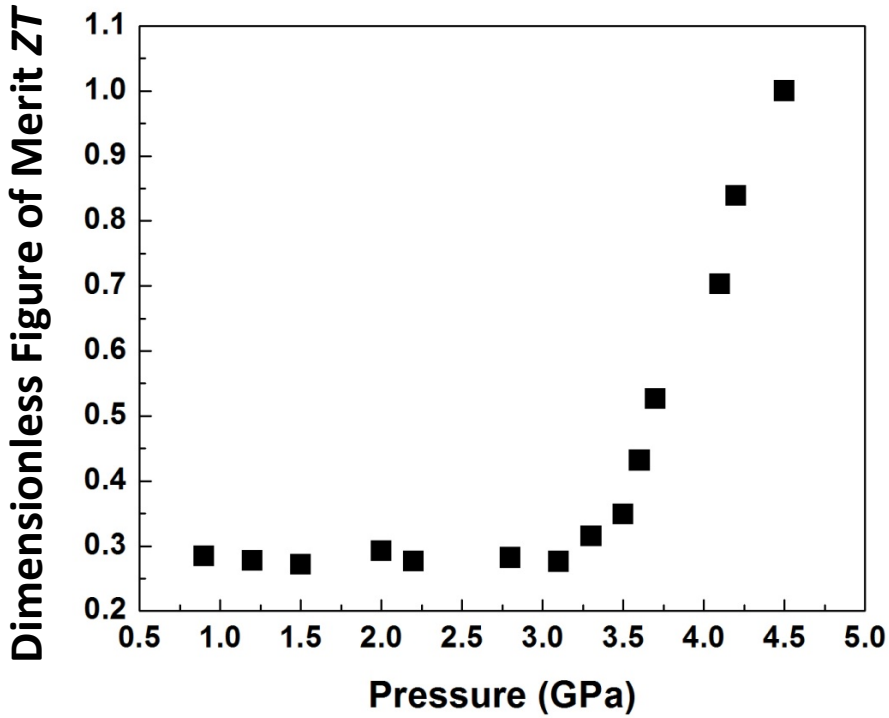
$$ZT = \frac{\alpha^2 \sigma}{\boxed{\kappa}} T$$

Thermal Conductivity

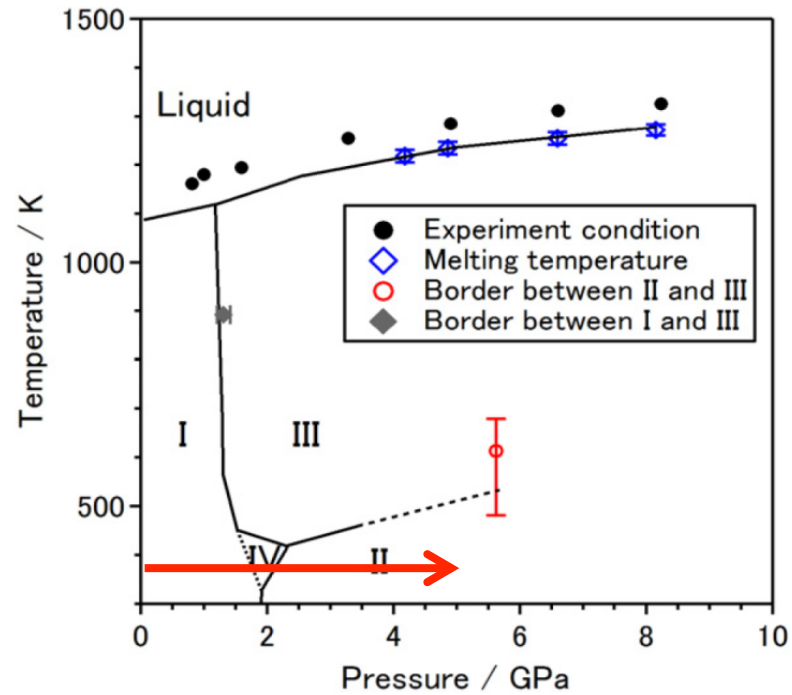
$$\kappa = \frac{P \Delta x}{A \Delta T}$$



SnTe Thermoelectric Properties



A Hinzmann *et al*



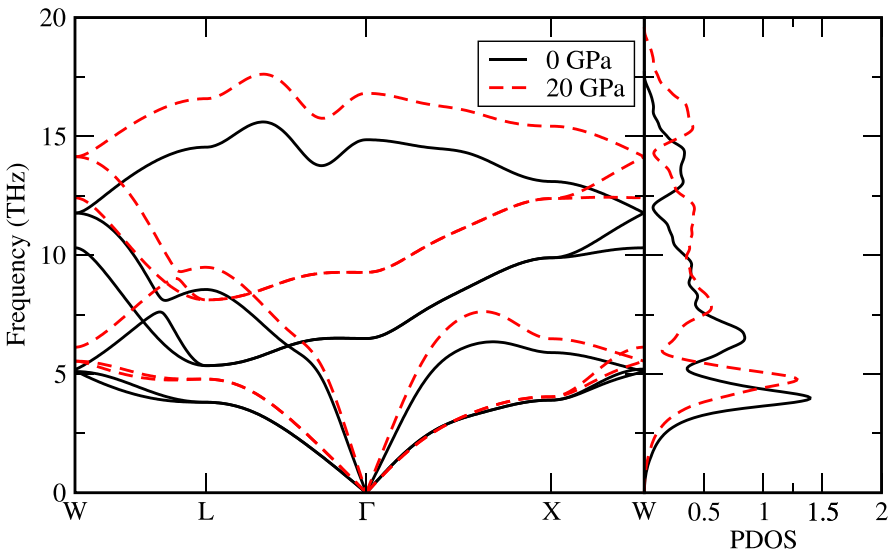
J. Phys.: Condens. Matter **24** (2012) 115103 (5pp)

Also perform simultaneous *in situ* XRD

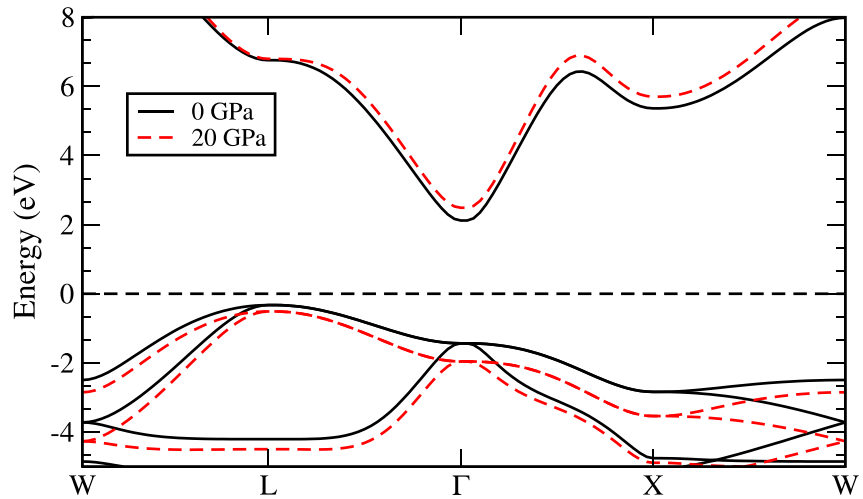
JOURNAL OF APPLIED PHYSICS **118**, 165101 (2015)

Thermoelectric properties of rocksalt ZnO from first-principles calculations

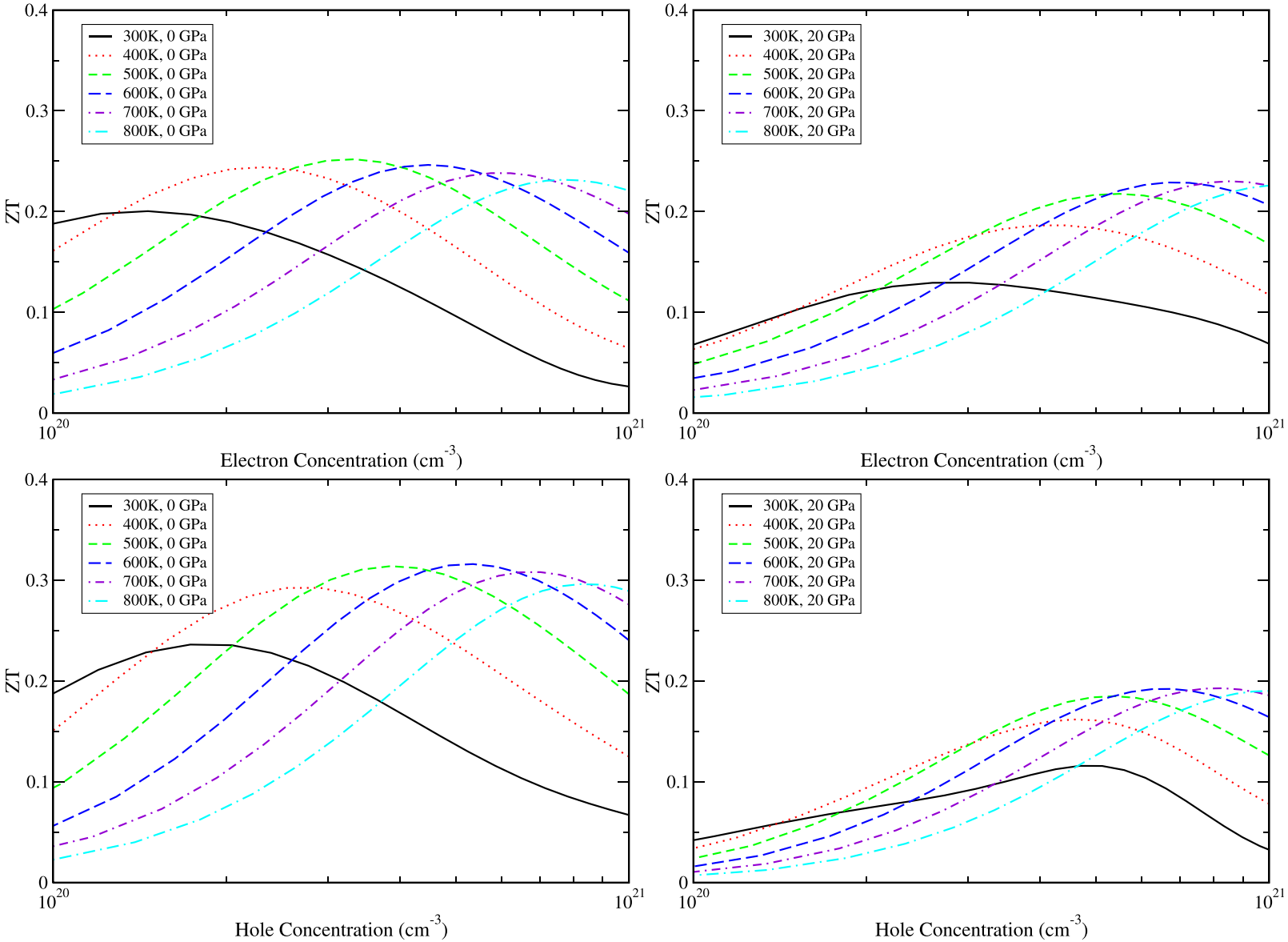
Andrew Alvarado, Jeevake Attapattu, Yi Zhang, and Changfeng Chen
Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA



Phonons



Electronic Band Structure


300K, 0 GPa
400K, 0 GPa
500K, 0 GPa
600K, 0 GPa
700K, 0 GPa
800K, 0 GPa
300K, 20 GPa
400K, 20 GPa
500K, 20 GPa
600K, 20 GPa
700K, 20 GPa
800K, 20 GPa
ZT
0
0.1
0.2
0.3
0.4
10^{20}
10^{21}
Electron Concentration (cm^{-3})
Hole Concentration (cm^{-3})

Conclusions

- HiPSEC gives students unique in depth training in high pressure techniques and synchrotron science
  - Large amount of time spent at HPCAT
  - Intimately involved with development at HPCAT
- HiPSEC is working with all DOE/NNSA laboratories
- Scope of work and productivity continues to increase
  - Two new faculty (one experiment and one theory) hired in last two years

UNLV
UNIVERSITY OF NEVADA LAS VEGAS

NNSA
National Nuclear Security Administration