XDL 2011

Time-domain experiments in diamond anvil cells

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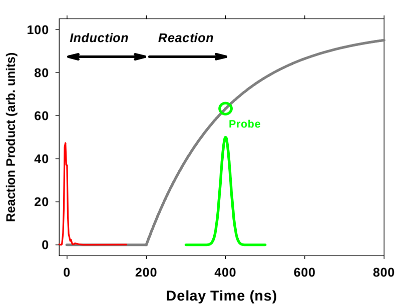
Geophysical Laboratory, Carnegie Institution of Washington

Challenges:

- Materials characterization under extreme conditions of high *P-T* -strain rate
- New materials synthesis under extremes including non-equilibrium conditions

New pulsed laser and X-ray techniques:

- Pulsed laser heating
- Ultrafast laser pump-probe techniques
- Combined Xray synchrotron-pulsed laser experiments
- Laser driven shock compression in the DAC



Themes:

- Metals thermal EOS and melting: Pt
- Simple diatomics- molecular dissociation: H_2, D_2, N_2, O_2
- Minerals: MgO
- Noble metals-thermal conductivity: Ar

Acknowledgements

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S. R. McWilliams
M. Mahmood

Howard University

M. R. Armstrong
J. C. Crowhurst

LLNL

V. Prakapenka
I. Kantor
M. Rivers

GSECARS, APS, ANL

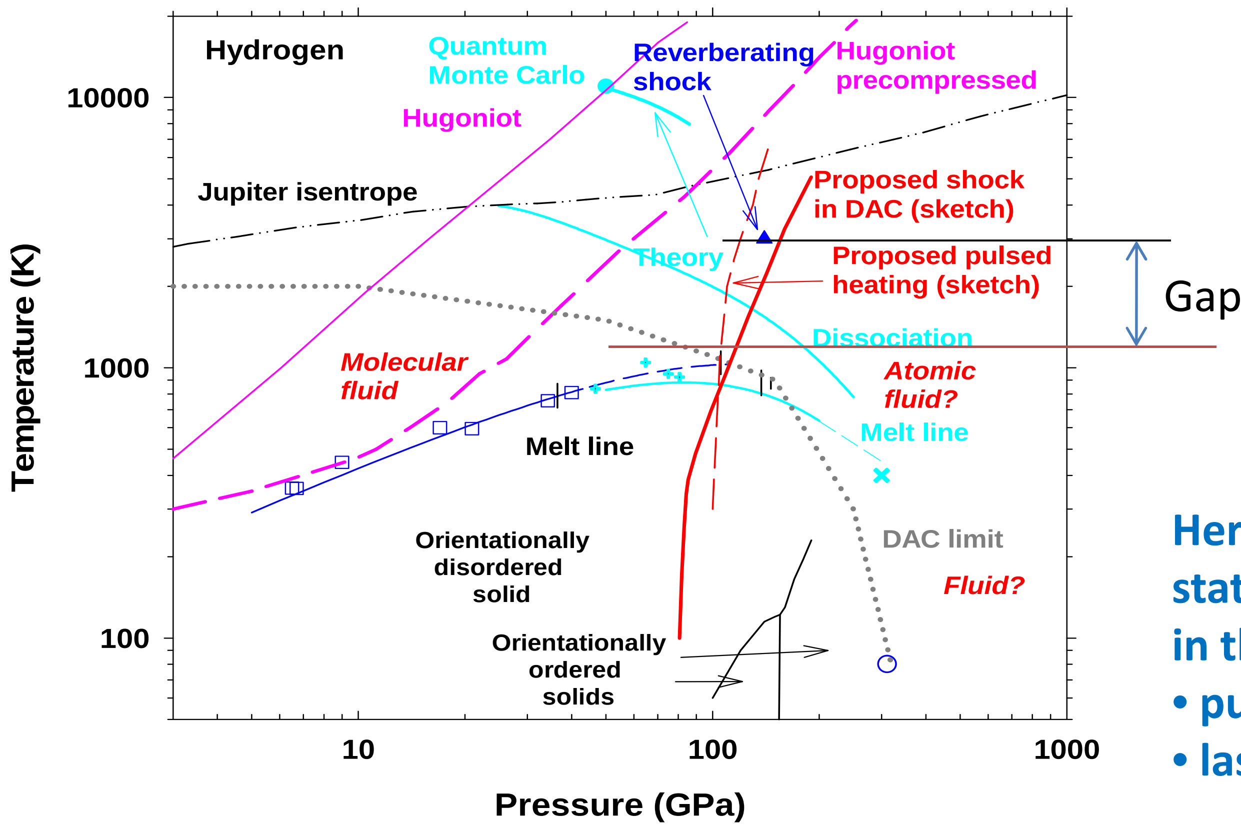
Support

NSF
DOE BES (EFree)
DOE NNSA (CDAC)
DCO
ARO
CIW

Carnegie Washington DC campus

Scientific challenges: bridge the gap between static and dynamic experiments in P-T-strain rate conditions reached & probed

<u>Phase diagram of hydrogen</u>

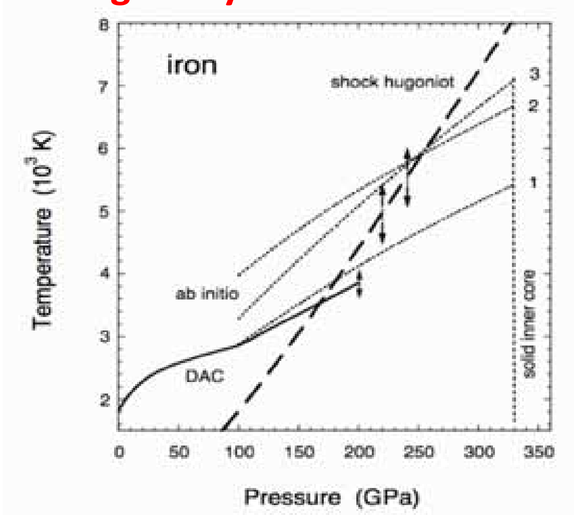


Extreme P-T conditions are relevant for:
- **-warm dense matter**
- **-new materials synthesis**
- **-fast chemical reactivity**
- **- materials strength**
- **- melting curves**
- **- planetary interior**

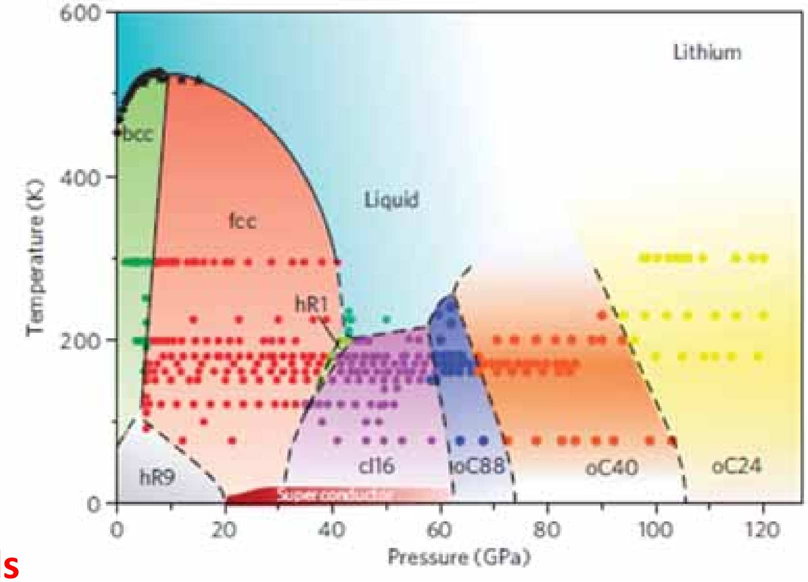
Here we propose to combine static and dynamic experiments in the DAC by performing
- **pulsed laser heating**
- **laser driven shock in the DAC**

Melting phenomena and properties of fluids at high P-T condition

Shock & static experiments disagree by 1000's K



Dramatic decline of melting line?!
Diagnostics of melting is scarce



Guillaume et al., 2011

Problems with static methods

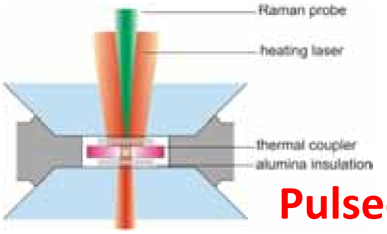
- **Instabilities (e.g., diffusion)**
- **chemical reaction**
- **indirect criteria and lack of positive observations**

New techniques are needed to enable accurate measurements of melting phenomena
improved laser heating techniques:

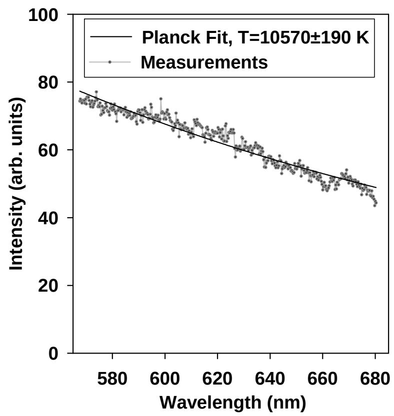
Time-resolved X-ray & optical techniques :

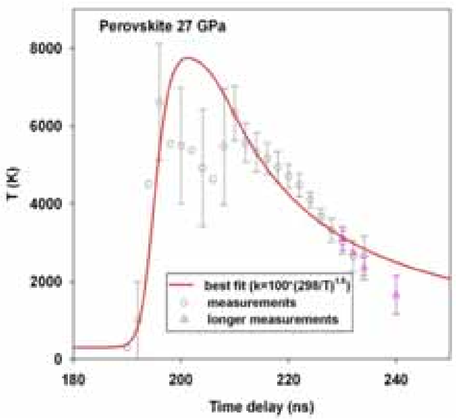
- **diffuse peak in XRD**
- **XAS spectroscopy**
- **elastic, optical, and vibrational properties**

Pulsed versus continuous laser heating in the DAC

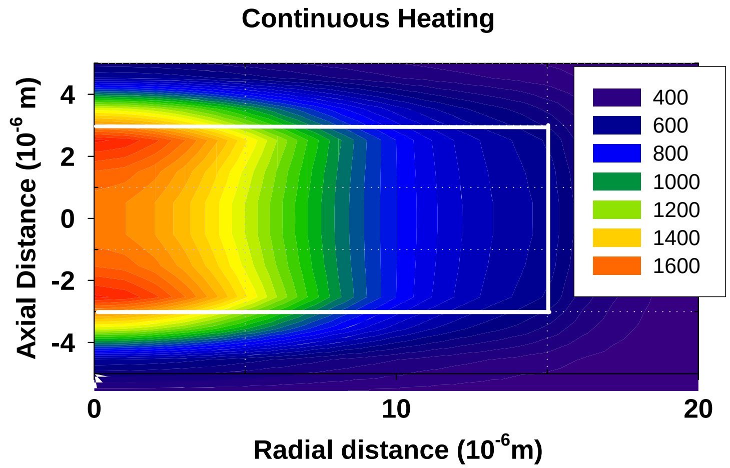


Pulsed laser heating: experiment

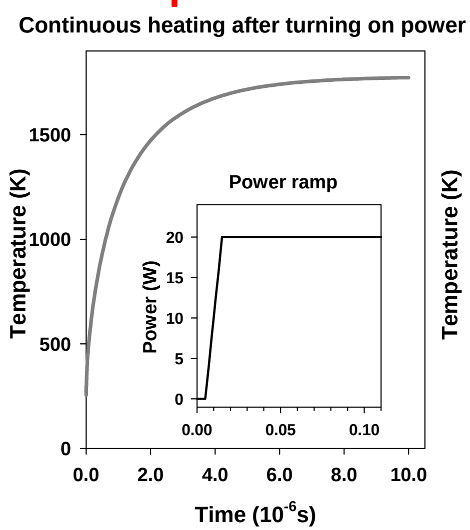


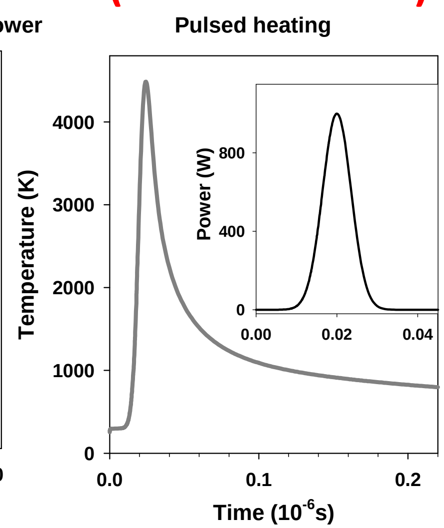


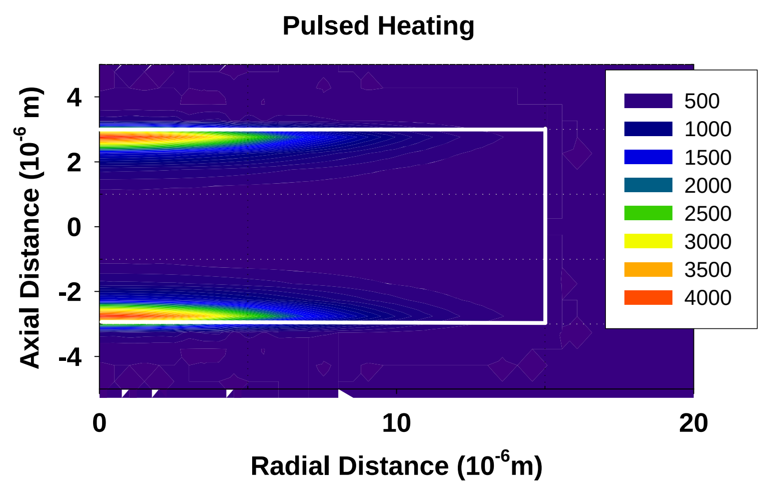
Finite element calculations, maps



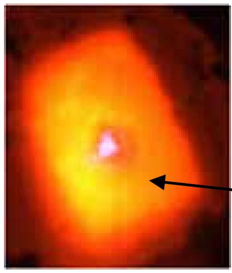
Temperature histories (FE calculations)







- Measurements are very challenging (small volume, strong thermal radiation)
- Uniform in space and time heating in the DAC require longer pulses

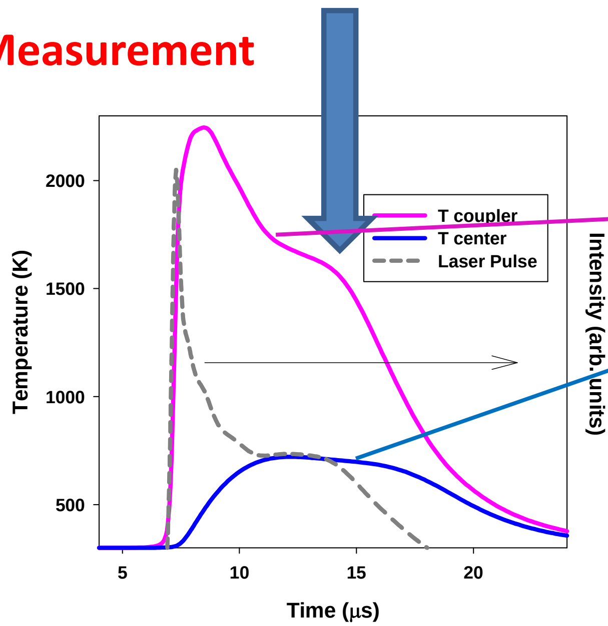


Time-domain experiments in laser heated DAC: thermal radiation & chemical reactivity suppression

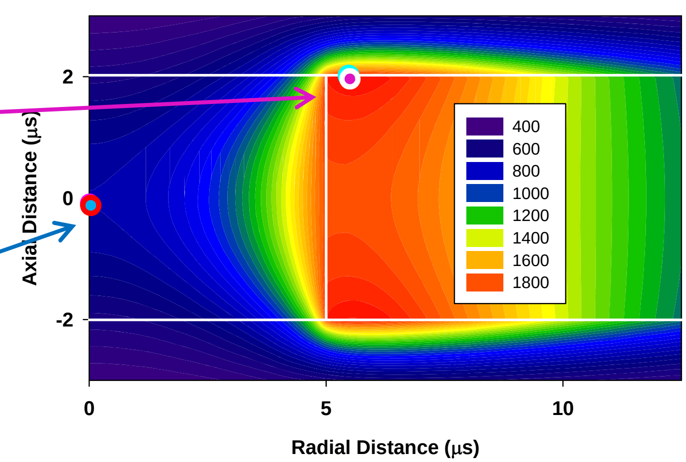
Coupler

Timing for pulsed heat + pulsed Raman operation:

Measurement



T map: FE calculations

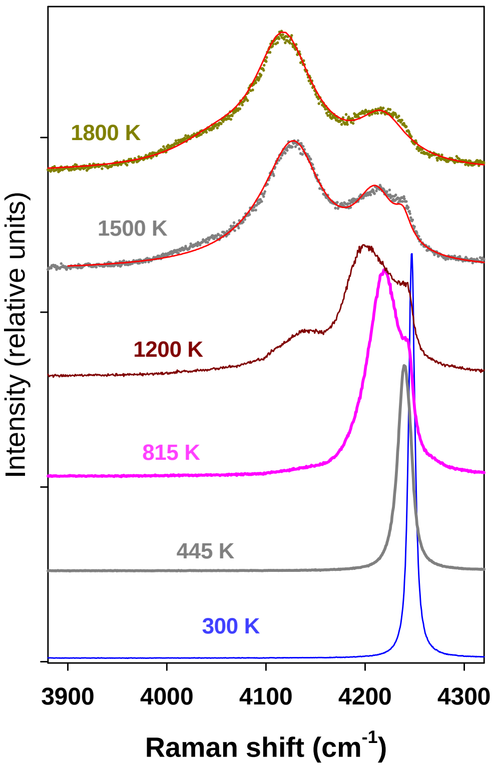


Pulsed heating (ns and μs): we discriminate spatially and temporally (by measuring ~5-10 μs after the arrival of the heating pulse).

A. F. Goncharov & J. Crowhurst (2005); Goncharov et al., 2008; Goncharov et al., 2010

Time-Resolved Raman Spectra of Hydrogen with double-sided microsecond laser heating

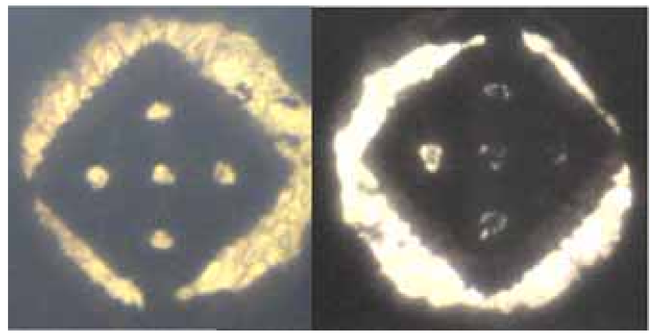
Raman spectra
CW excitation 60 GPa



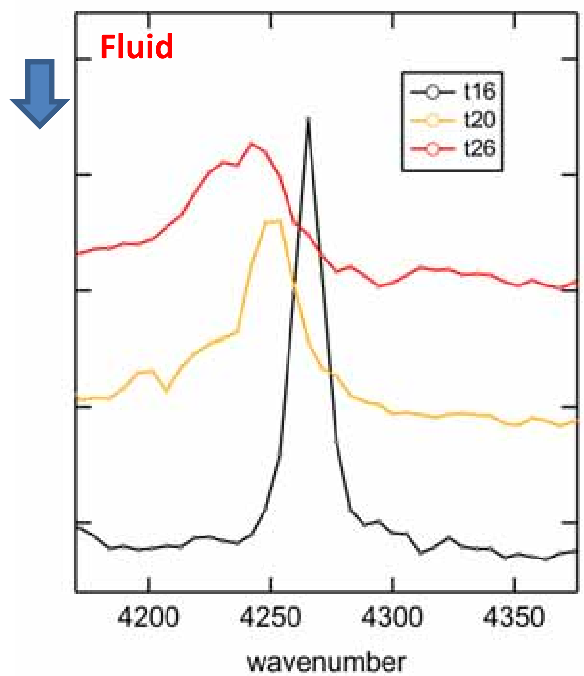
Rapidly collected Raman spectra show modified intramolecular bonds above 40 GPa.
Subramanian et al. PNAS, 2011

Sample: H_2, Ir Coupler P = 10-25 GPa

before *after*

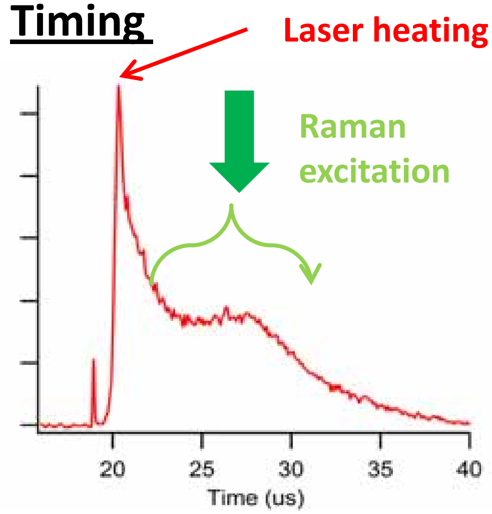


Raman spectra

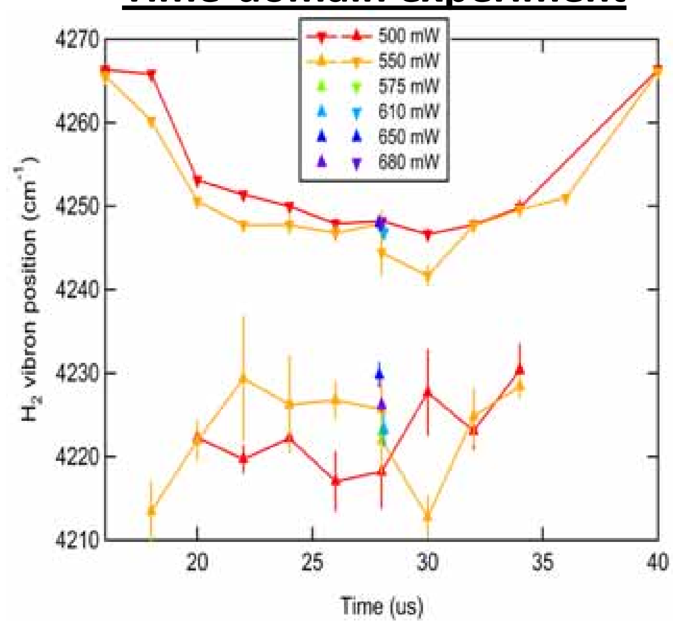


S. R. McWilliams

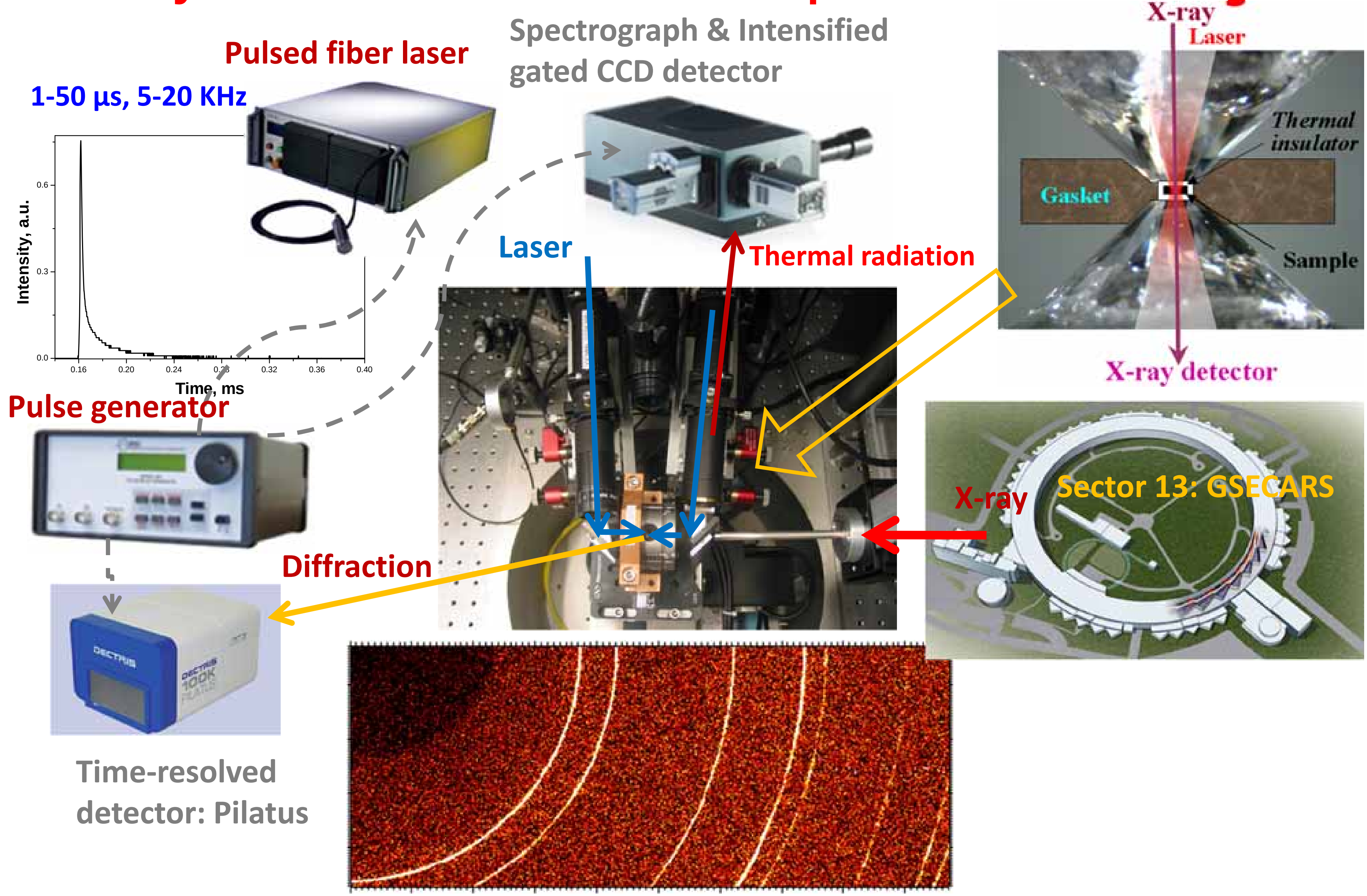
Timing



Time-domain experiment



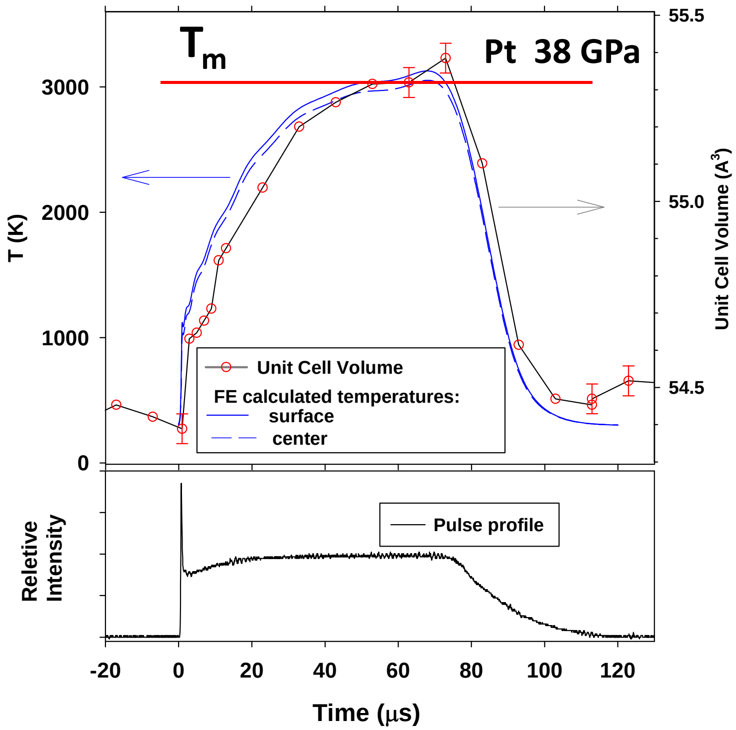
X-ray diffraction combined with pulsed laser heating



Goncharov, Struzhkin, Prakapenka, Kantor, Rivers, Dalton

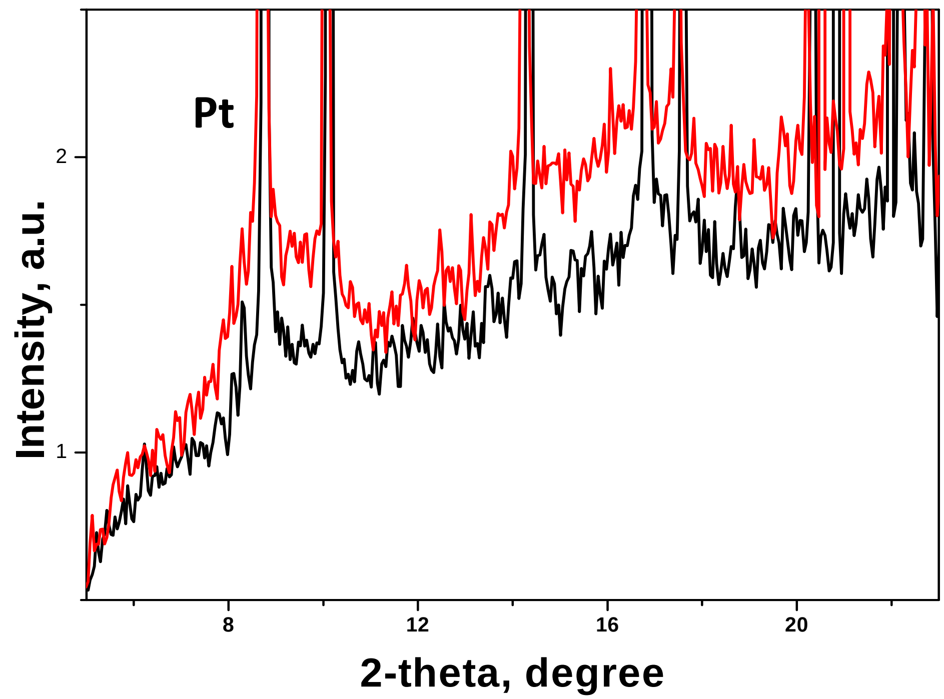
Pulsed laser heating in the DAC: μs timescales

Pulse profile vs
Thermal expansion
& temperature histories



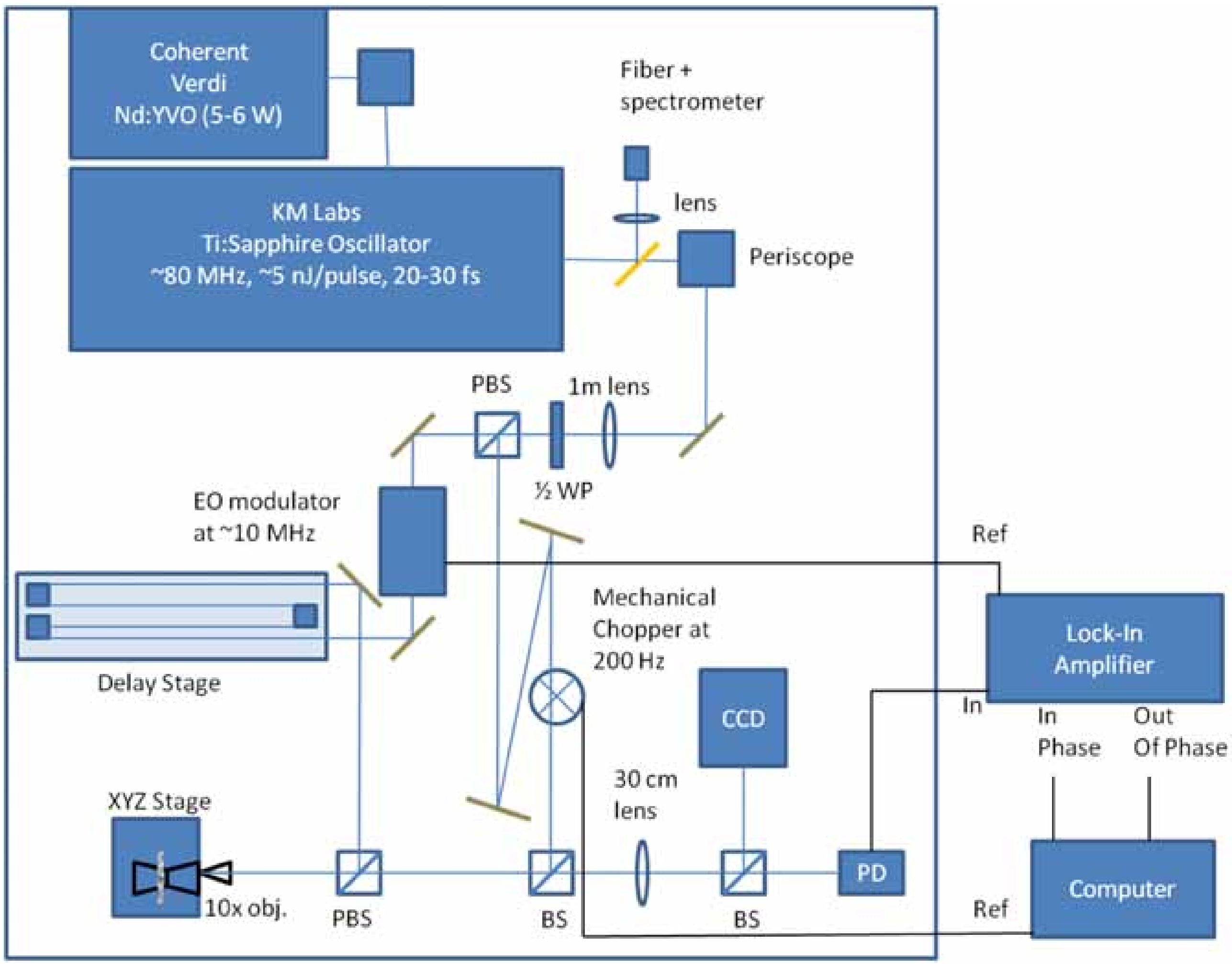
Time-resolved X-ray diffraction

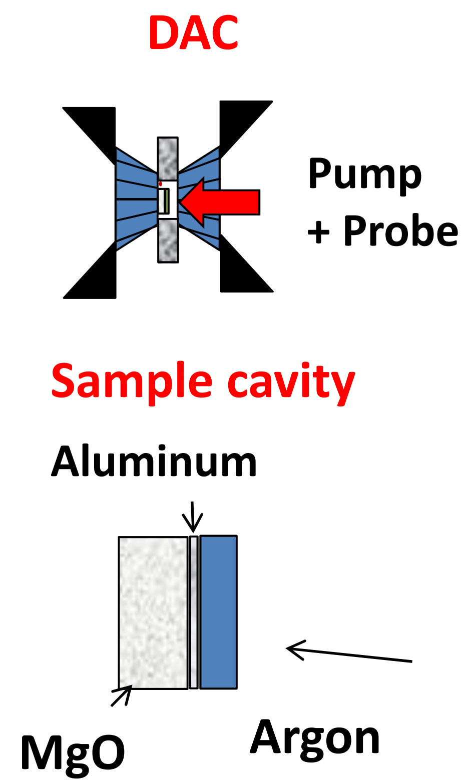
Detection of melting



GL: A. Goncharov, V. Struzhkin, A. Dalton; GSE CARS: V. Prakapenka, M. Rivers, I. Kantor

Optical Pump-Probe System for Time Domain Thermoreflectance experiments use a double modulation approach

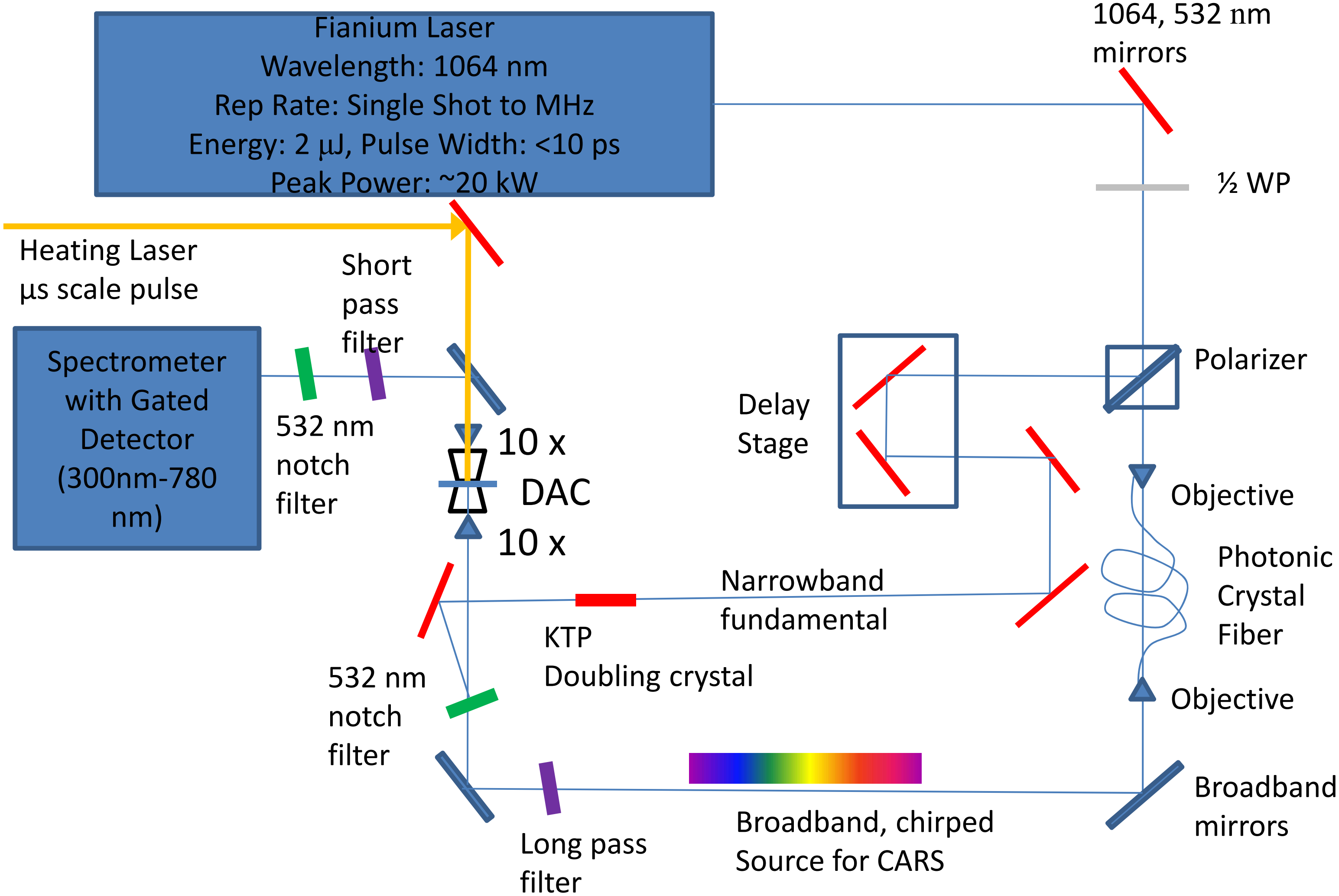




$$\Delta T = \frac{(1-R)Q}{C_{Al} A d_{Al}}$$

D. Dalton, A. Goncharov, W.-P. Hsieh, D. Cahill

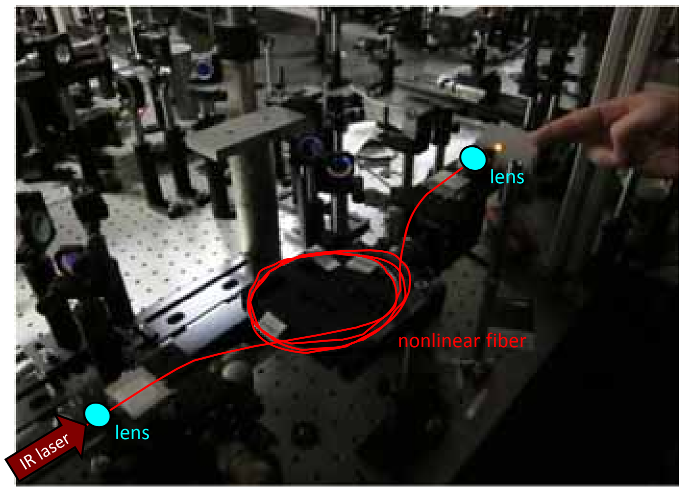
We are developing a new coherent Antistokes Raman and broad band spectroscopy systems

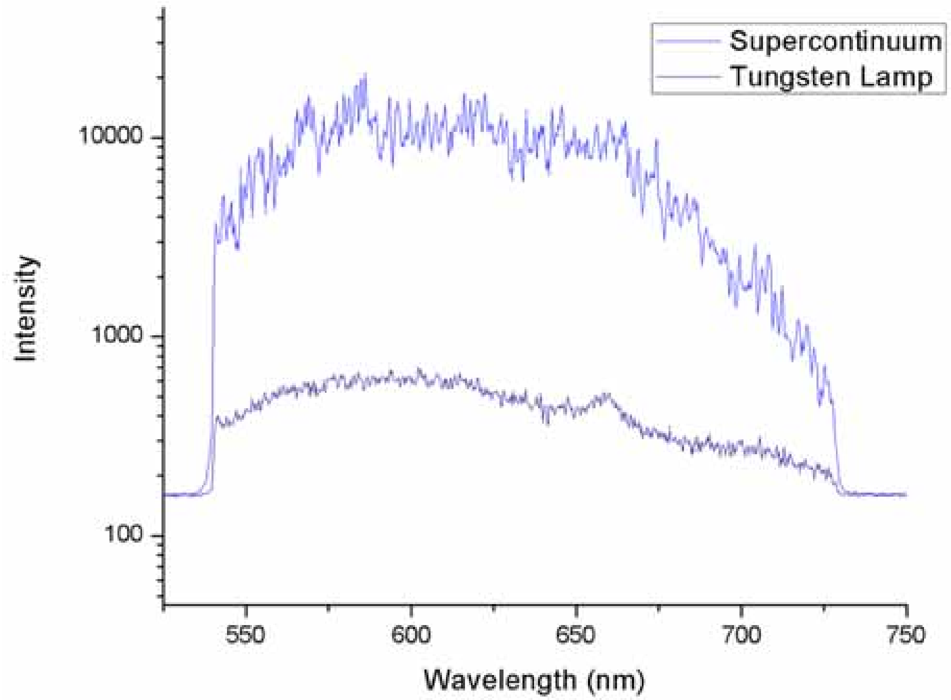


D. A. Dalton, McWilliams

Broadband Optical Spectroscopy will enable single shot study of optical properties at the extreme environments attainable in the DAC.

Supercontinuum Generation (SG) results in a very bright, white light source.





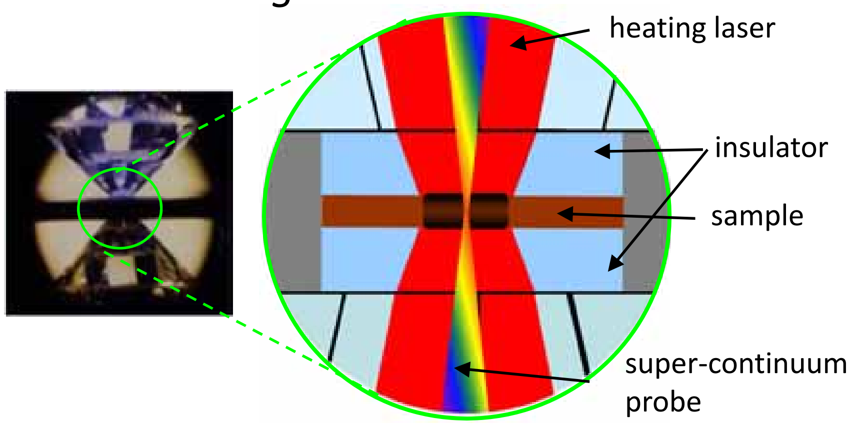
The supercontinuum data was collected in a single shot manner at ~180 nJ/pulse into the fiber

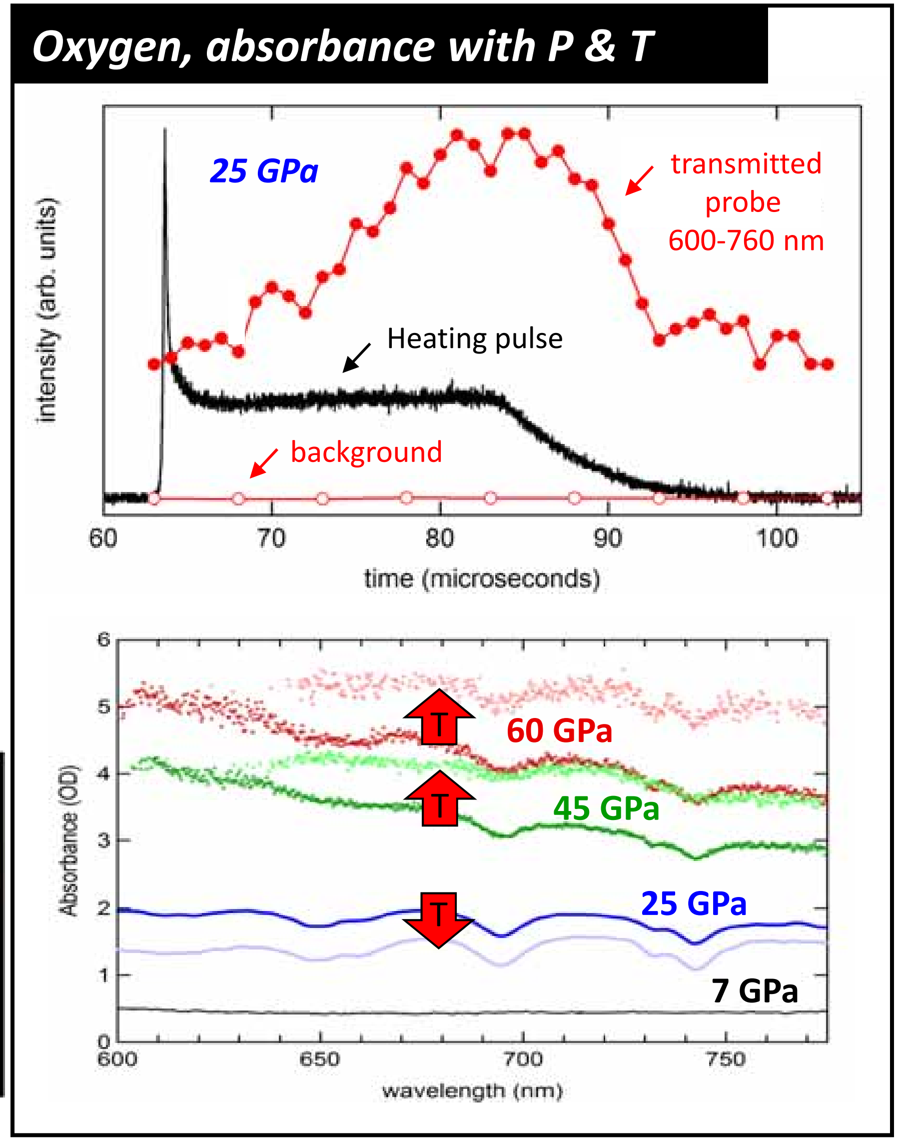
Tungsten lamp (~3000 K) data collected at 10^3 longer accumulation time.

D. A. Dalton & S. McWilliams

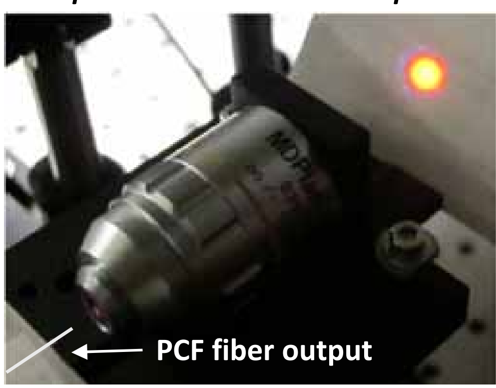
Time-domain optical spectroscopy in the diamond-anvil cell.

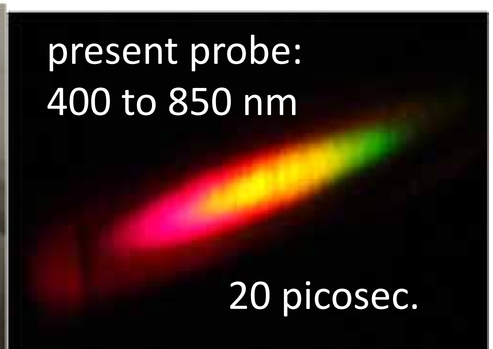
Transient extreme conditions; diamond anvil cell combined with pulsed laser heating.





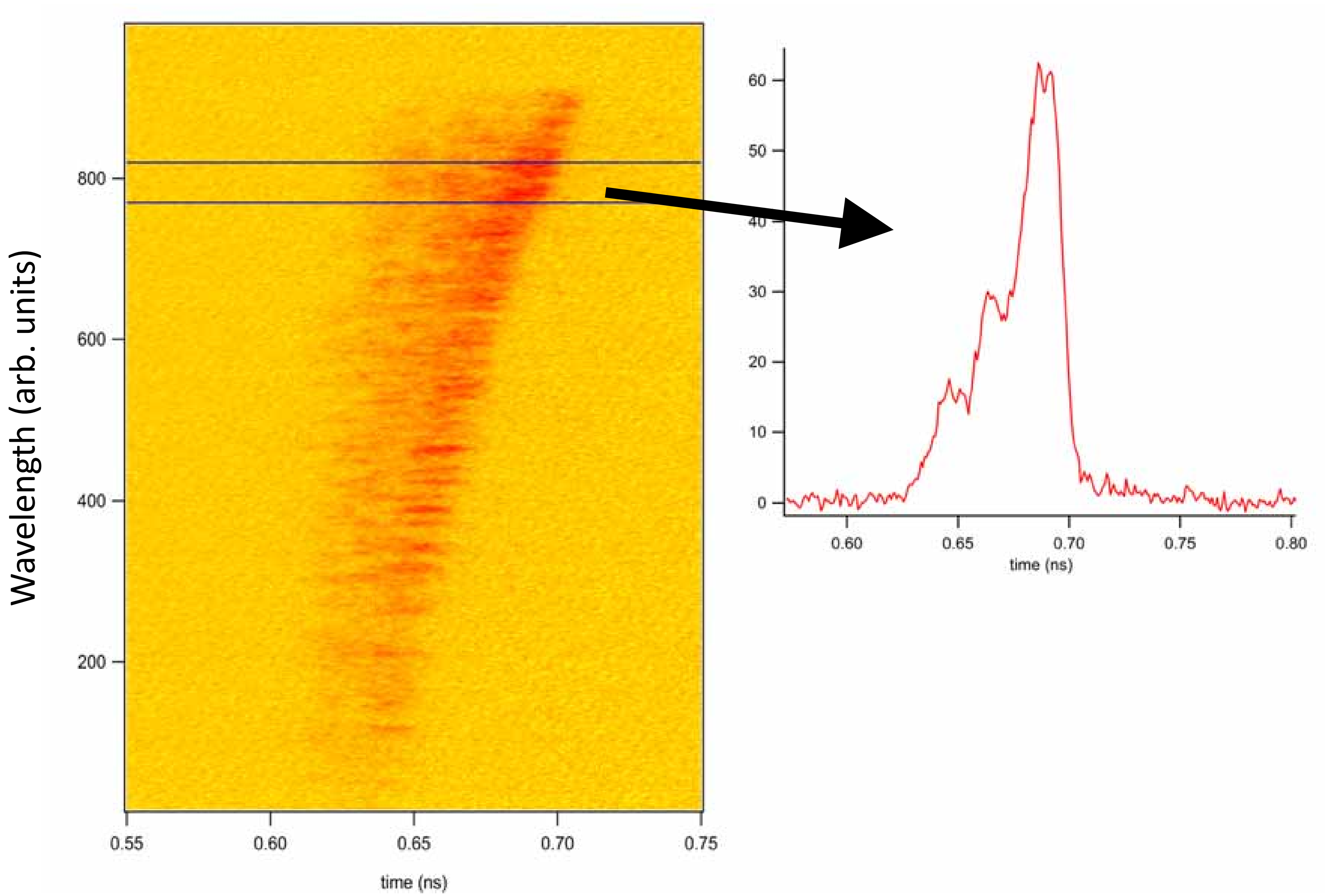
Ultrafast absorption spectroscopy using super-continuum optical probe.





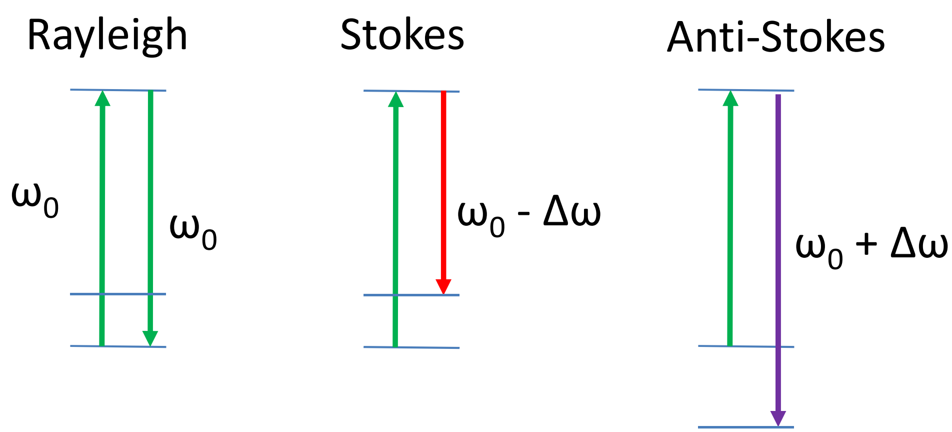
Goncharov, McWilliams, Dalton, Geophysical Lab

First Sweep of the Supercontinuum using a streak camera

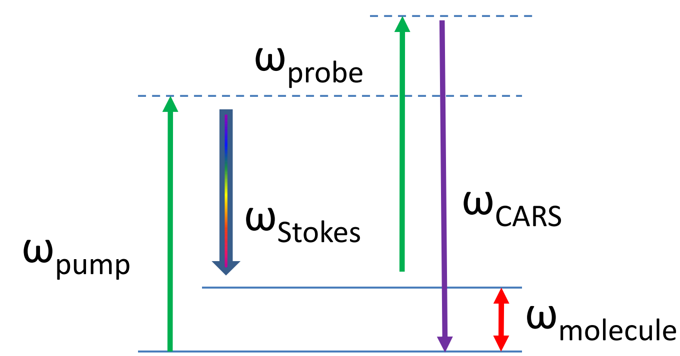


Coherent Anti-Stokes Raman Spectroscopy (CARS) will be used for time resolved chemistry in the DAC

Raman Effect



CARS



CARS has better conversion efficiency that Raman
CARS can discriminate from fluorescense and thermal background
CARS does have non-resonant background

ω_{pump} $=\omega_{probe}$ λ=532 nm

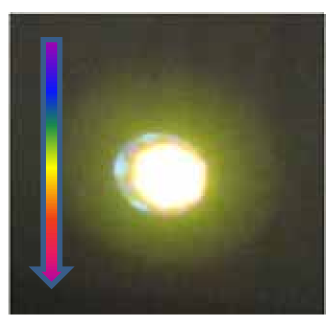
ω_{Stokes} λ= 532 nm-2 μm

ω_{CARS} λ= ~300-532 nm

$\omega_{molecule} = \omega_{pump} - \omega_{Stokes}$

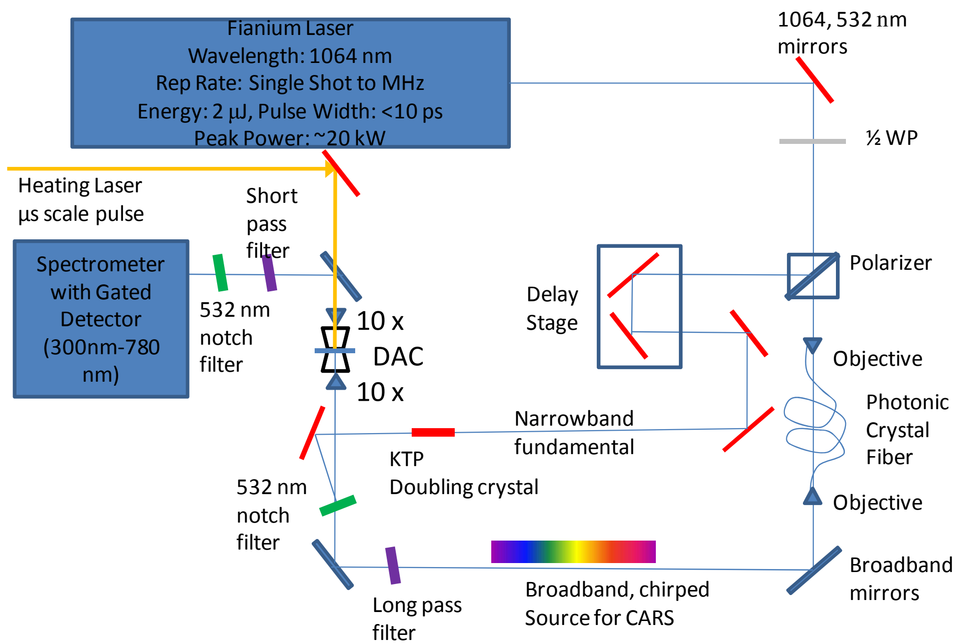
$$I_{CARS}(\Omega) \propto \left|\chi_{CARS}^{(3)}(\Omega)\right|^2 I_p^{\,2} I_s$$

Second harmonic **Supercontinuum**



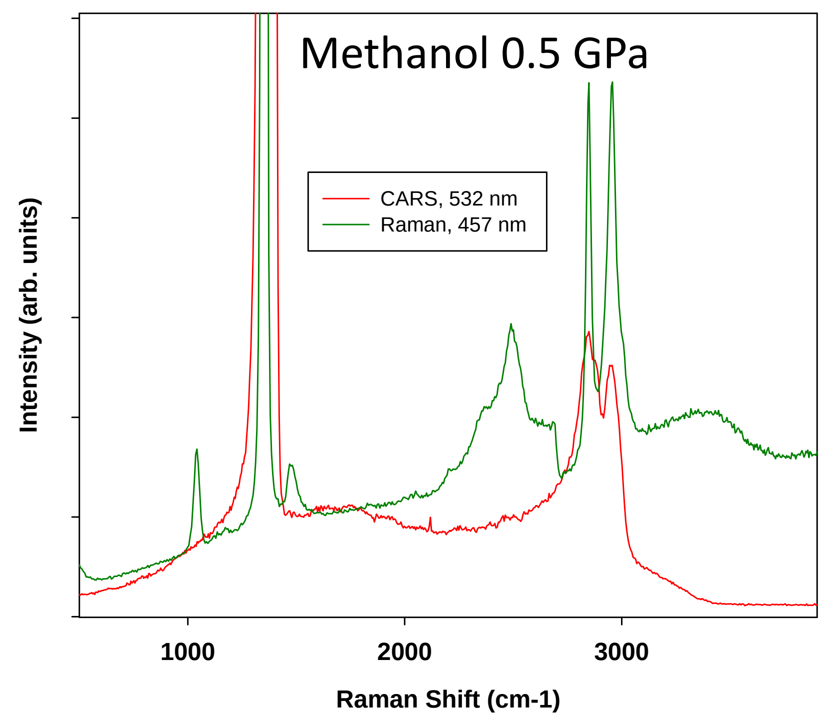
Broadband Coherent Anti-Stokes Raman Spectroscopy (CARS) is planned to perform single shot study of optical properties at the extreme environments attainable in the DAC: first tests at CIW

CARS spectra with supercontinuum at CIW



Dalton, McWilliams, & Goncharov

CARS spectra with supercontinuum



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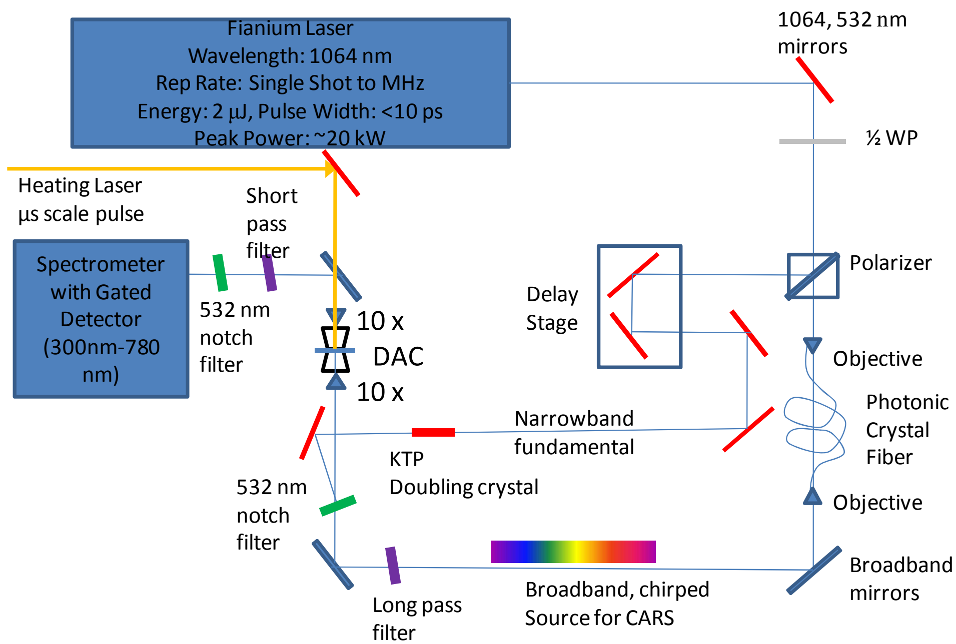
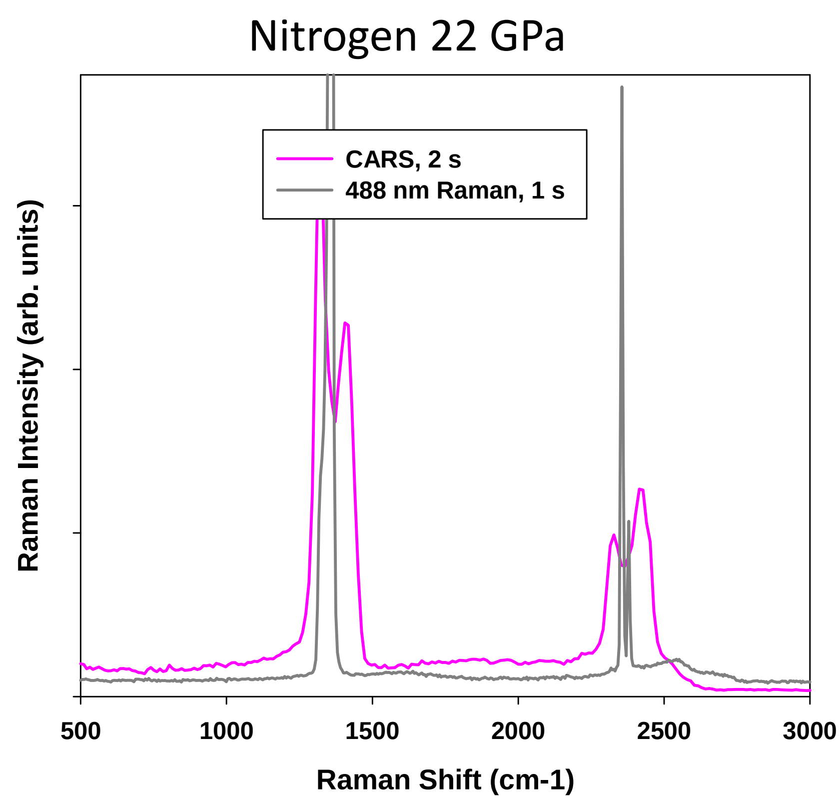
CARS spectra with supercontinuum at CIW



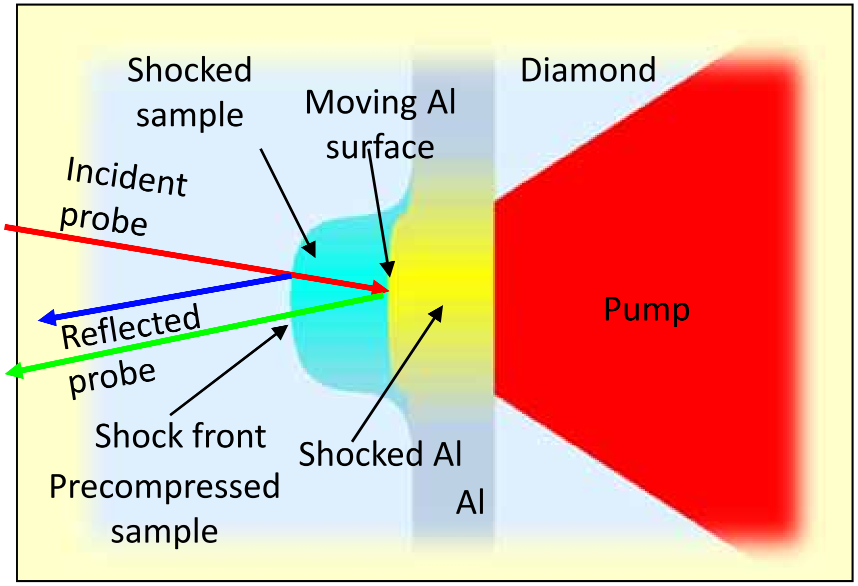
Dalton, McWilliams, & Goncharov

CARS spectra with supercontinuum

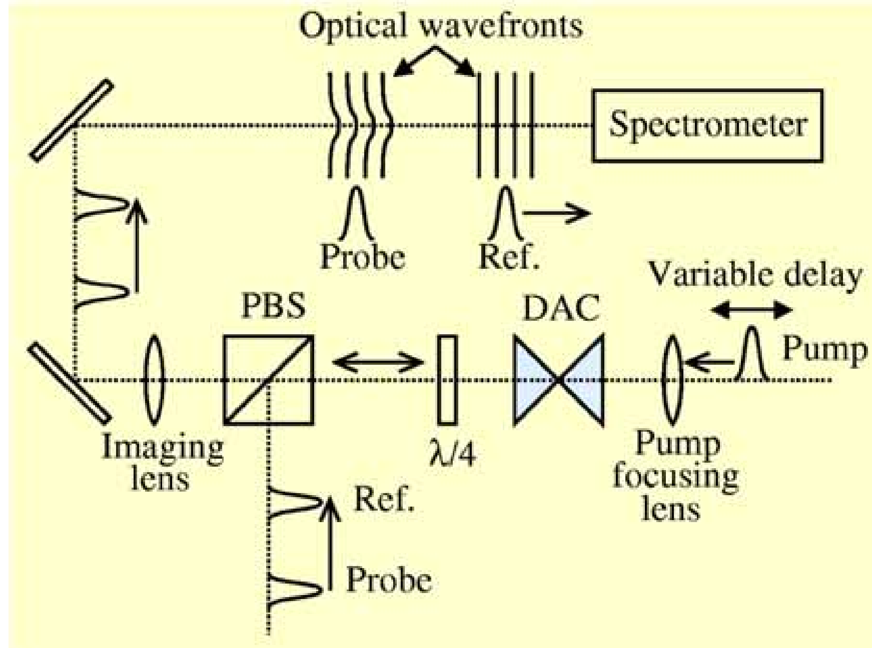


Laser driven shock compression in the DAC: samples are dynamically compressed in the DAC

Schematic



Ultrafast interferometry diagnostics



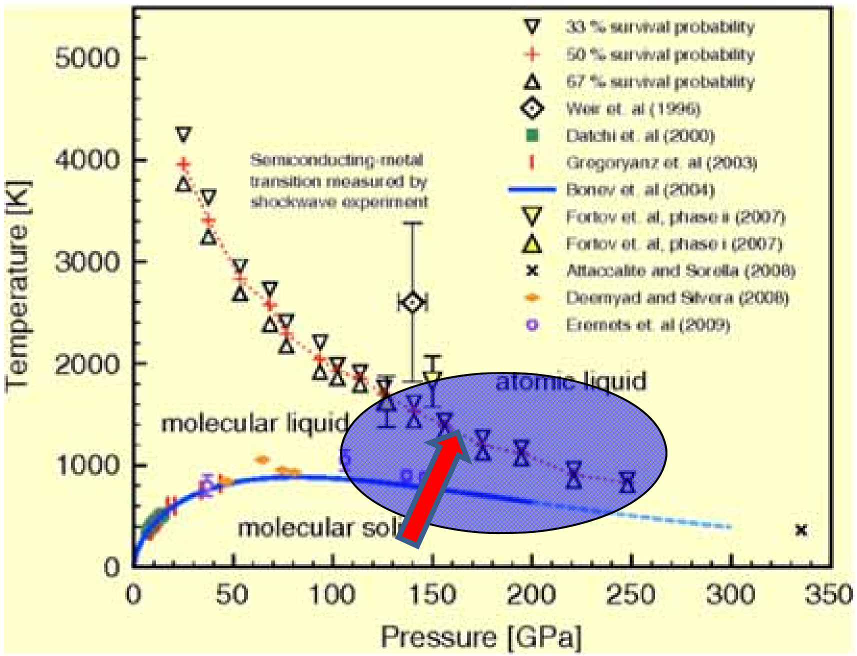
- Precompression in 100 GPa range is possible
- Preheating and precooling if needed
- <u>Ultrafast experiments can be small scale</u>:

Table top system, unlike currently better known technique of laser shocks which involves large laser facilities (such as NIF)

Armstrong and Crowhurst, LLNL

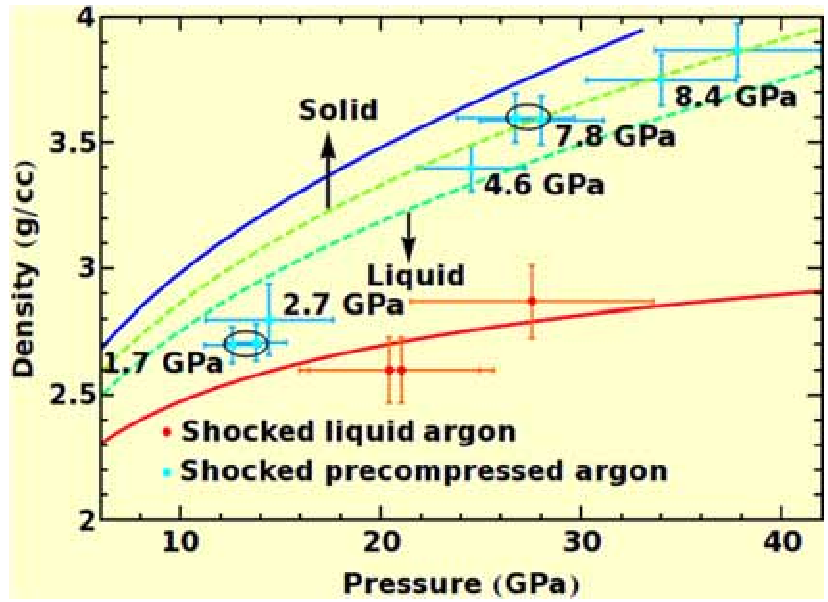
Observation of Off-Hugoniot Shocked States with Ultrafast Time Resolution: Probing High-pressure, Low-temperature States

Phase diagram of hydrogen



Bonev et al., (2010)

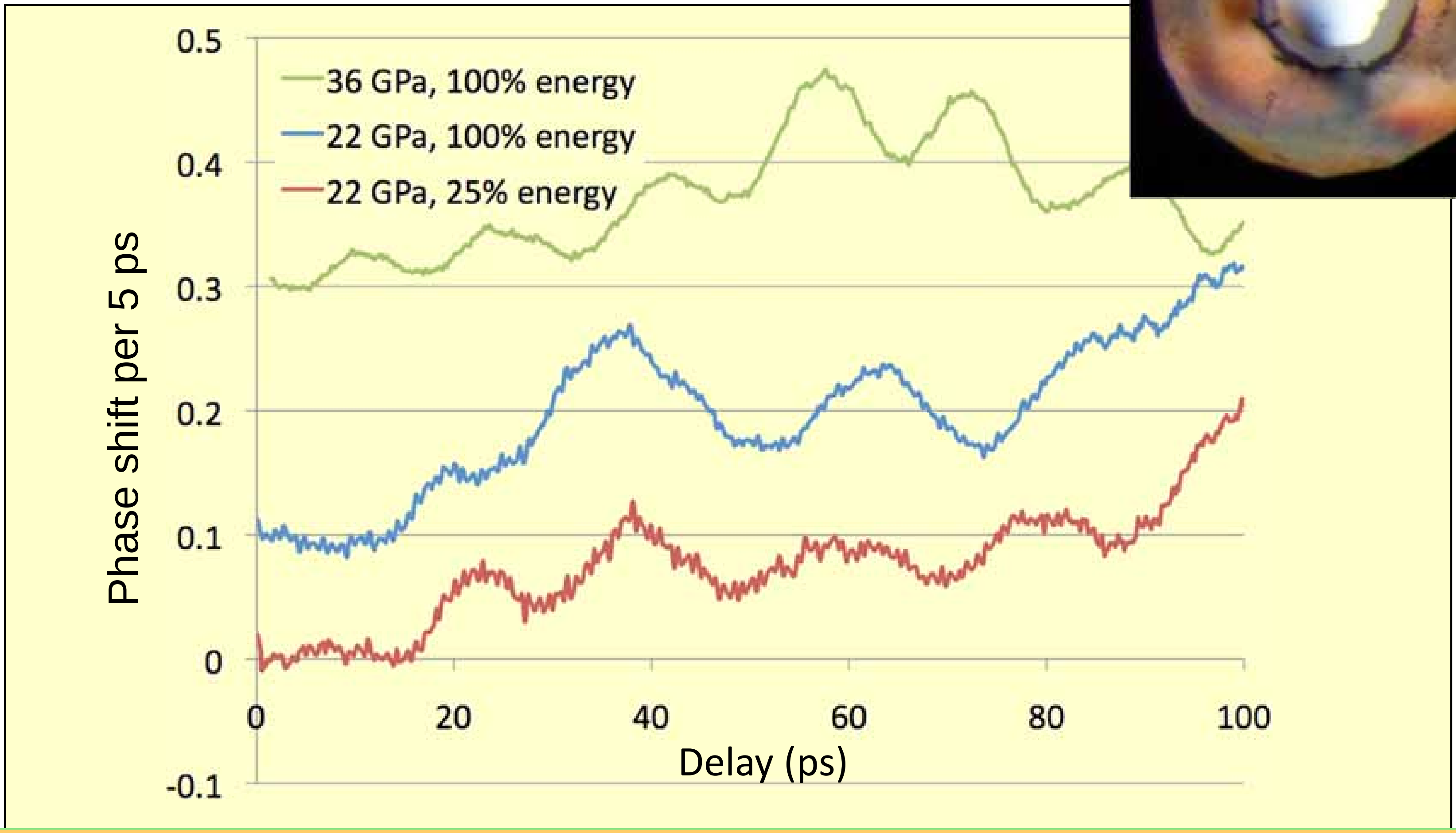
Example of data for Ar

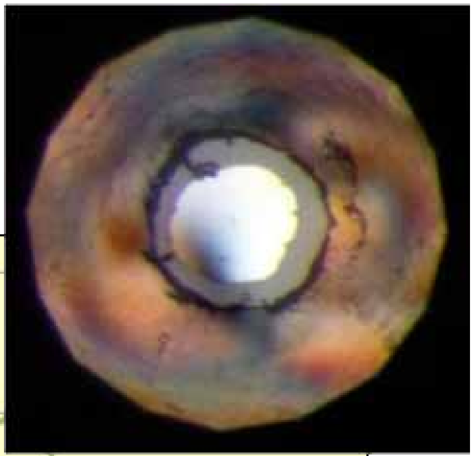


Armstrong et al ., in press

Laser shocks in the DAC can generate and detect 10s GPa shock waves (and low pressure acoustic waves) in materials under precompression of 10s GPa

First shots on deuterium





•Shock and particle velocities of ~12-13 km/s and ~1 km/s for precompression ranging up to 36 GPa, giving a shock pressure ~10 GPa.

•Possible phase transition over the duration of the probe window

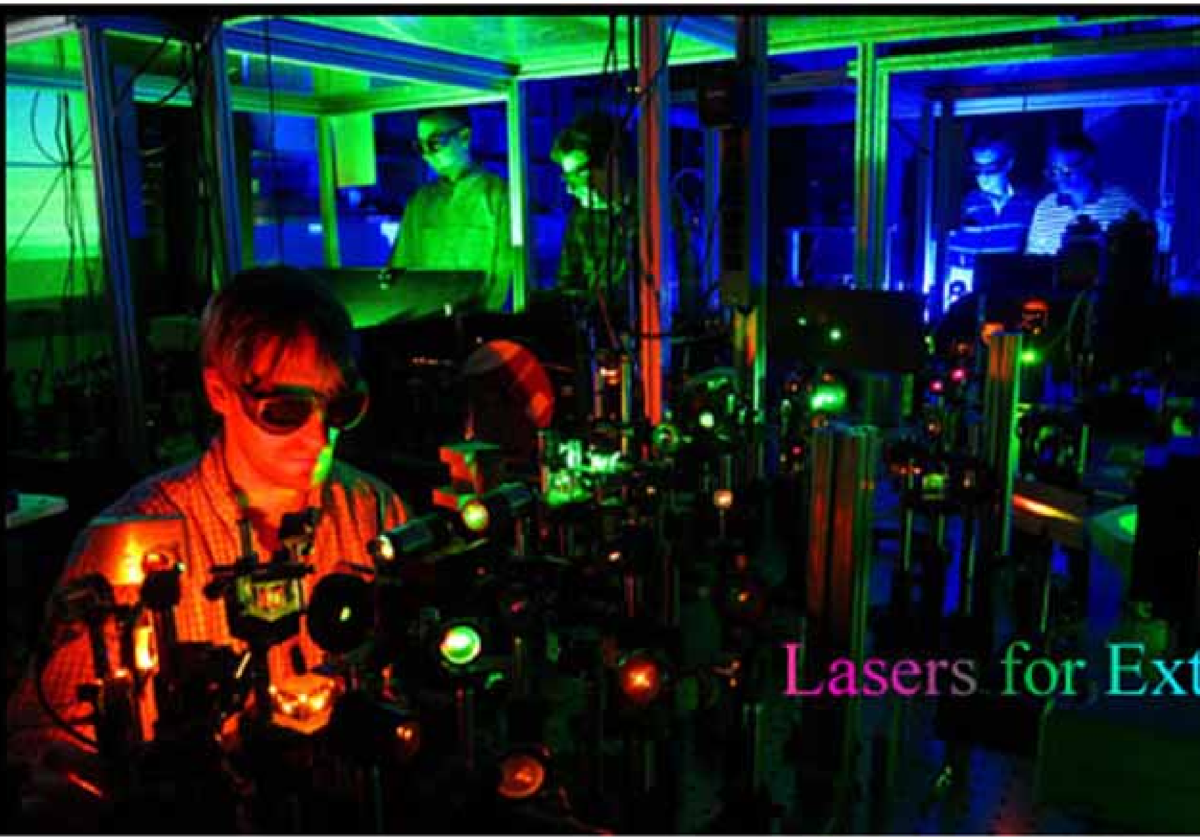
M. Armstrong. J. Crowhurst, LLNL

Outlook: the field is mature
We are looking for new opportunities which will be given by new generation synchrotron sources

➢ **Pulsed laser techniques have a great abilities to:**
- access unavailable previously extreme P-T conditions
- overcome problems of containing and probing chemically reactive and mobile materials
-study vibrational, optical, elastic, transport properties under extreme conditions

➢ **The full potential of these techniques will be reached with further development of ultrafast (ps to fs) pump-probe & single –shot techniques coupled to pulsed laser heating and laser shocks in the DAC.**
-perform experiments in a time domain to access the time scale and dynamics of phase transitions & chemical reactions

➢ **We are looking forward for developing new combined X-ray – optical techniques at synchrotron beamlines (e.g., ERL, Petra III, XFEL, NSLS-II)**



Lasers for Extreme Conditions