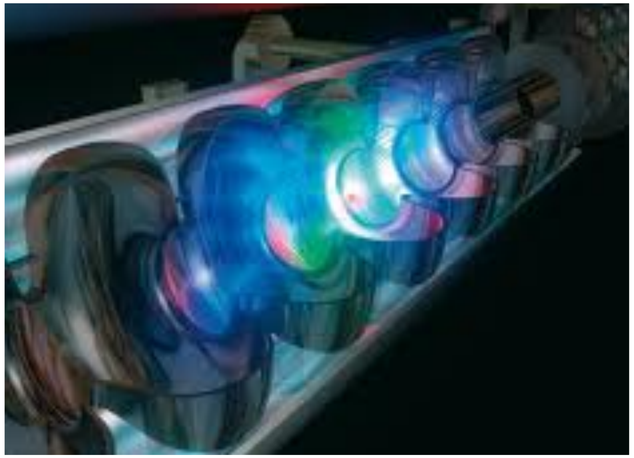
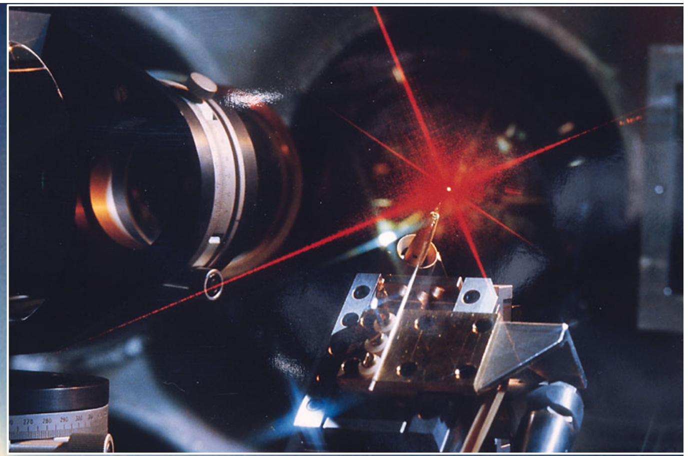




# Hard X-ray FEL for matter under extreme conditions

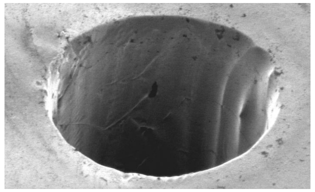
Marion Harmand et al.

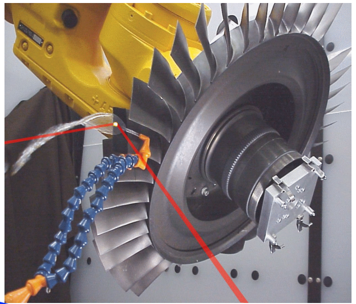
IMPMC – CNRS, Sorbonne Université, MNHN - France

# Matter under extreme conditions - large range of application, topics… and time scales

fs

### Laser industrial processes

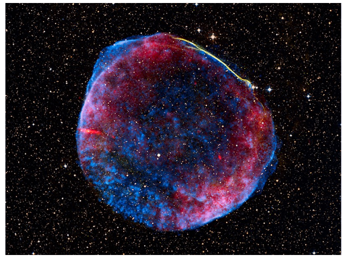

fs drilling


Laser shock hardening

μs - days

### Astrophysical shock wave

Polar Accretion column


Supernovae remnant

$10^6$ years

### High velocity impacts


Space debris impacts

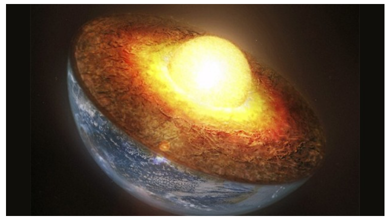

Meteorite craters


Giant impacts

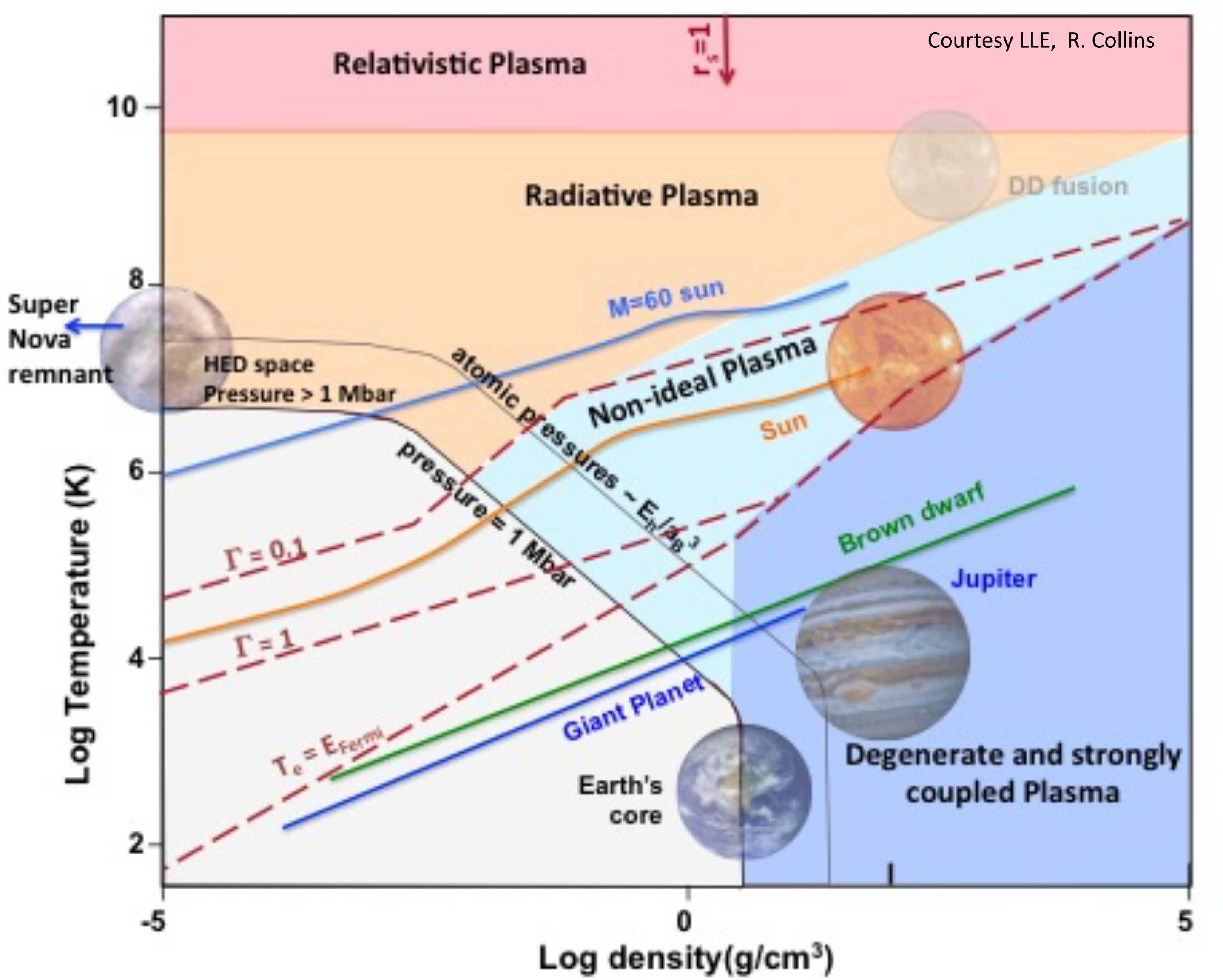
$10^9$ years

### (Exo)-Planetary interiors and (exo)-planet properties


Trapist system

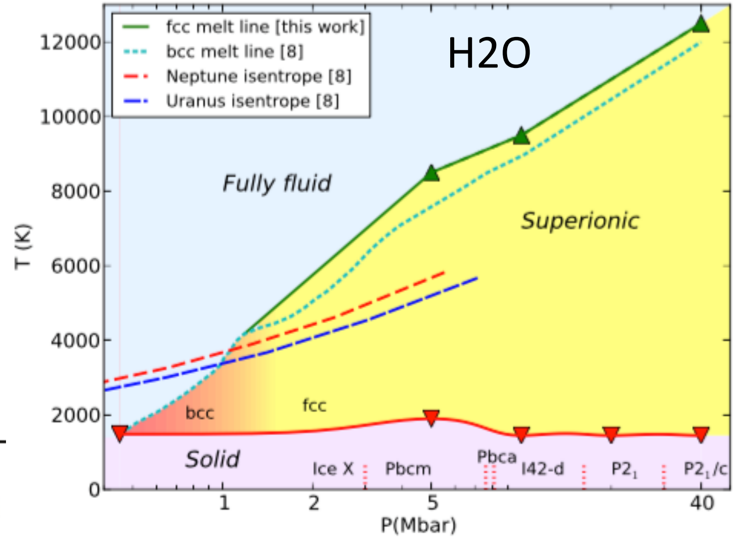

Earth interior

# Matter under extreme conditions - large range of thermodynamic conditions

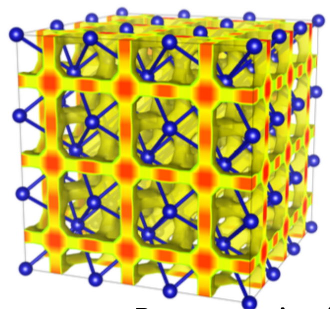


# Non expected physical properties of matter

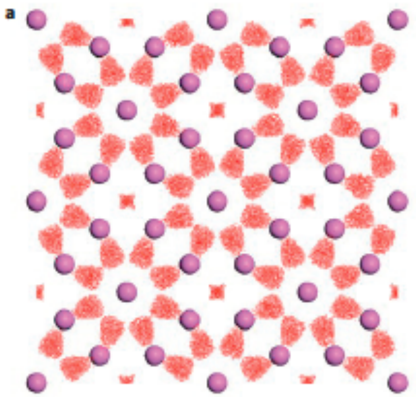
At high pressures and high temperature, the interplay between electron and ions play a major role
- Orbital hybridation
- Interstitial, localized electron bonding
- Gap changes, mettalization…



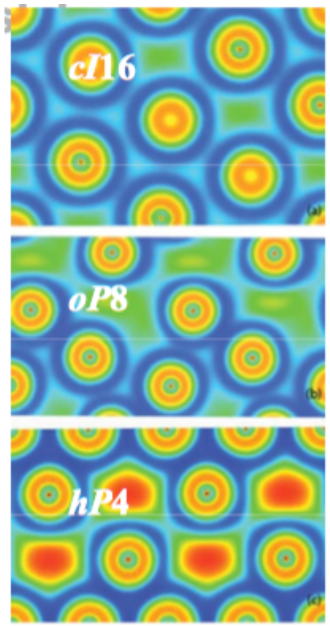

*Wilson et al PRB 2013*



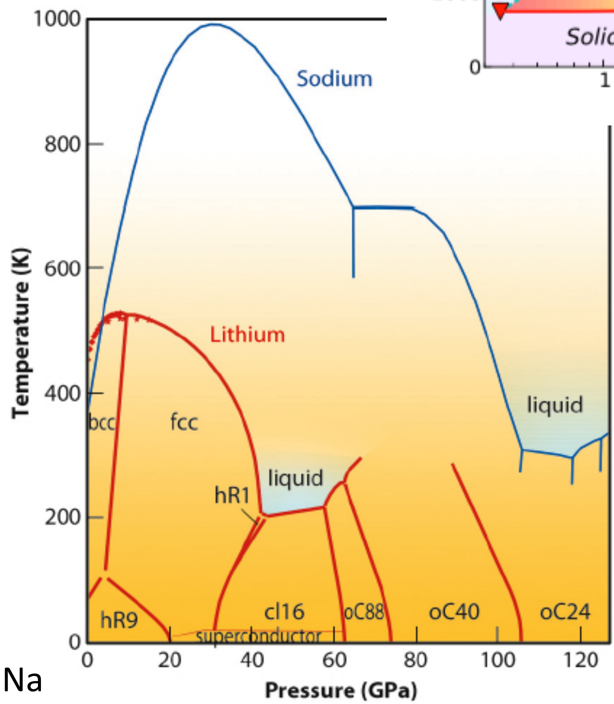
Bcc superionic



Host guest structures in Al at Tpa pressures
*Pickard, Nature Materials 9, 2019*



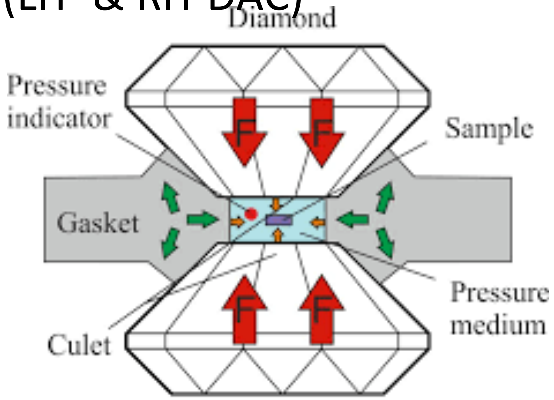

Electron localized function of Na
*Marques et al, PRB 2009*

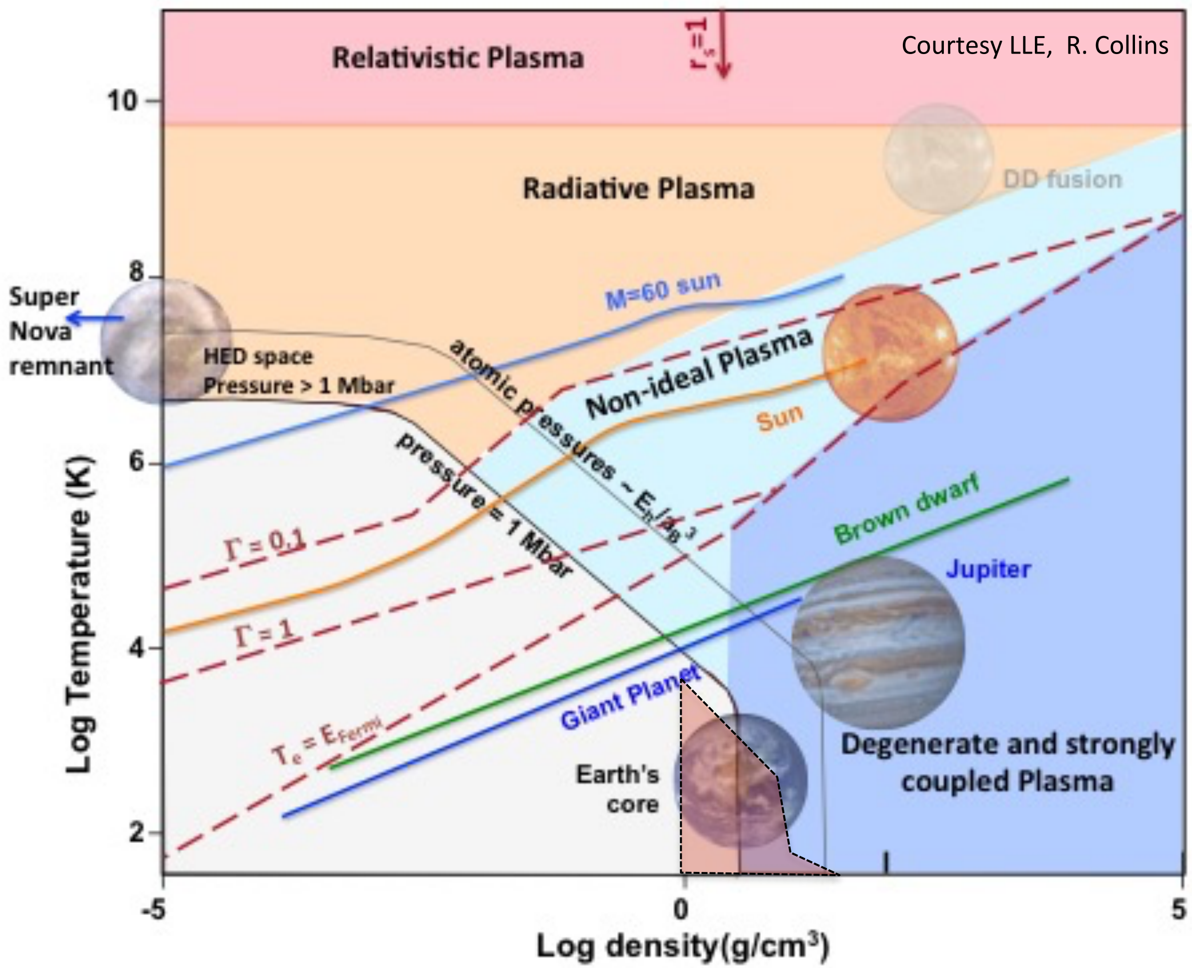



*Gregoryanz et al., Science 2008*

# … studied in laboratories

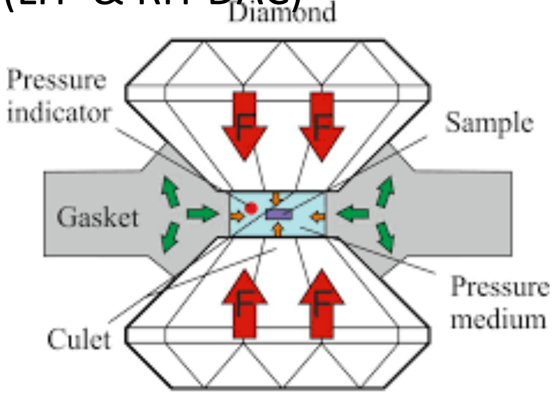
Static compression heating
(LH- & RH-DAC)



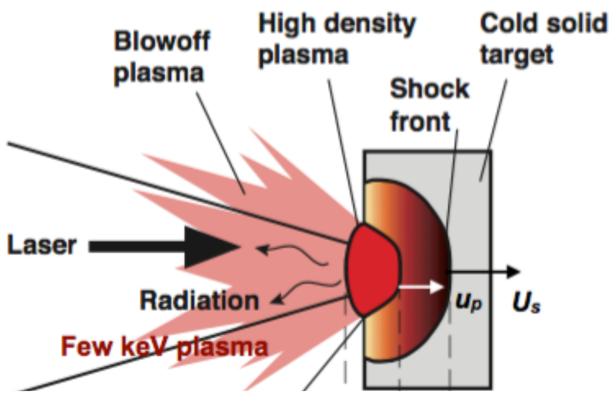



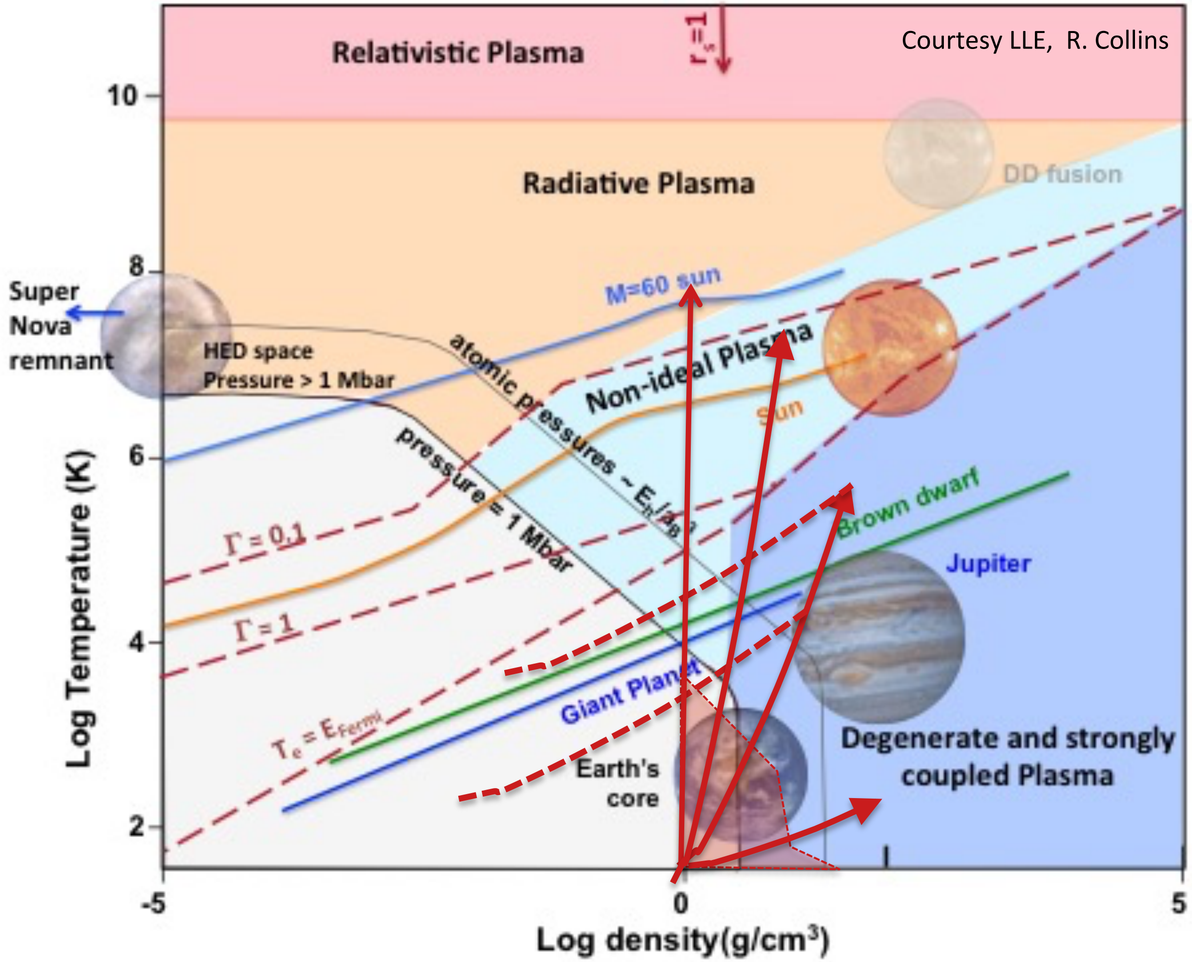
# … in laboratories

Static compression heating
(LH- & RH-DAC)




Dynamic compression and
ultrafast heating with Lasers



# Extreme conditions in laboratory : Time scales

100fs — 1ps — 10ps — 100ps — 1ns — 10ns

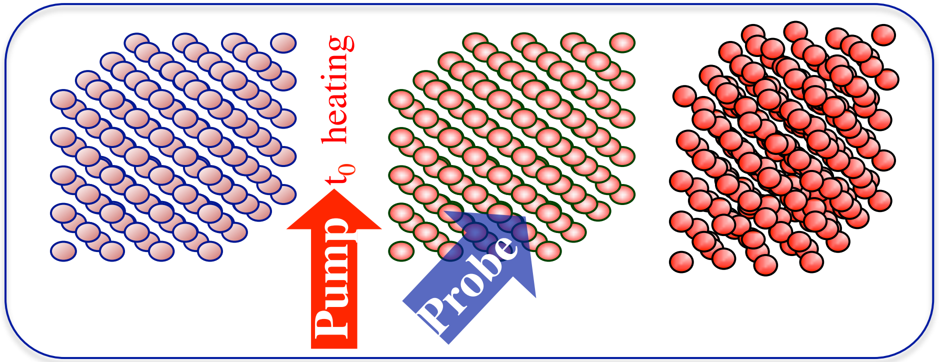
Energy depostion on electrons

Energy transfer and thermic equilibration (e- ion coupling)

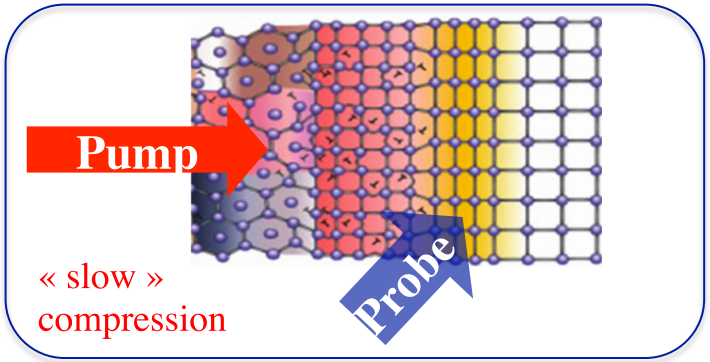
Nucleation process and phase transition

Plasticity and deformation

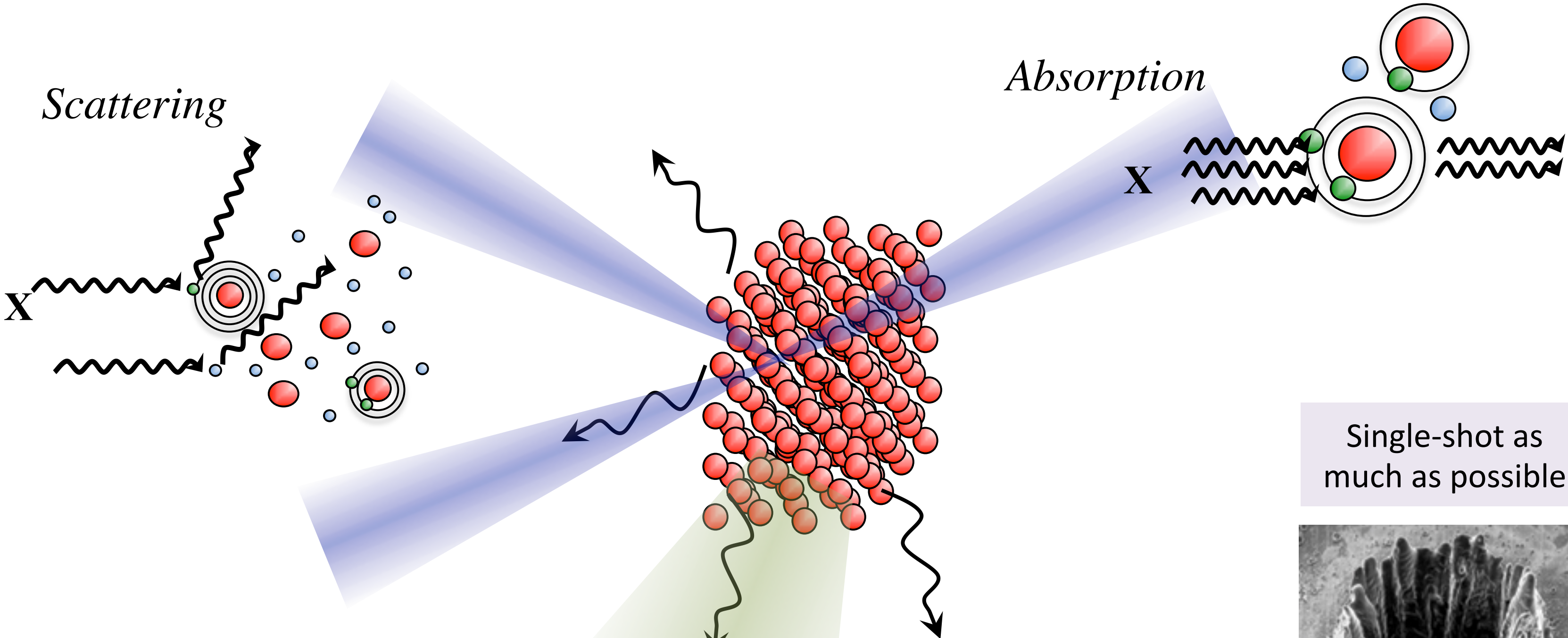
Isochoric heating
(FEL, intense lasers, secondary sources)



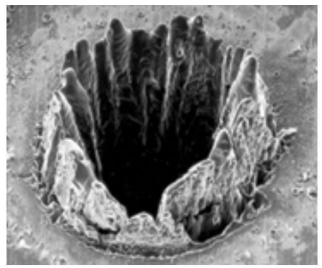

Compression
(high energy lasers)



# X-ray diagnostics for probing extreme conditions




Single-shot as much as possible



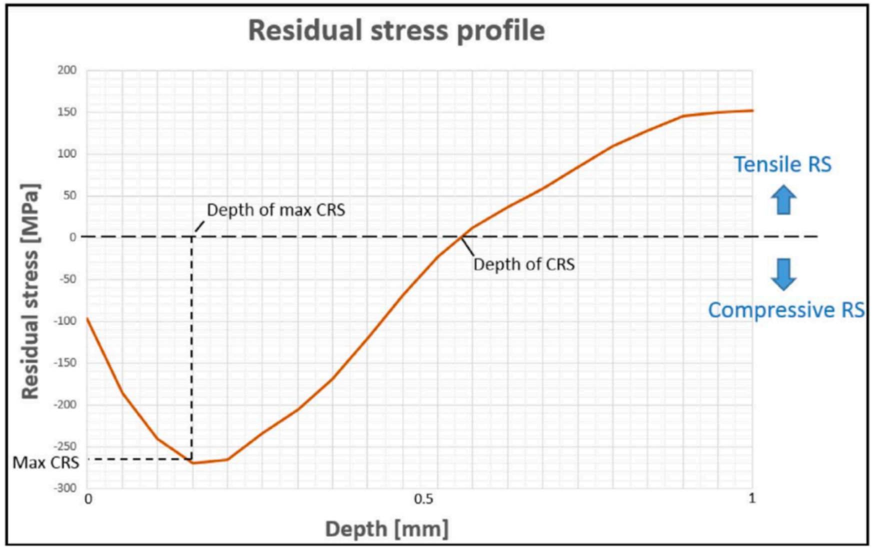
XFEL facilities have already completly modified our experimental approaches giving access to structural, bulk, electronic and atomic properties as well as allowing  X-ray ultrafast heating

New opportunities with Hard X-rays

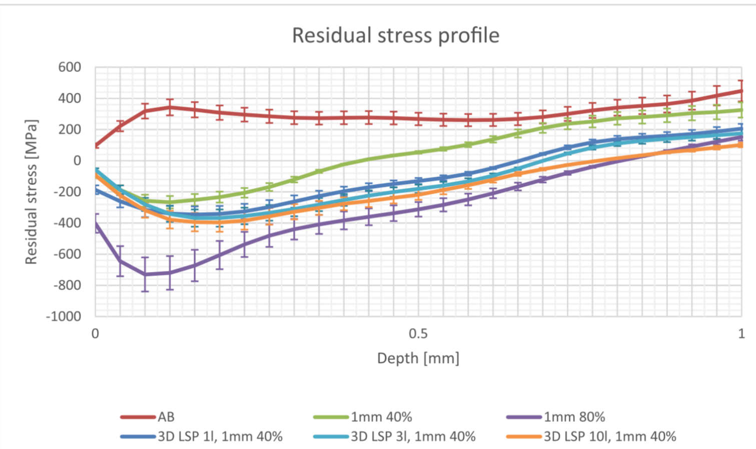
- Probing and heating Larger Volume
- Liquid scattering (PDF) with a unique Q-range
- Extend the accessible range of XAS edges

# Hard X-rays for probing large volume

Caracterizing the bulk stress properties of **real size samples** is crtitical for industrial applications such as Laser shock peening
→ mm to cm size volume of interest for aeronautic applications




N. KALENTICS et al - Materials and Design - Vol. 130 - 2017



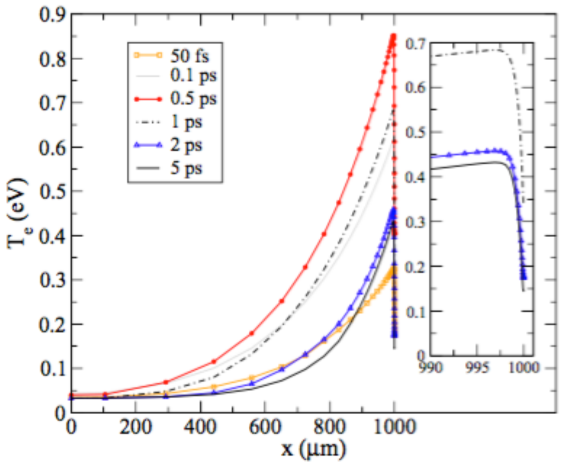

Residual stress measured with a hole drilling model… no in-situ, non destructive bulk method for characterisation of LSP treatment
→ High resolution at depth

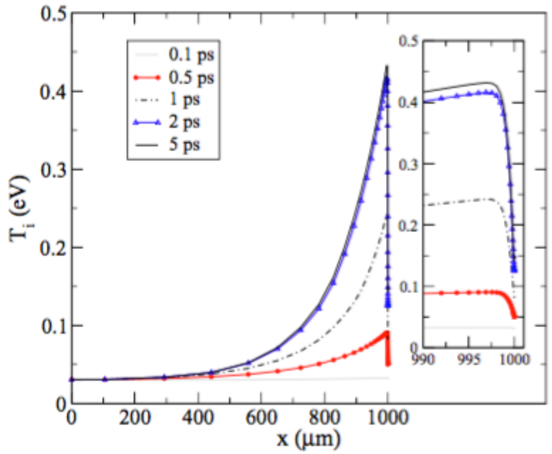
# Hard X-rays for ultrafast heating of large volumes

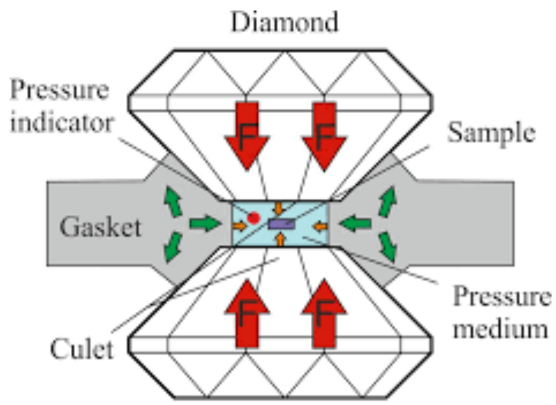
Ultrafast heating produces non thermal equilibrium Te ≠ Ti and allows following thermalisation and e-ion coupling

- Laser heating only on the skin depth (<100nm)
- X-ray heating in volume

10keV simulations on Si



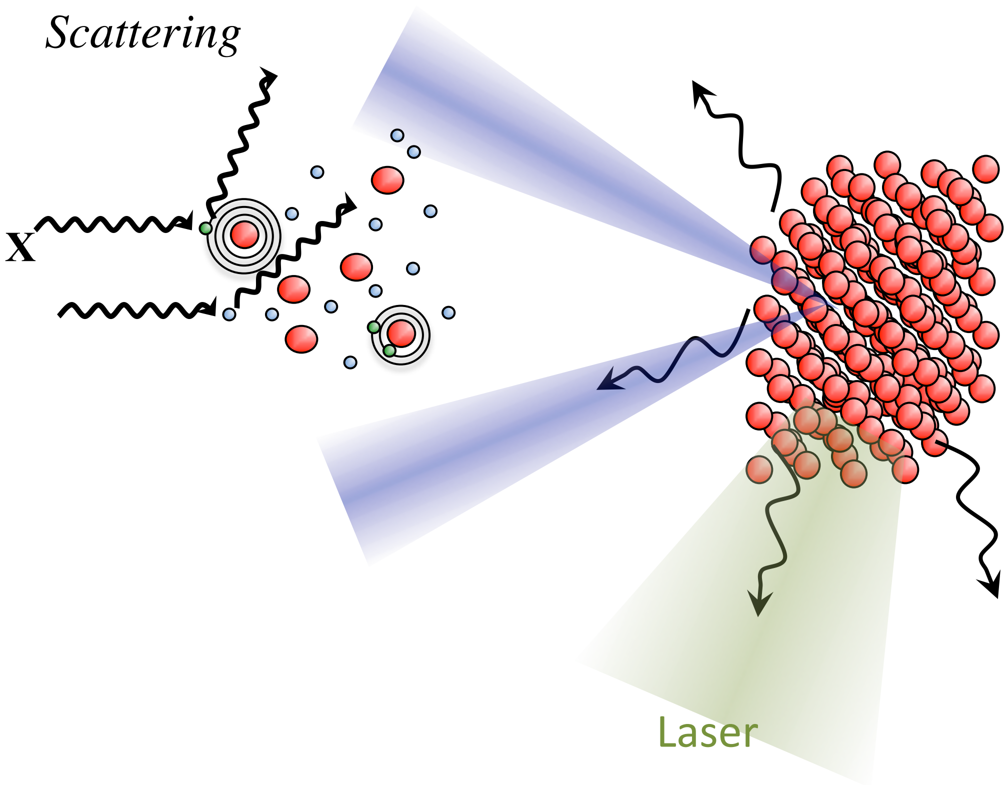




New capabilities for heating complex and large samples such as DAC

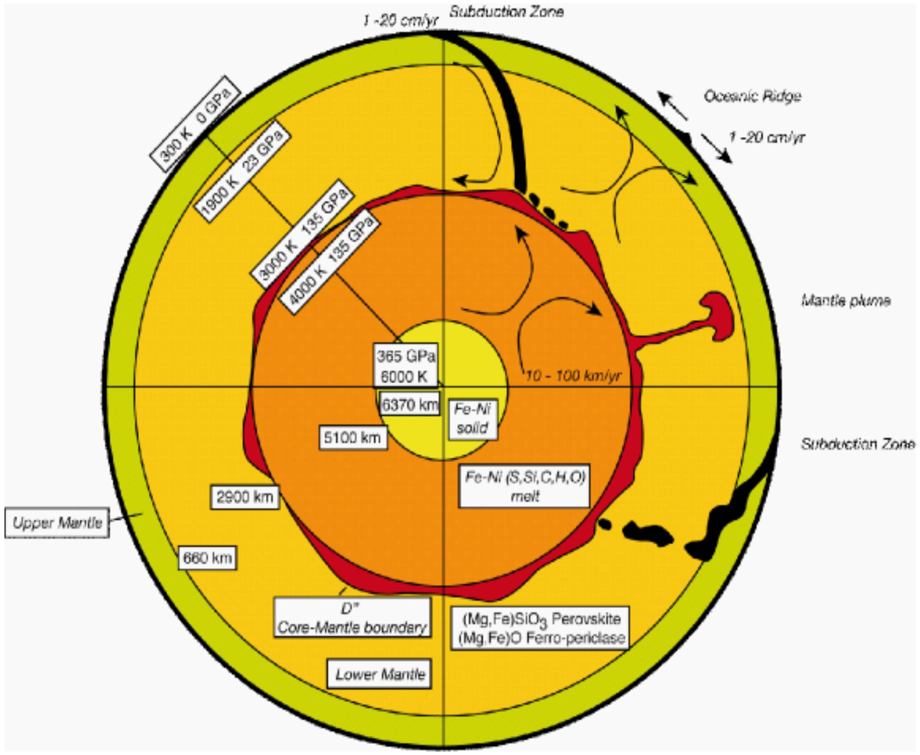
*O. Peyrusse et al. PRE 2017*

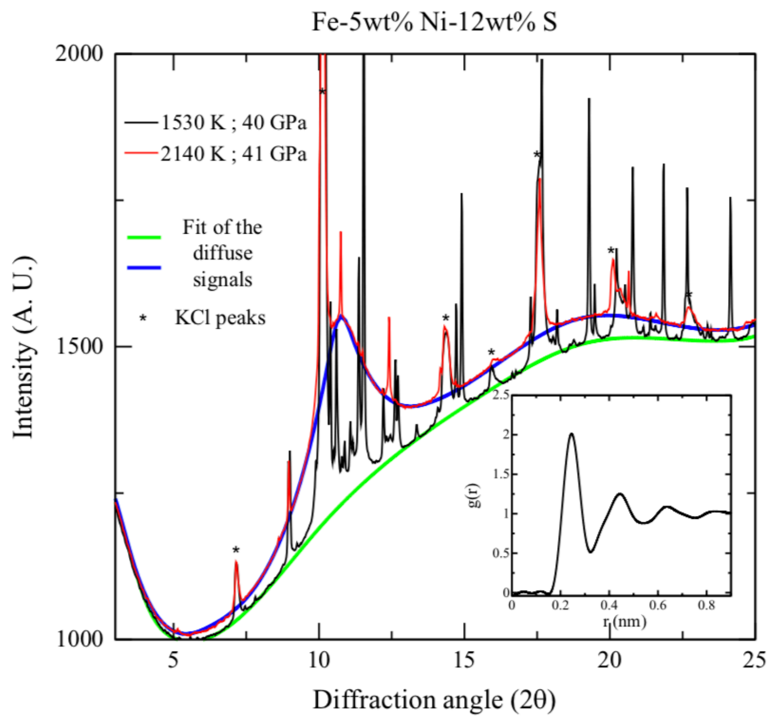
# X-rays Scattering for liquids and amorphs
# Pair Distribution Function




With Hard X-rays
- Probing and heating Larger Volume
- **Liquid scattering (PDF) with a unique Q-range**
- Extend the accessible range of XAS edges

# Liquid studies for Earth interiors




- Generation of Magnetic field
- Constraing the PREM (P,T within Earth)
- Deep magma ocean

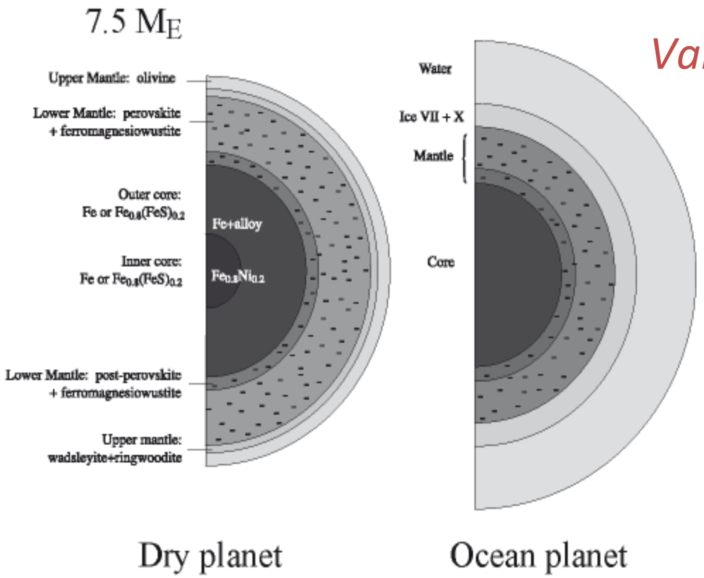
→ Study melting curve and liquid properties of Fe and Fe alloys (Fe-Si, S, Ni, O, C, H)

→ Amorphous properties and coordination (Silcates)

*Morard et al. EPSL 2013*

# Exoplanets Interiors and properties

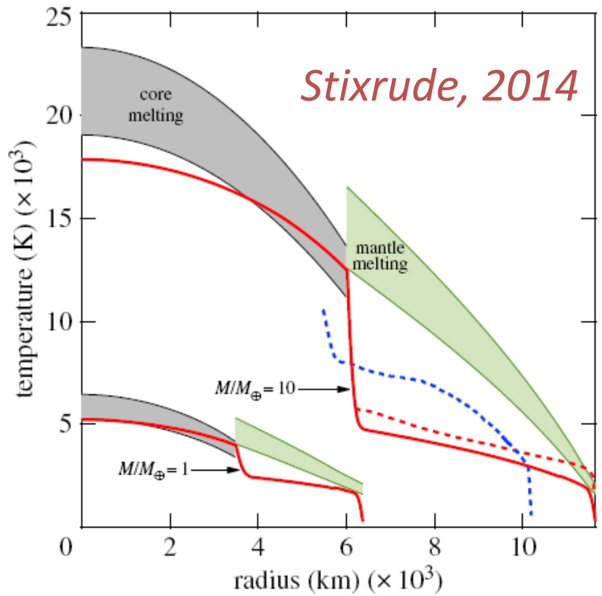
*Valencia 2007*




Core-Mantle Boundary
P = 1100 GPa
T = 5000 K

Center of the planet
P = 3400 GPa
T = 7000 K

*Stixrude, 2014*



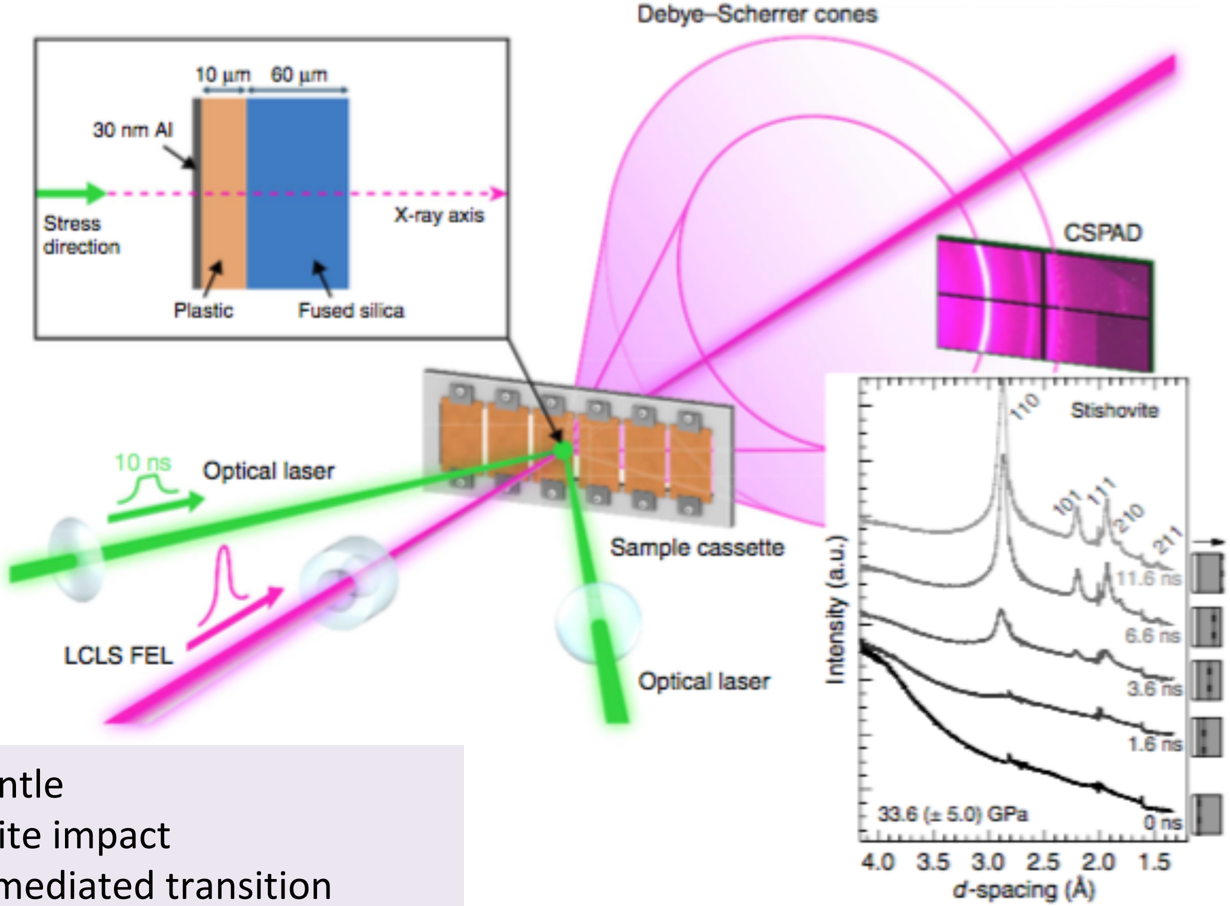

- Big inner core, entirely solid?
- Tectonic?
- Dynamo and Magnetic field? From liquid Fe alloy core? From silicates

→Extend studies to much higher pressure (several Mbar) with Laser compression

→ Very weak scattering signal … It needs high brightness as XFEL's

# Amorphisation under high-velocity impact

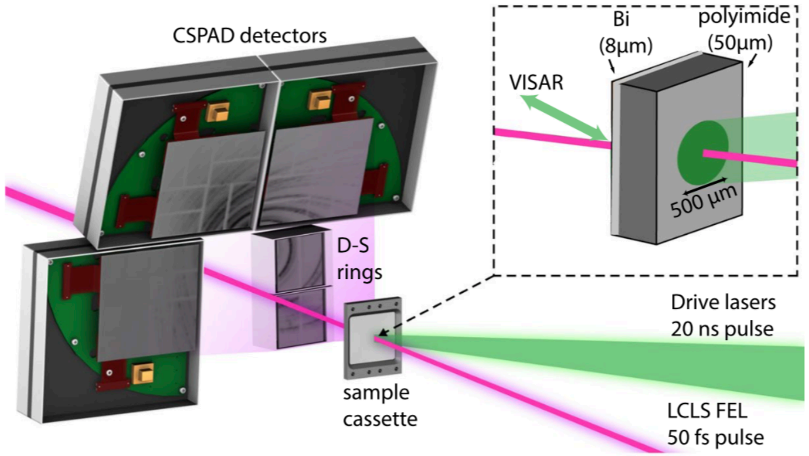
Production of nm-size stichovite under shock
as example of an ultrafast reconstructive Phase Transitions

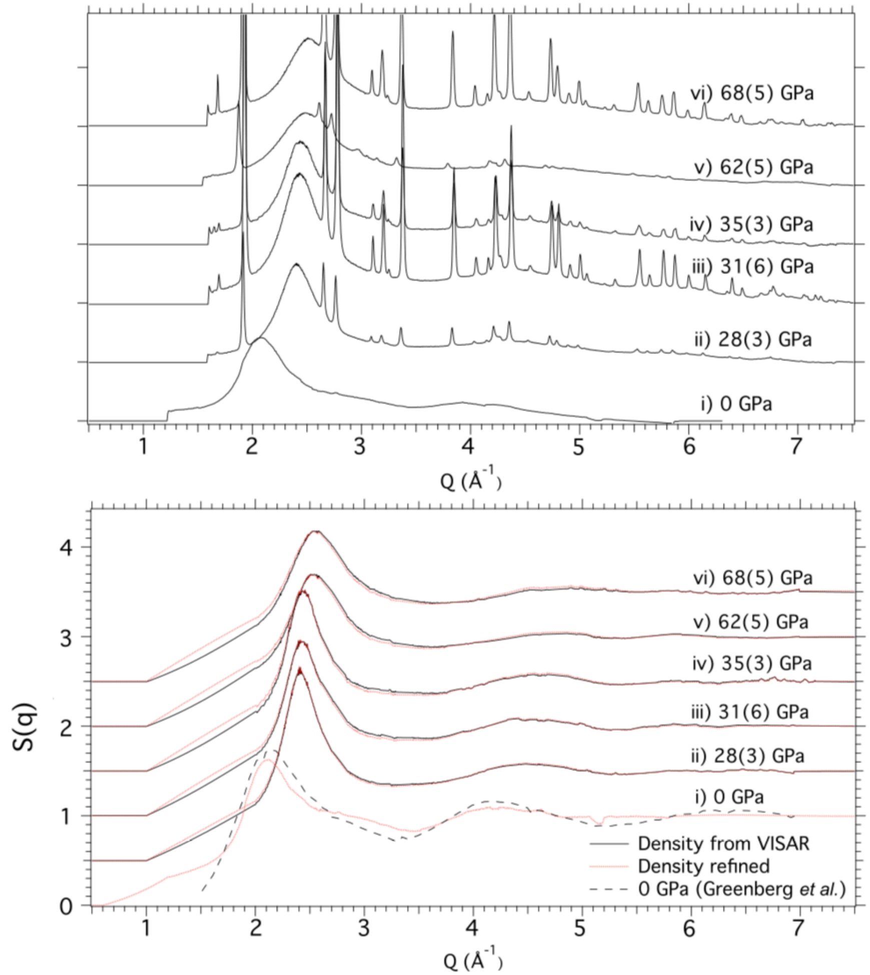



One of the major mineral of the mantle
Observed on hyper-velocity meteorite impact
→ Very fast process for a diffusion mediated transition
→ Was expected to require an amorphous PT
→ Needs further detailled studies to track the PT process

*Gleason et al. Nature Com. 2015*

# Recent Liquid scattering at LCLS on Bi

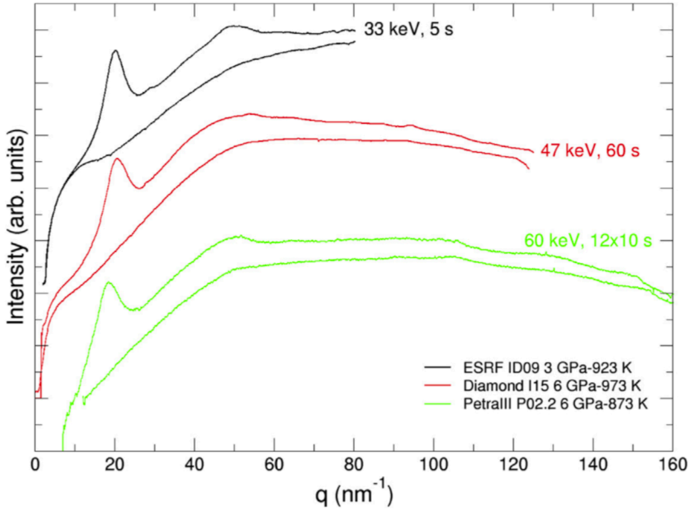


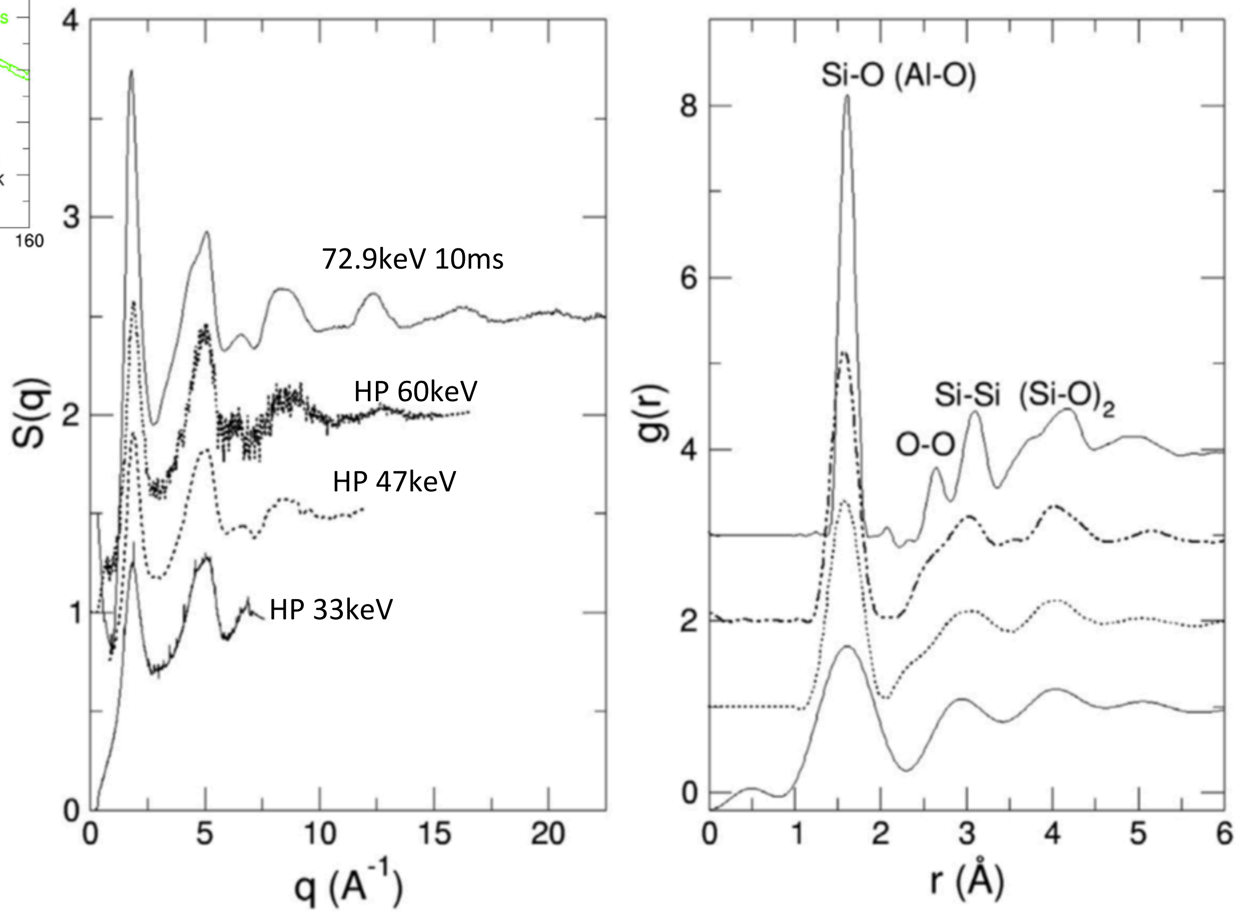

- Significant Improvements of the melting signal
- Should be even better at the HED-HIBEF beamline with large area detectors
- Q range still limited…

*Gorman et al. Scientific Report (2018)*

# Hard X-ray Scattering for liquids and amorphs

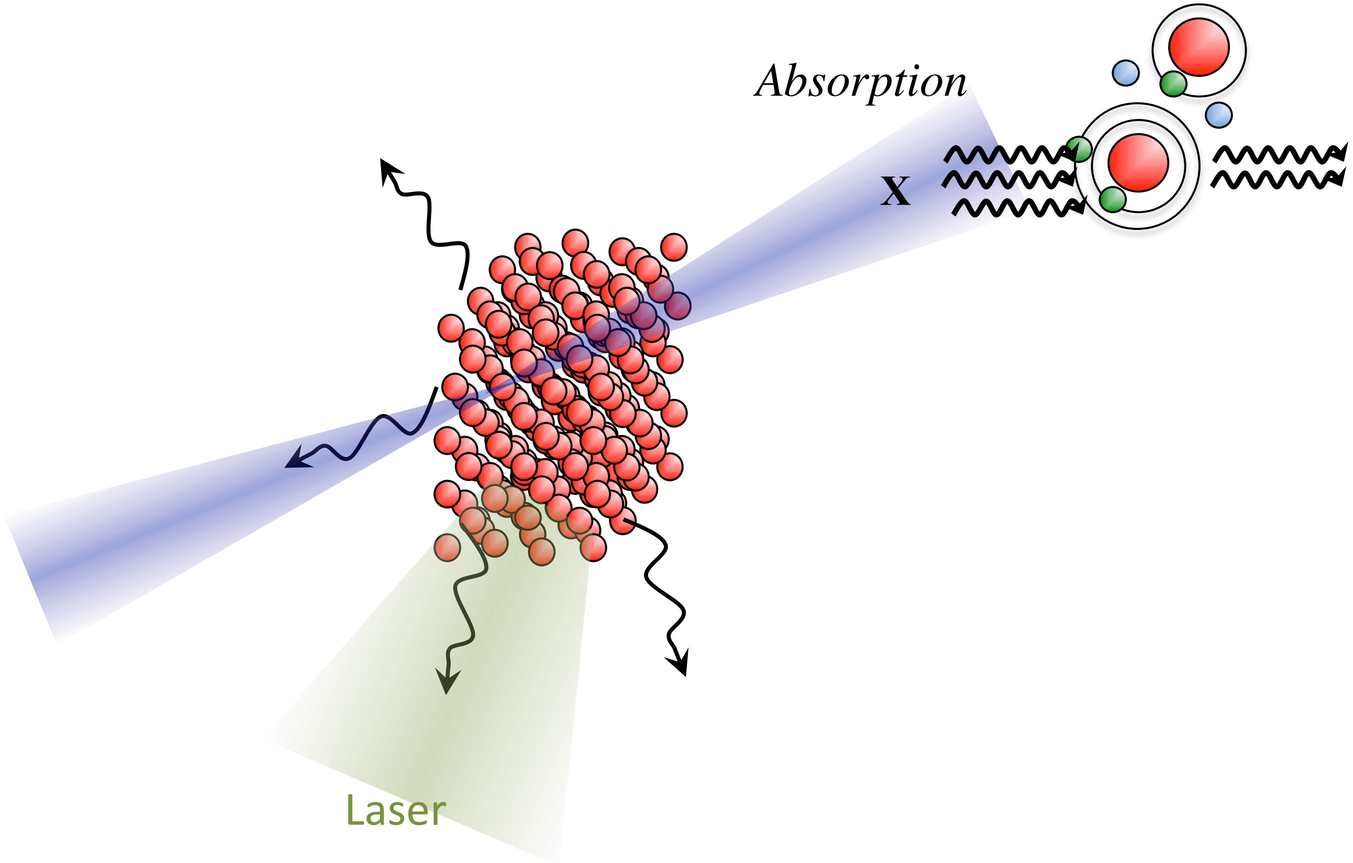



HPG glass



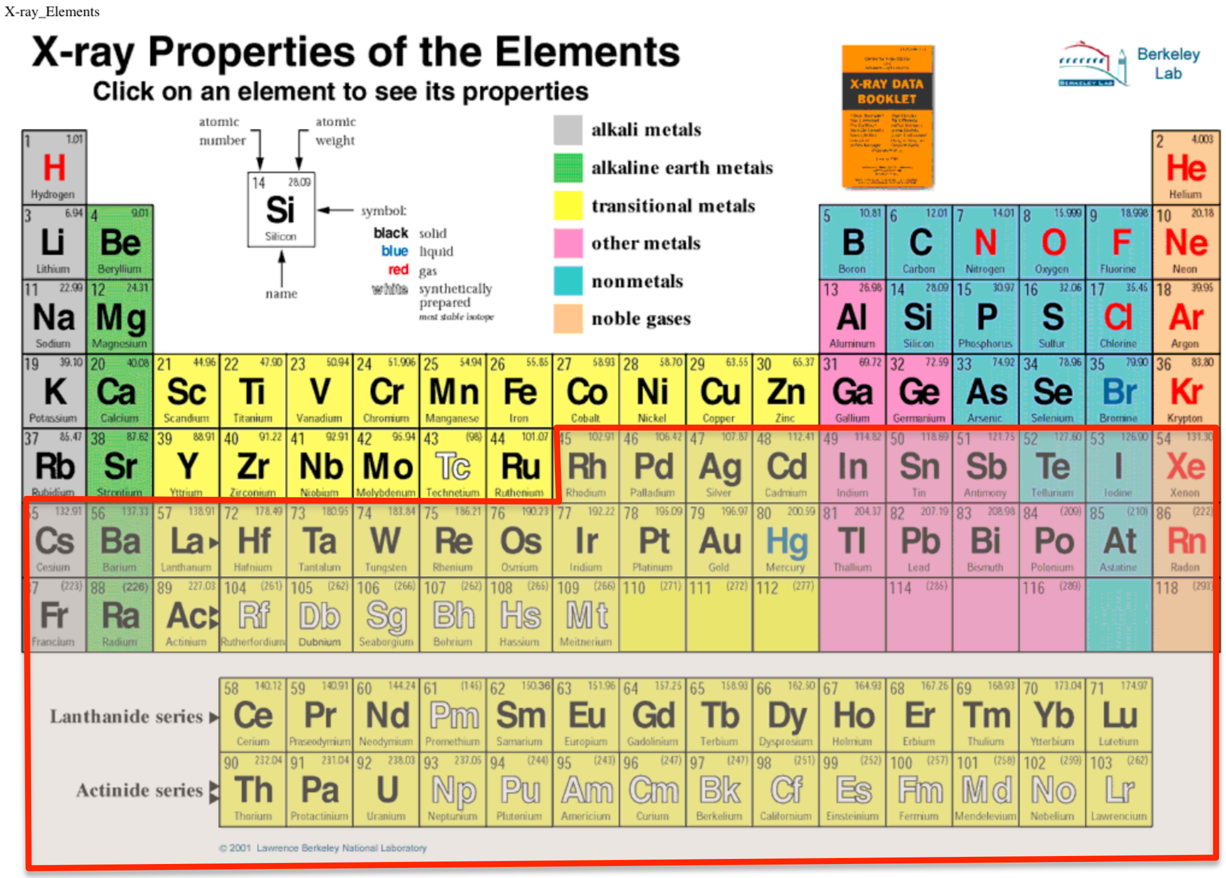

*C. Sanloup, Chap.5 - Magmas under high pressure, Elsevier 2018*

# X-ray diagnostics for probing extreme conditions




With Hard X-rays
- Probing and heating Larger Volume
- Liquid scattering (PDF) with a unique Q-range
- **Extend the accessible range of XAS edges**

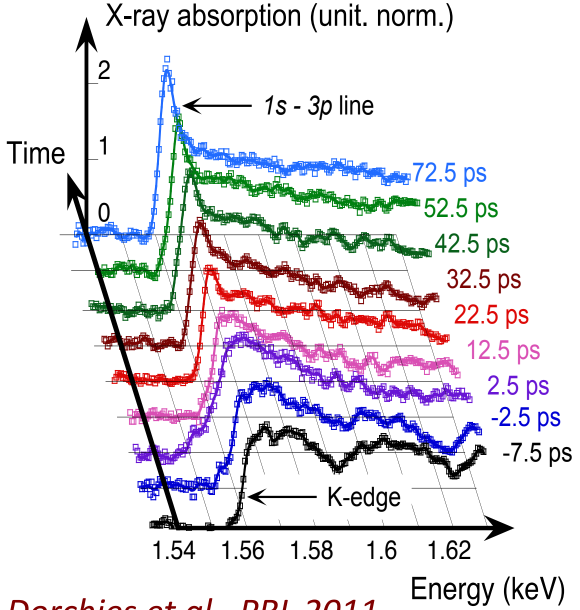
# High-energy absorption edge spectroscopy




K-edges above 24keV

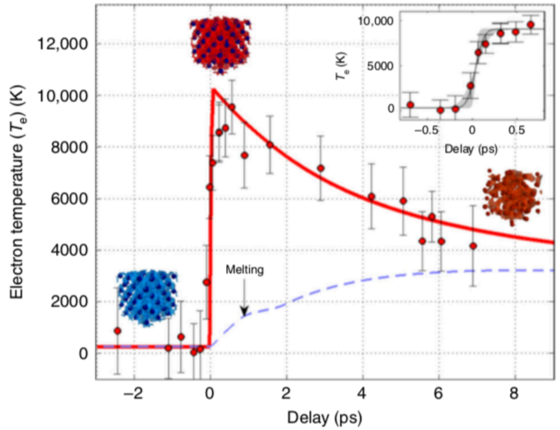
# XAS for ultrafast laser heating on Higher Z-elements

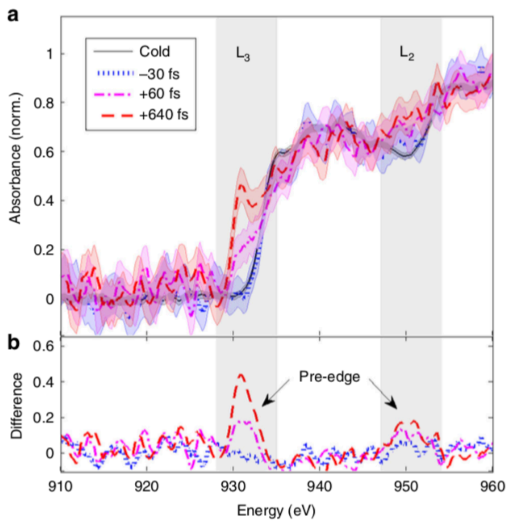
Solid-liquid-vapor transition with ultrafast laser heating




*Dorchies et al., PRL 2011*

Bond hardening and anomalous melting for 3d metals under ultrafast heating



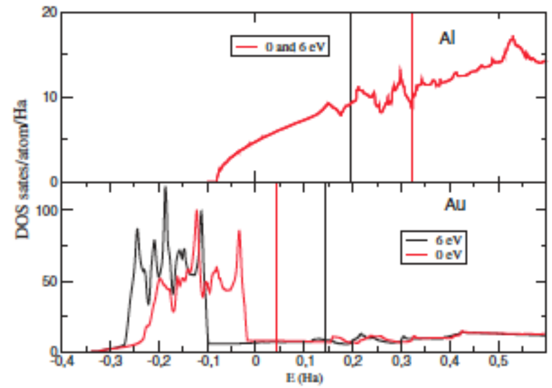




*Recoules et al, PRL 2006*
*Mahieu et al. 2018*

- Understanding how electron structure affect the melting under ultrafast heating

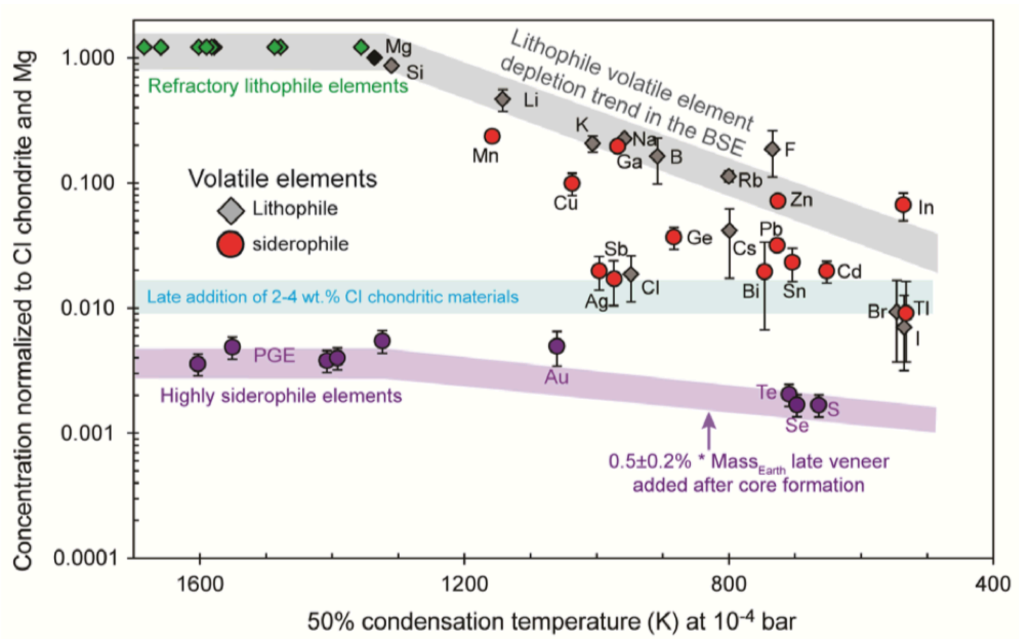
→ Reconstruct the full DOS ( p, d ) at the L-edge and K-edges of Sn, Au, Ta, Bi

→ Access fs temporal resolution and go further than actual limitations of secondary X-ray sources

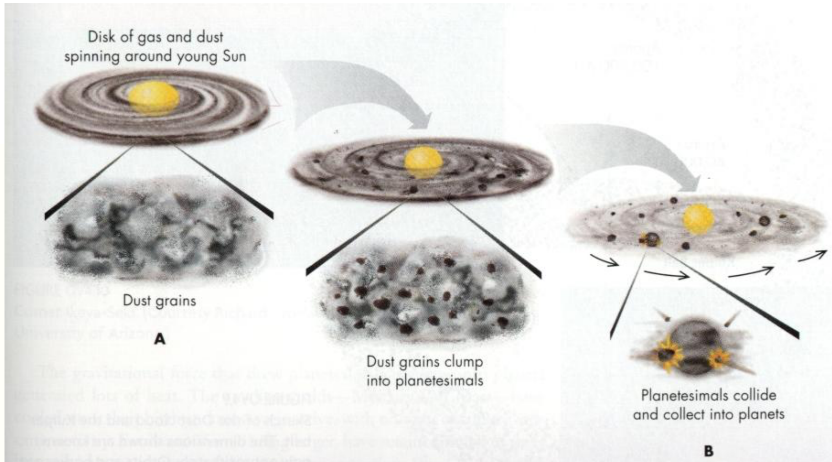


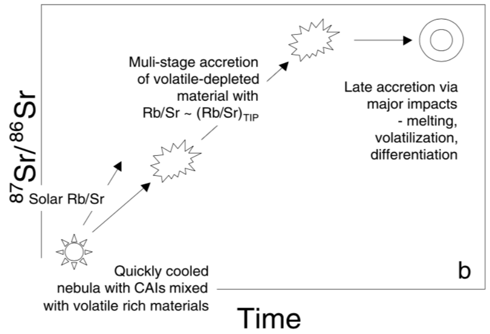
# Trace Elements for understanding the Earth and Moon formations

- The Earth Bulk Silcate has a slighlty different composition than the Sun
  → studies of the trace elements in function of P,T
  → PaleoCosmoChemistry : Life-time of traces elements are used for datation and planet formation history
- The moon does not have the same composition of the Earth → giant impact from a mars-size object




Wang et al

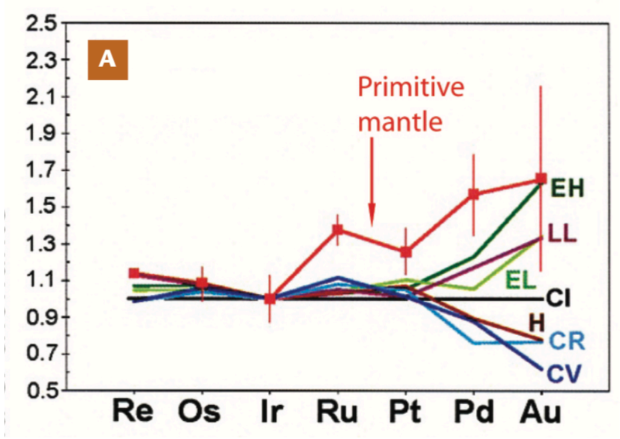



*Halliday et al.*

# X_ray absorption of trace elements

- What happen to traces elements during impact?
- What about the impactor?
- What about the effect of the debris accretion?

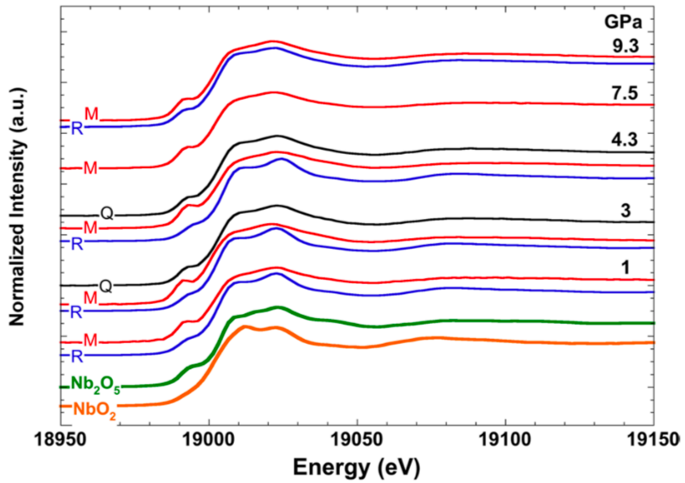



*Lorand et al. Elements, VOL. 4, PP. 247–252 (2008)*

Siderophile K-edges
- Ir 76,1keV
- Au 80,7keV
- Pt 78,3 keV

Rare Earth Lithophile
- Xe 34,5keV
- Ce 40,4keV
- Eu 48,5keV
- …

Nb local structure and oxidation state in silicate melts




*Sanloup et al. Jour. Phys. Cond. Matter 2018*

- XAS is element selective and would allow to track local order and valence state under shock
- Many elements have energy edges above 24keV

# Conclusion

- Wide range of extreme conditions applications would benefit from 100keV XFELs
  - Material science
  - Industrial applications
  - Geoscience and (exo)-planetary science

- Unique abilities for
  - Probing and heating large volume samples
  - Liquid and amorph pair distribution functions
  - High-energy edges for XAS