

Hard X-ray FEL for matter under extreme conditions

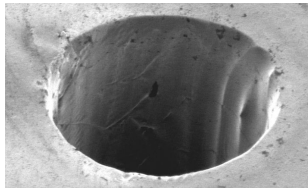
Marion Harmand et al.

IMPMC – CNRS, Sorbonne Université, MNHN - France

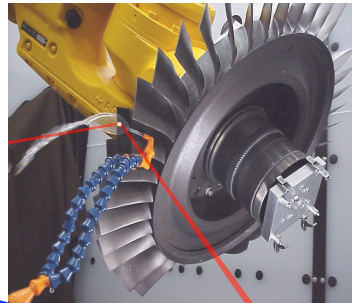


Matter under extreme conditions - large range of application, topics... and time scales

Laser industrial processes



fs drilling

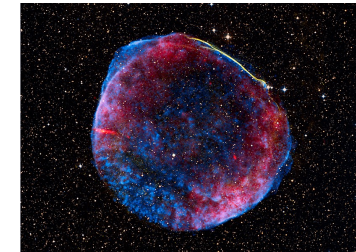


Laser shock hardening

Astrophysical shock wave



Polar Accretion column



Supernovae remnant

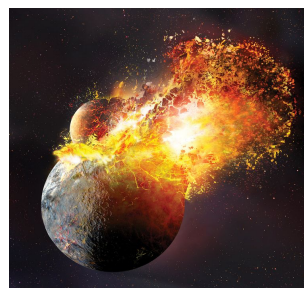
High velocity impacts



Space debris impacts



Meteorite craters



Giant impacts

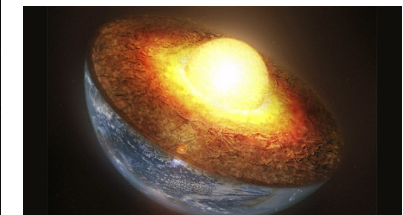
10^6 years

10^9 years

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

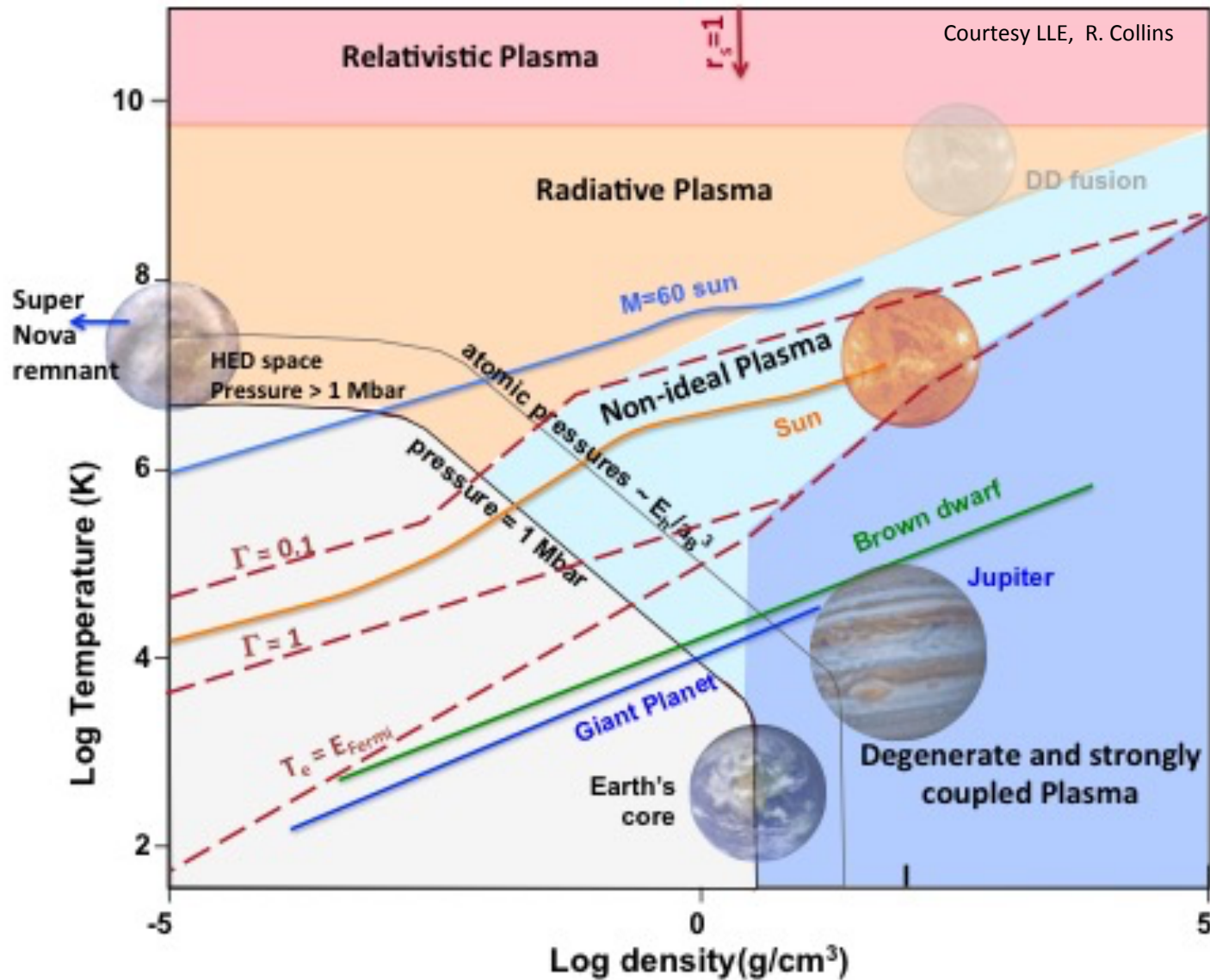


Trappist system



Earth interior

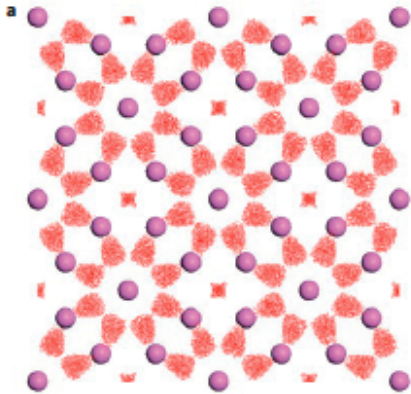
Matter under extreme conditions - large range of thermodynamic conditions



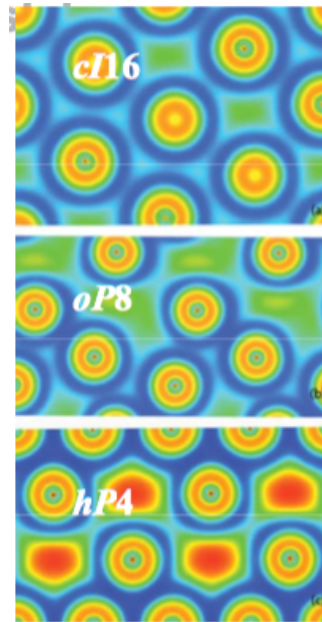
Non expected physical properties of matter

At high pressures and high temperature, the interplay between electron and ions play a major role

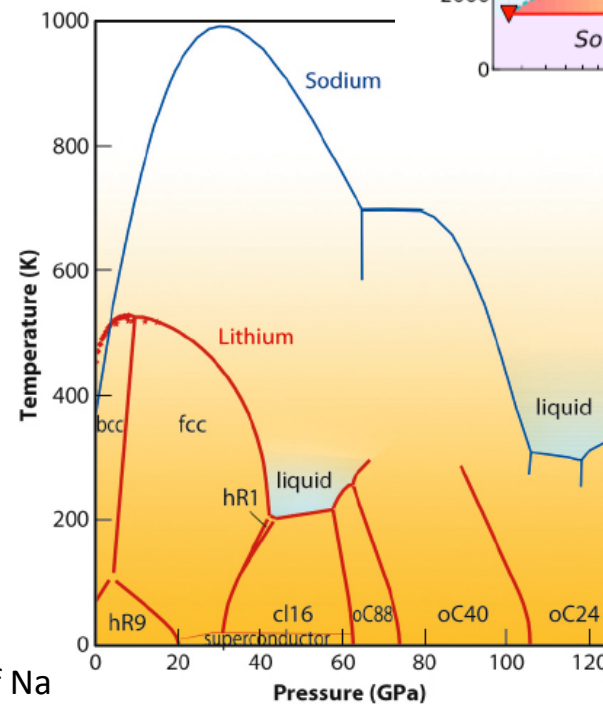
- Orbital hybridization
- Interstitial, localized electron bonding
- Gap changes, metallization...



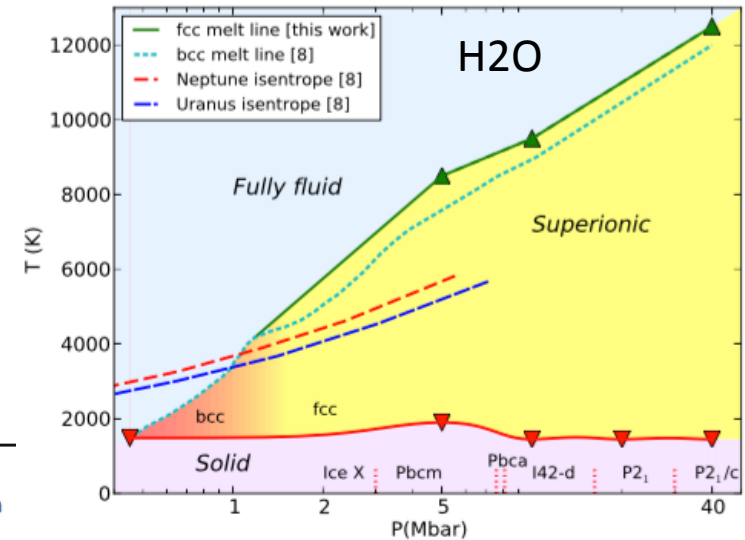
Host guest structures in Al at Tpa pressures
Pickard, Nature Materials 9, 2019



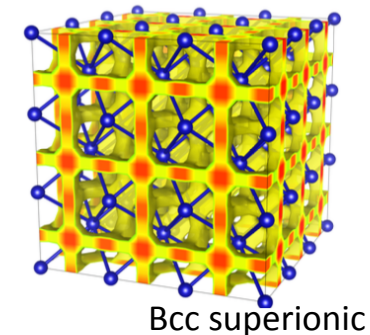
Electron localized function of Na
Marques et al, PRB 2009



Gregoryanz et al., Science 2008



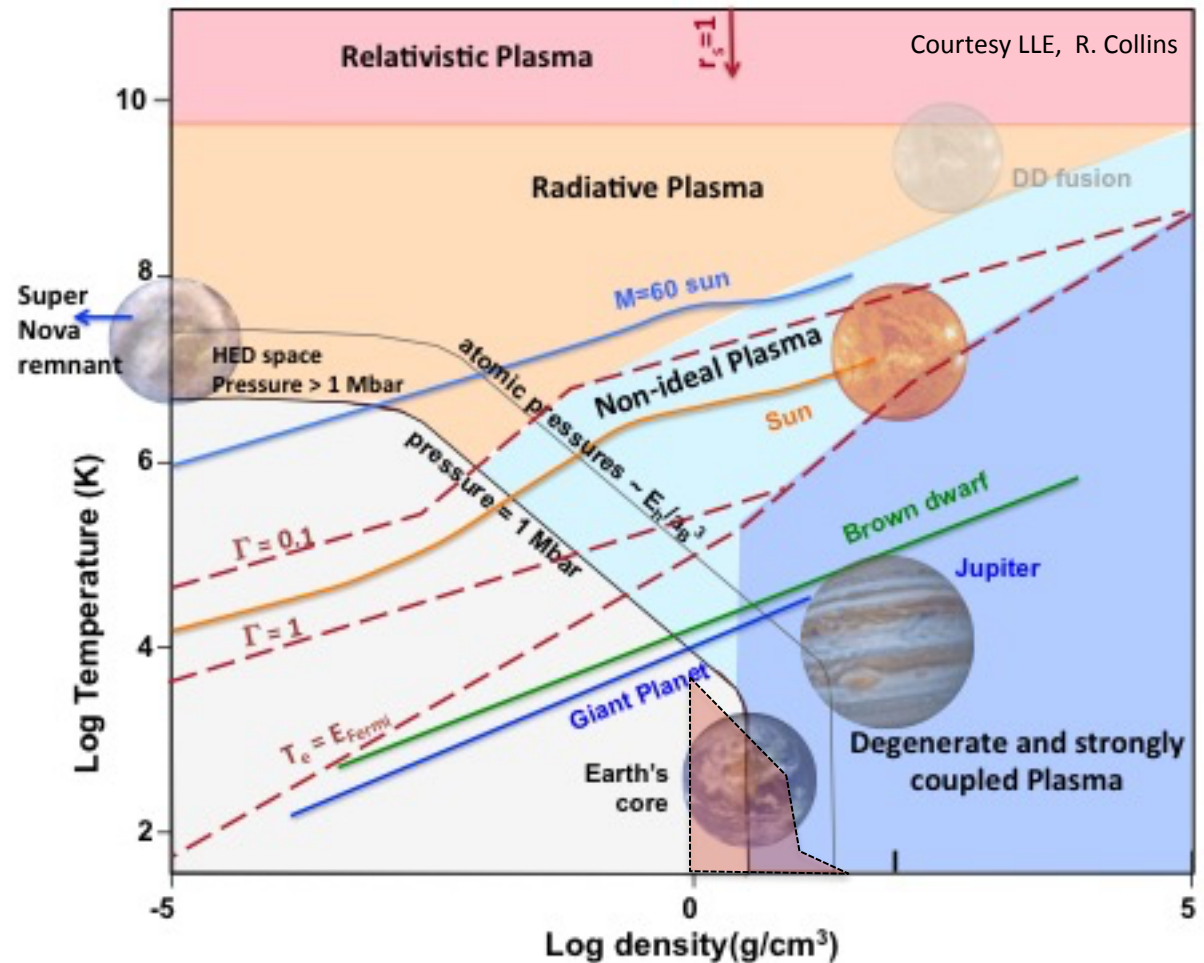
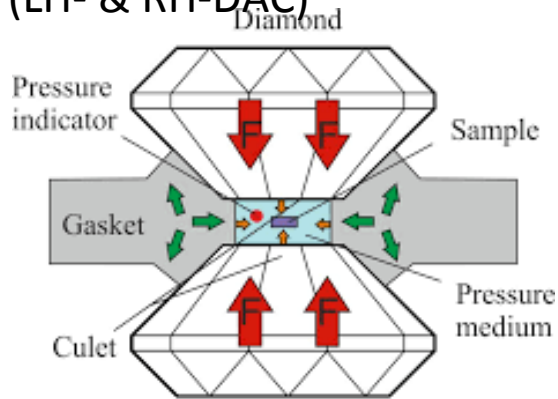
Wilson et al PRB 2013



Bcc superionic

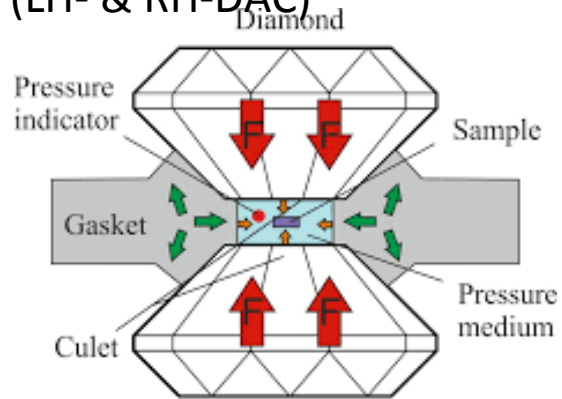
... studied in laboratories

Static compression heating (LH- & RH-DAC)

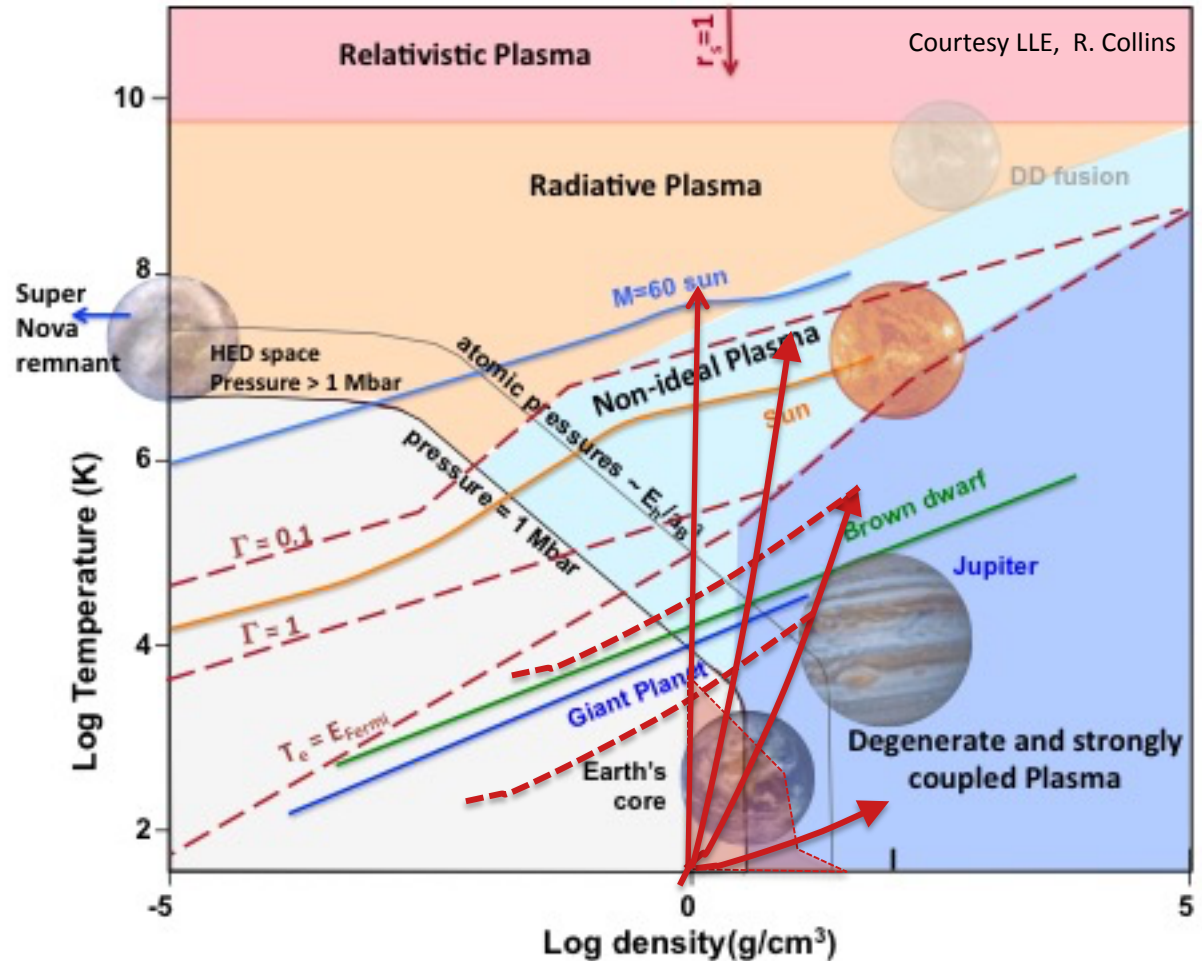
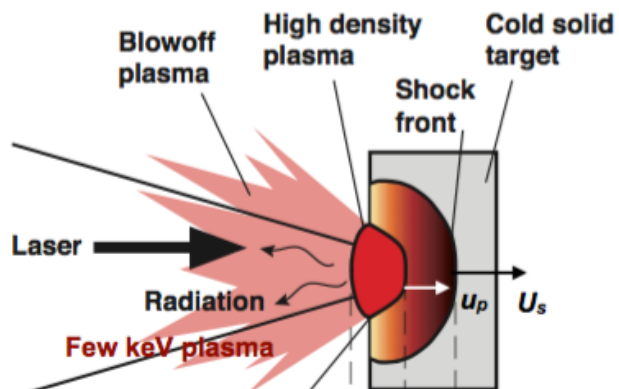


... in laboratories

Static compression heating
(LH- & RH-DAC)

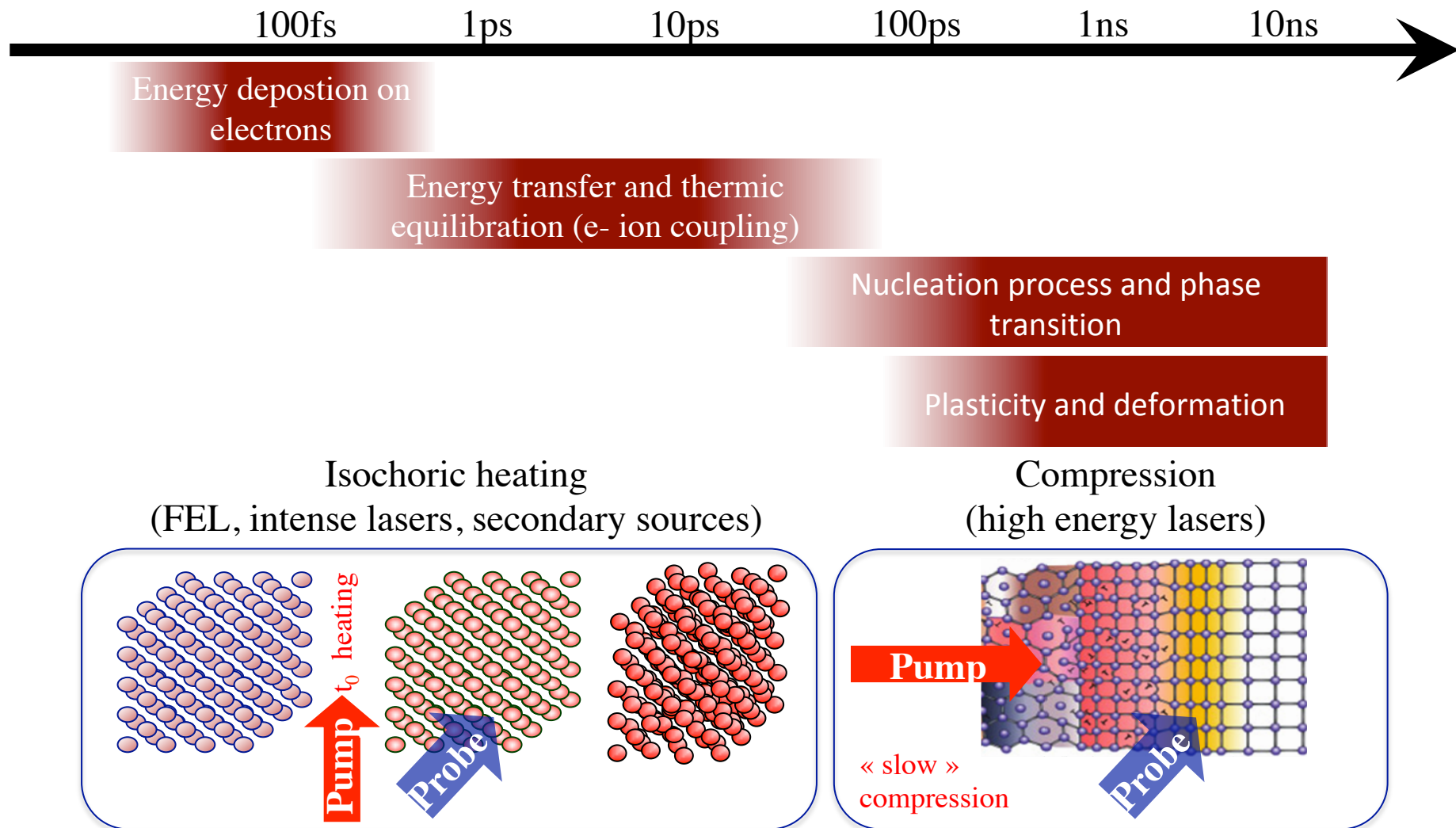


Dynamic compression and
ultrafast heating with Lasers

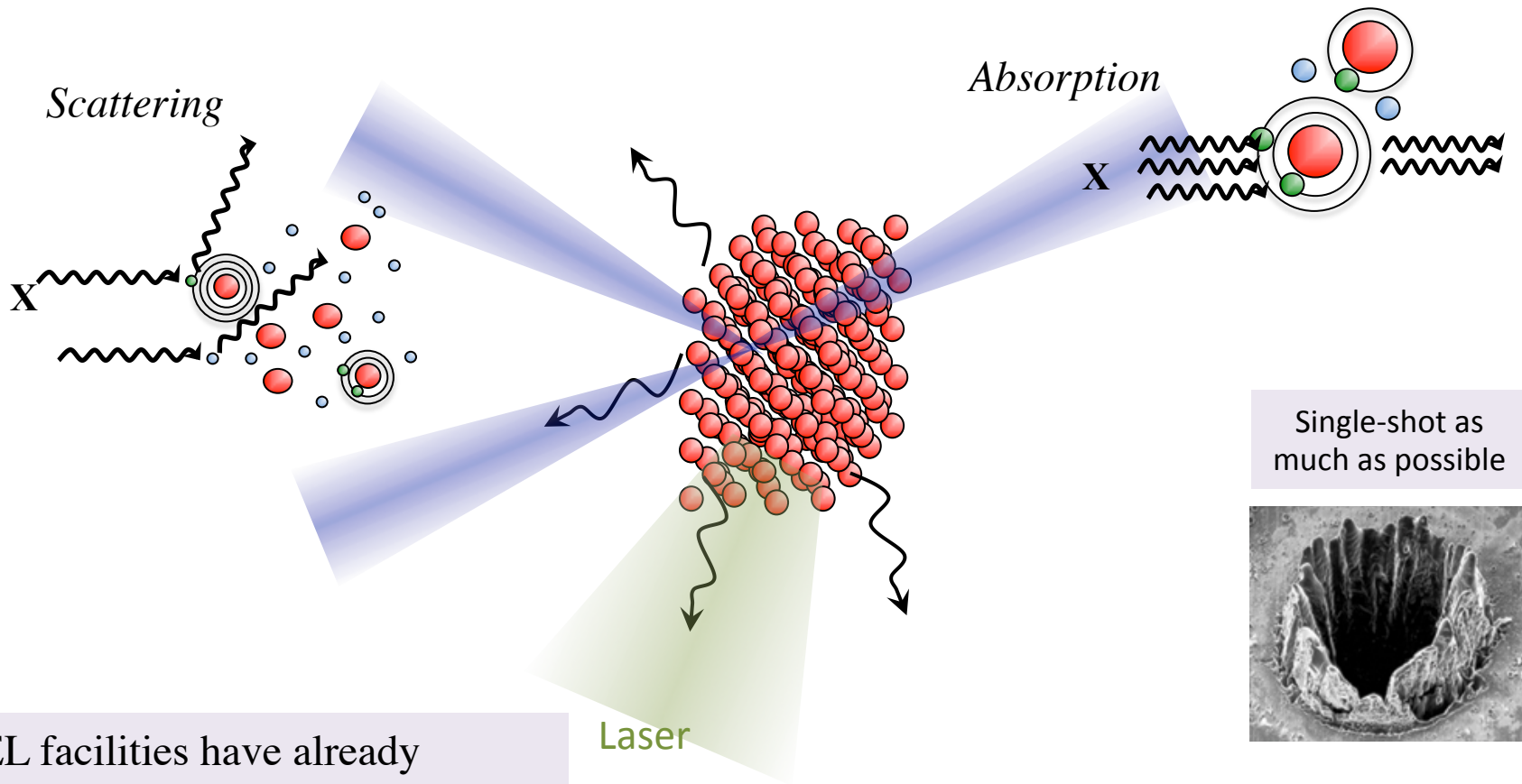


Courtesy LLE, R. Collins

Extreme conditions in laboratory : Time scales



X-ray diagnostics for probing extreme conditions



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

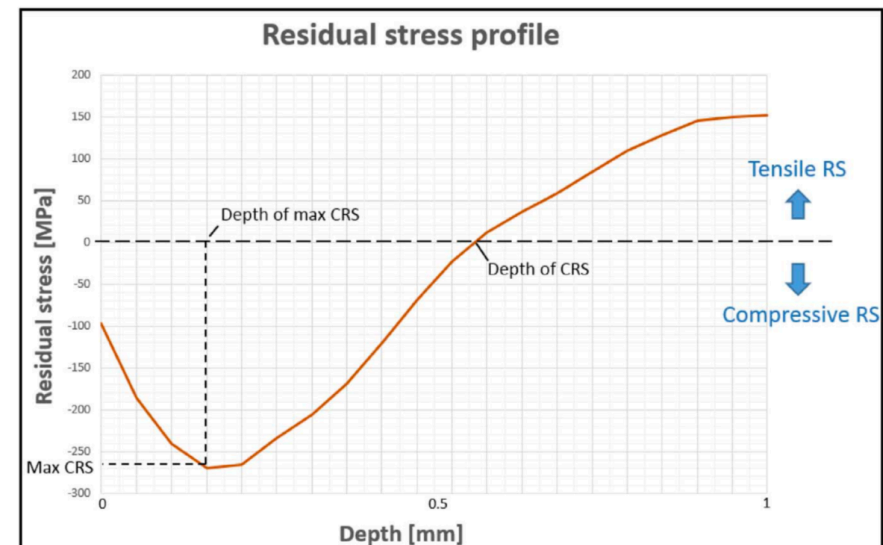
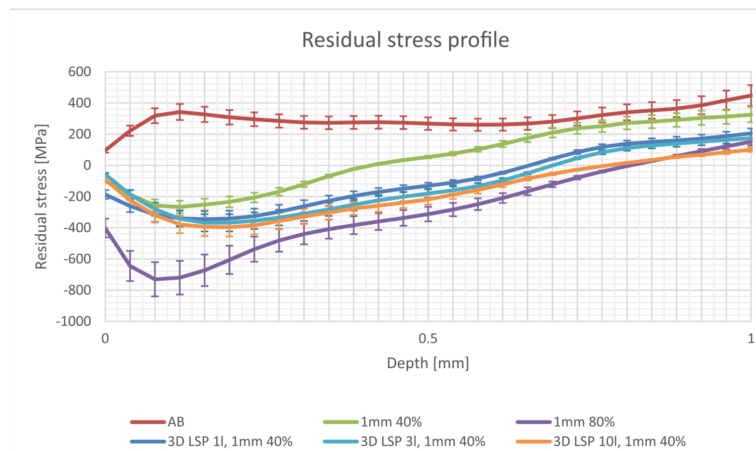
New opportunities with Hard X-rays

- 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

Characterizing the bulk stress properties of **real size samples** is critical 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

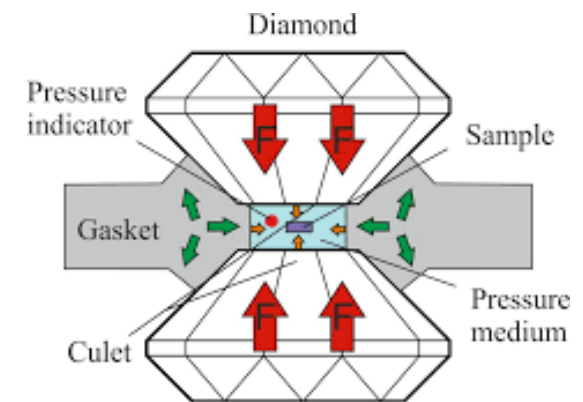
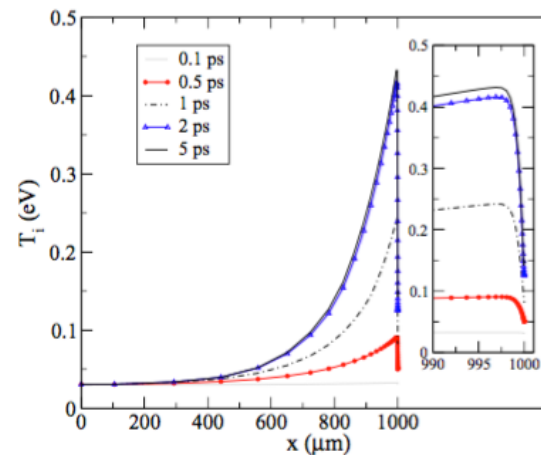
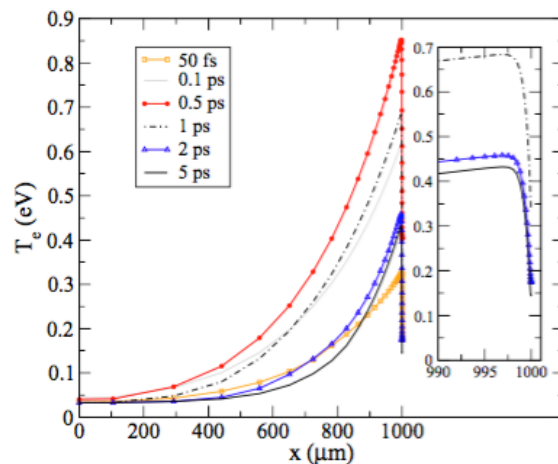
Residual stress measured with a hole drilling model... no in-situ, non destructive bulk method for characterisation of LSP treatment
→ High resolution at depth

Hard X-rays for ultrafast heating of large volumes

Ultrafast heating produces non thermal equilibrium $T_e \neq T_i$ and allows following thermalisation and e-ion coupling

- Laser heating only on the skin depth ($<100\text{nm}$)
- X-ray heating in volume

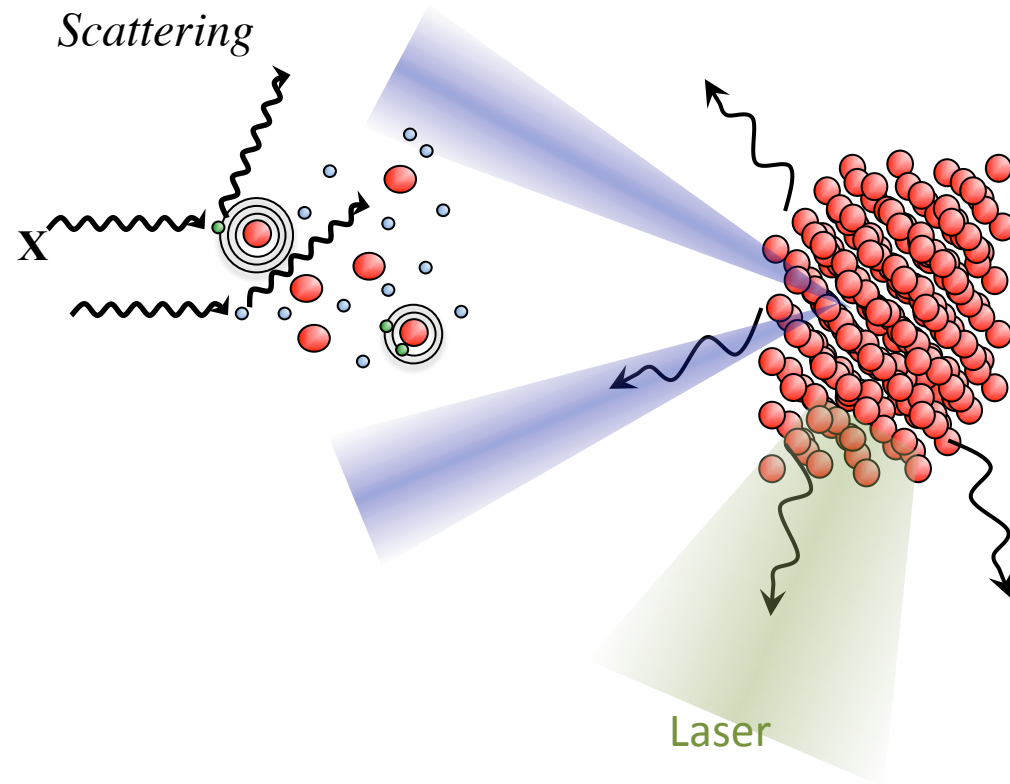
10keV simulations on Si



New capabilities for heating complex and large samples such as DAC

X-rays Scattering for liquids and amorphs

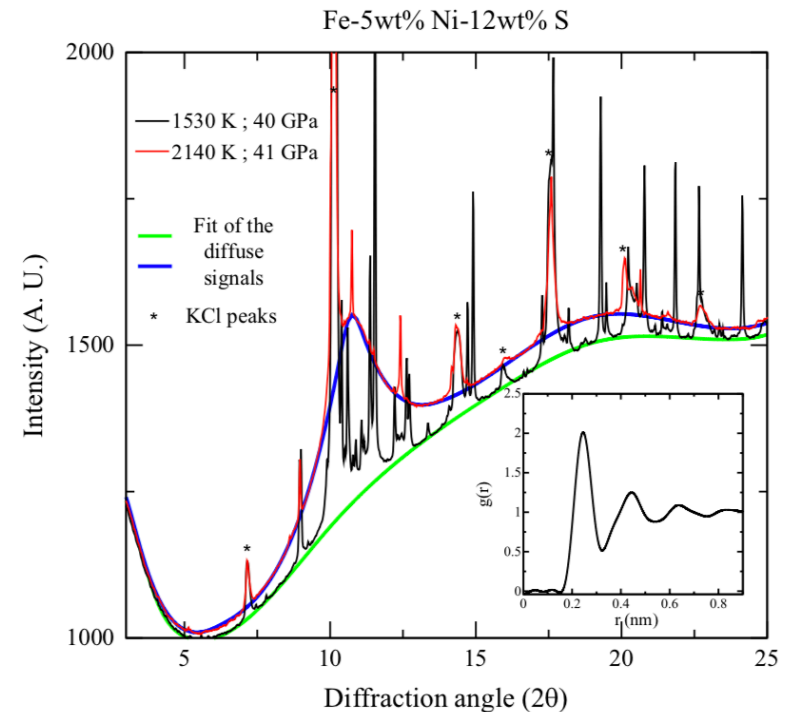
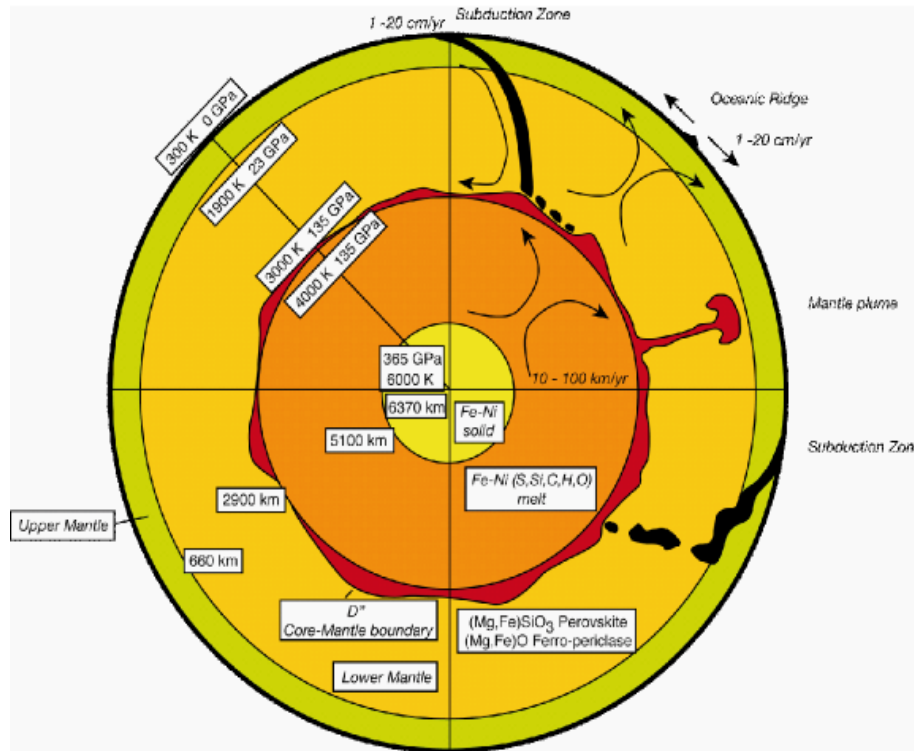
Pair Distribution Function



With Hard X-rays

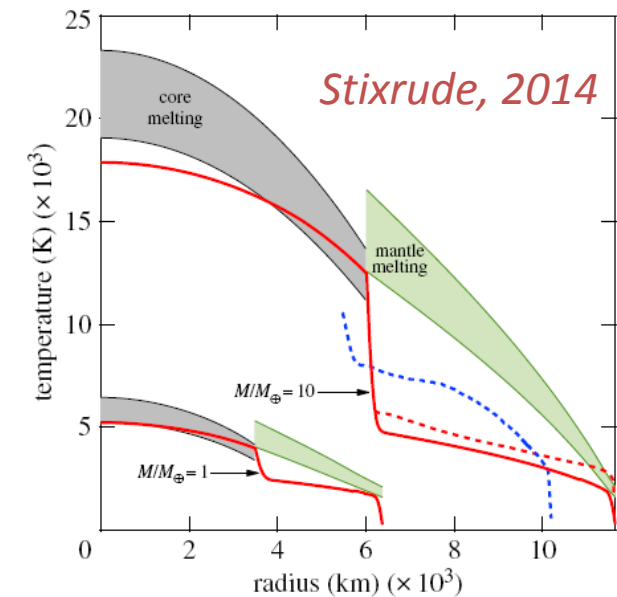
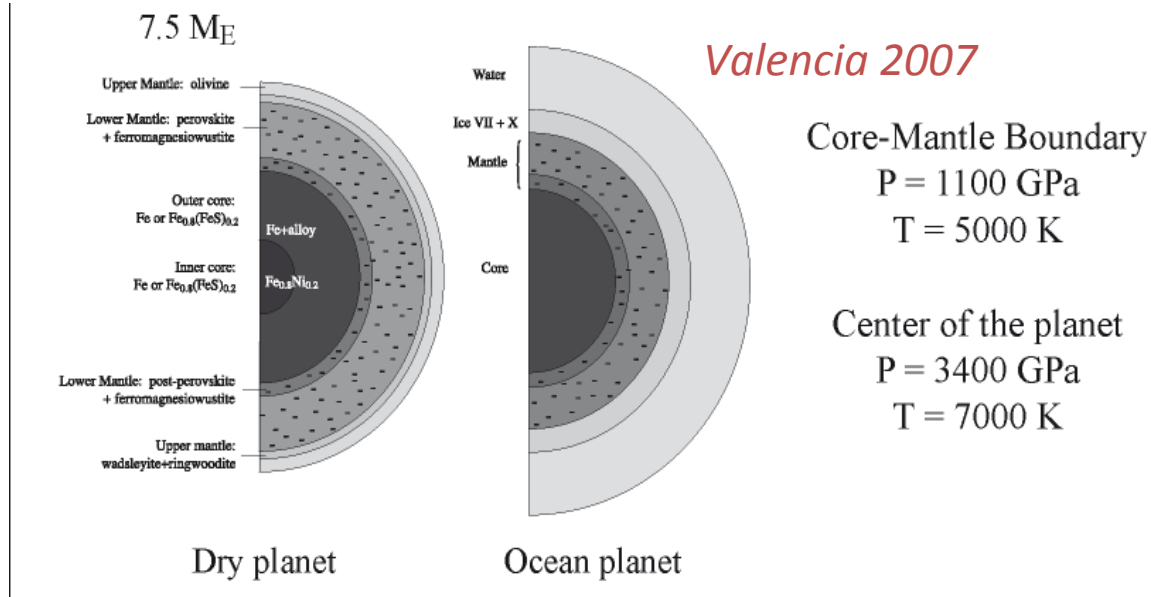
- Probing and heating Larger Volume
- **Liquid scattering (PDF) with a unique Q-range**
- Extend the accessible range of XAS edges

Liquid studies for Earth interiors



- Generation of Magnetic field
- Constraining 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 (Silicates)

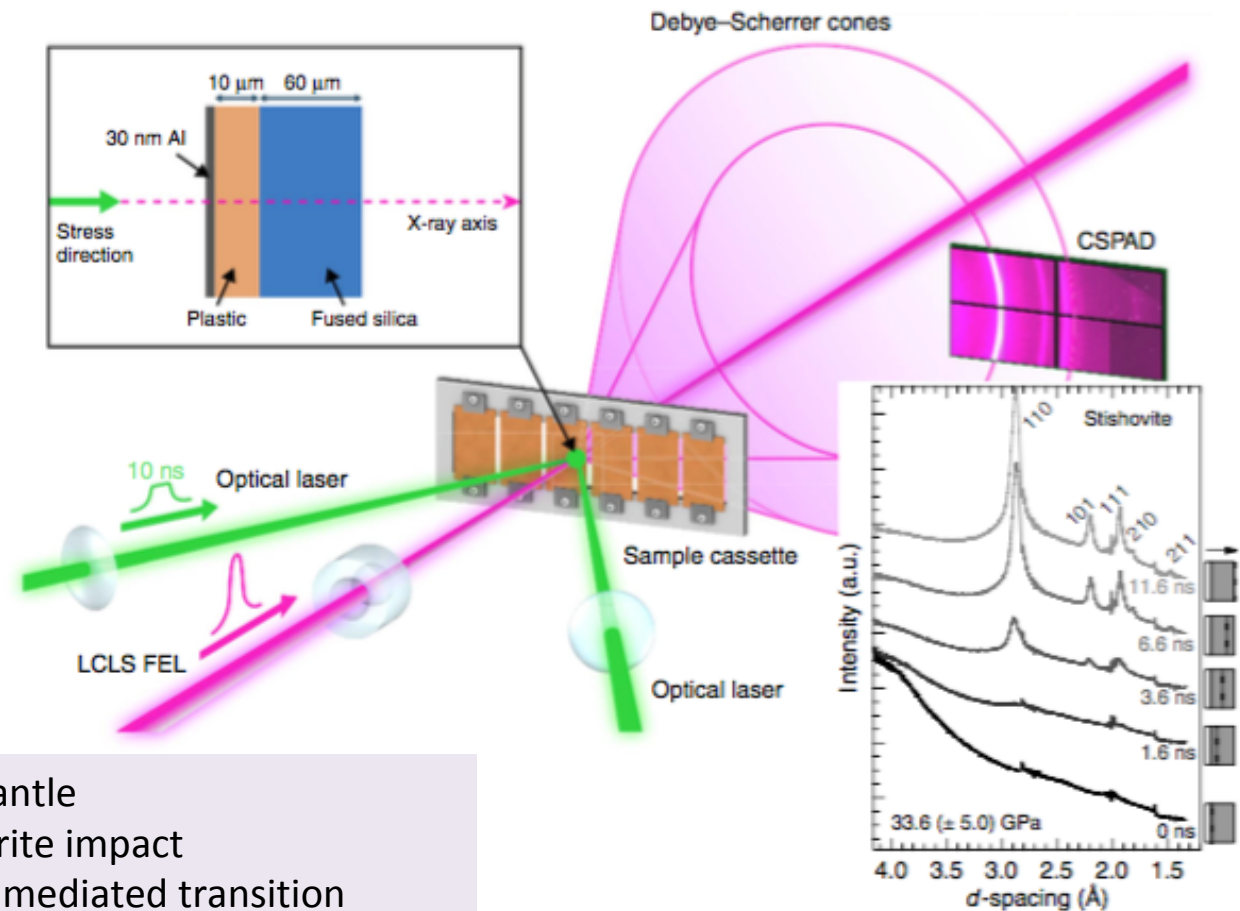
Exoplanets Interiors and properties



- 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

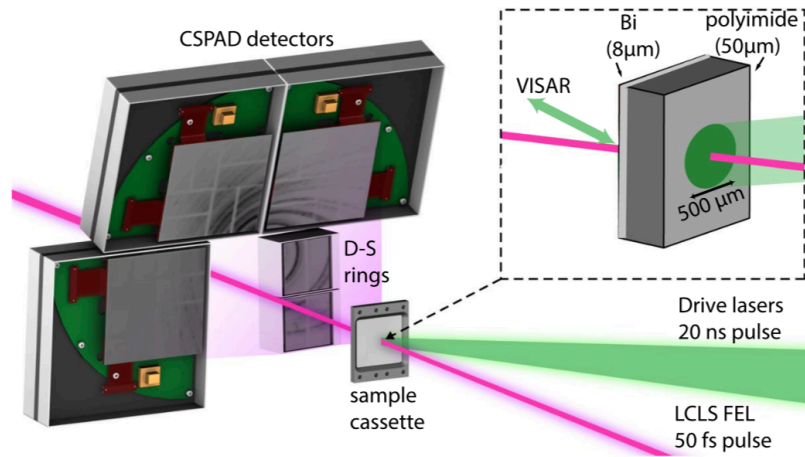
Production of nm-size stichovite under shock
as example of an ultrafast reconstructive Phase Transitions



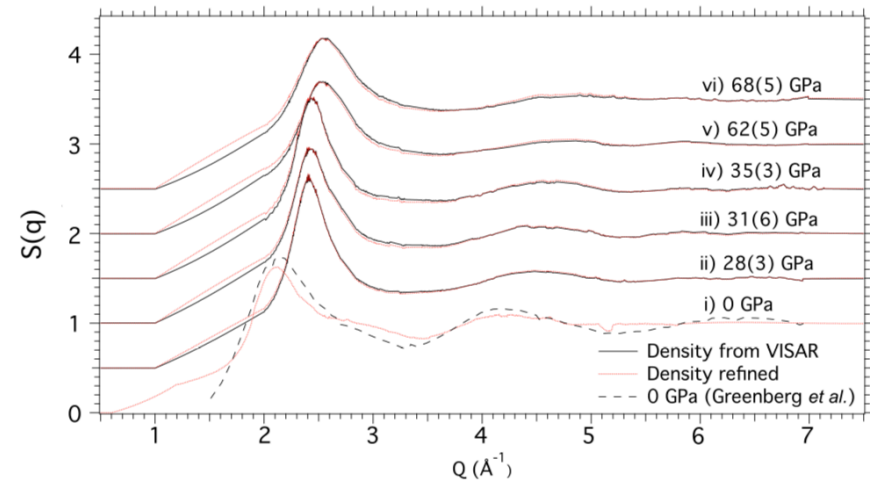
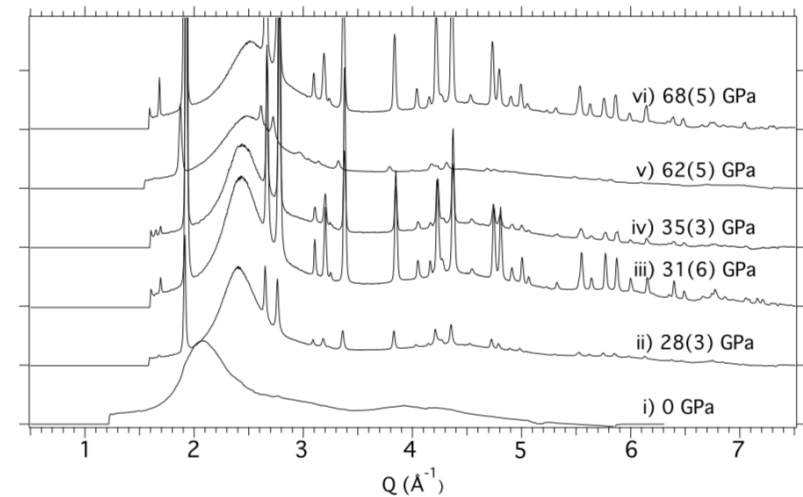
One of the major mineral of the mantle
Observed on hyper-velocity meteorite impact
→ Very fast process for a diffusion mediated transition
→ Was expected to require an amorphous PT
→ Needs further detailed studies to track the PT process

Gleason et al. Nature Com. 2015

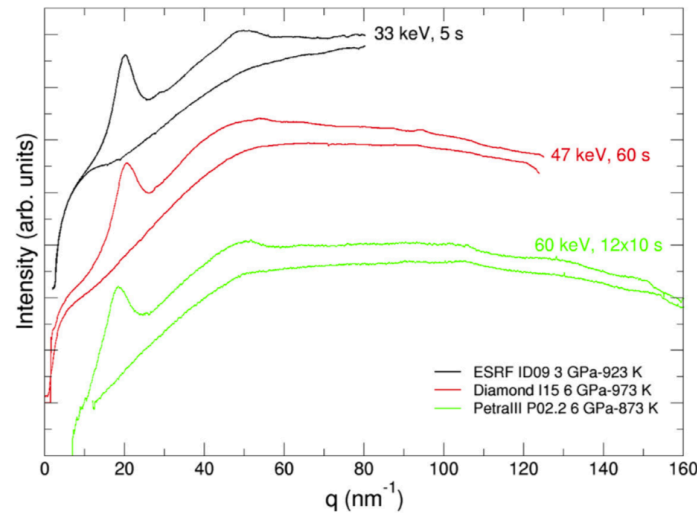
Recent Liquid scattering at LCLS on Bi



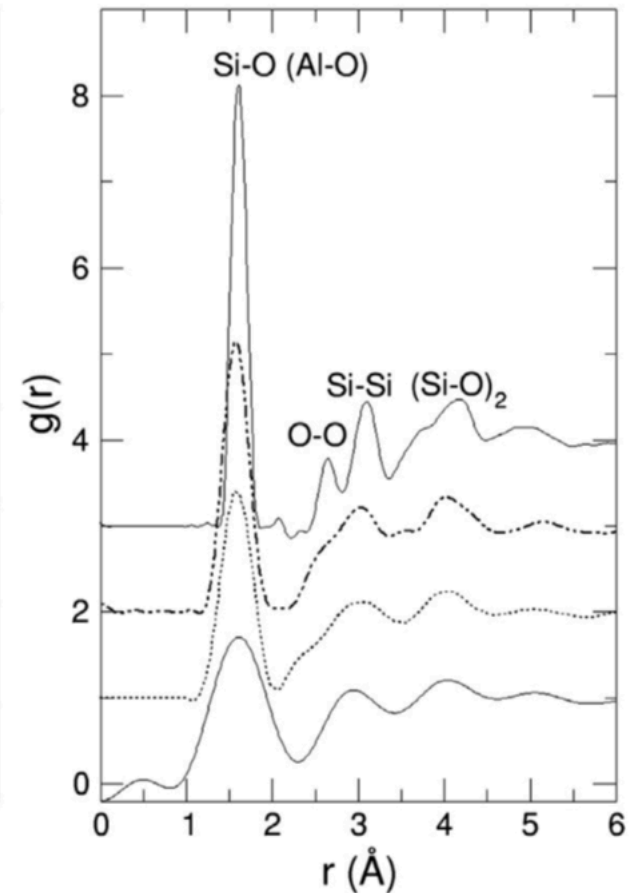
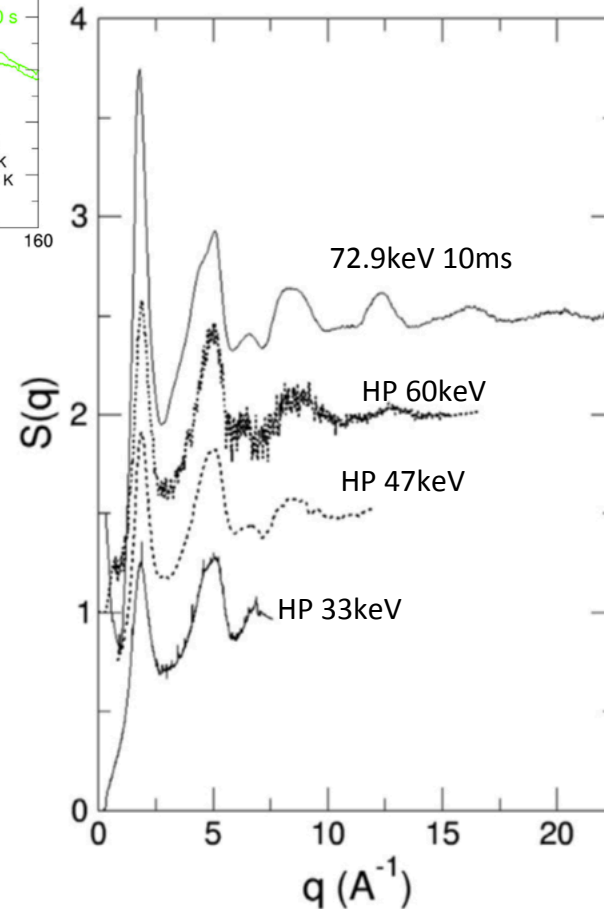
- Significant Improvements of the melting signal
- Should be even better at the HED-HIBEF beamline with large area detectors
- Q range still limited...



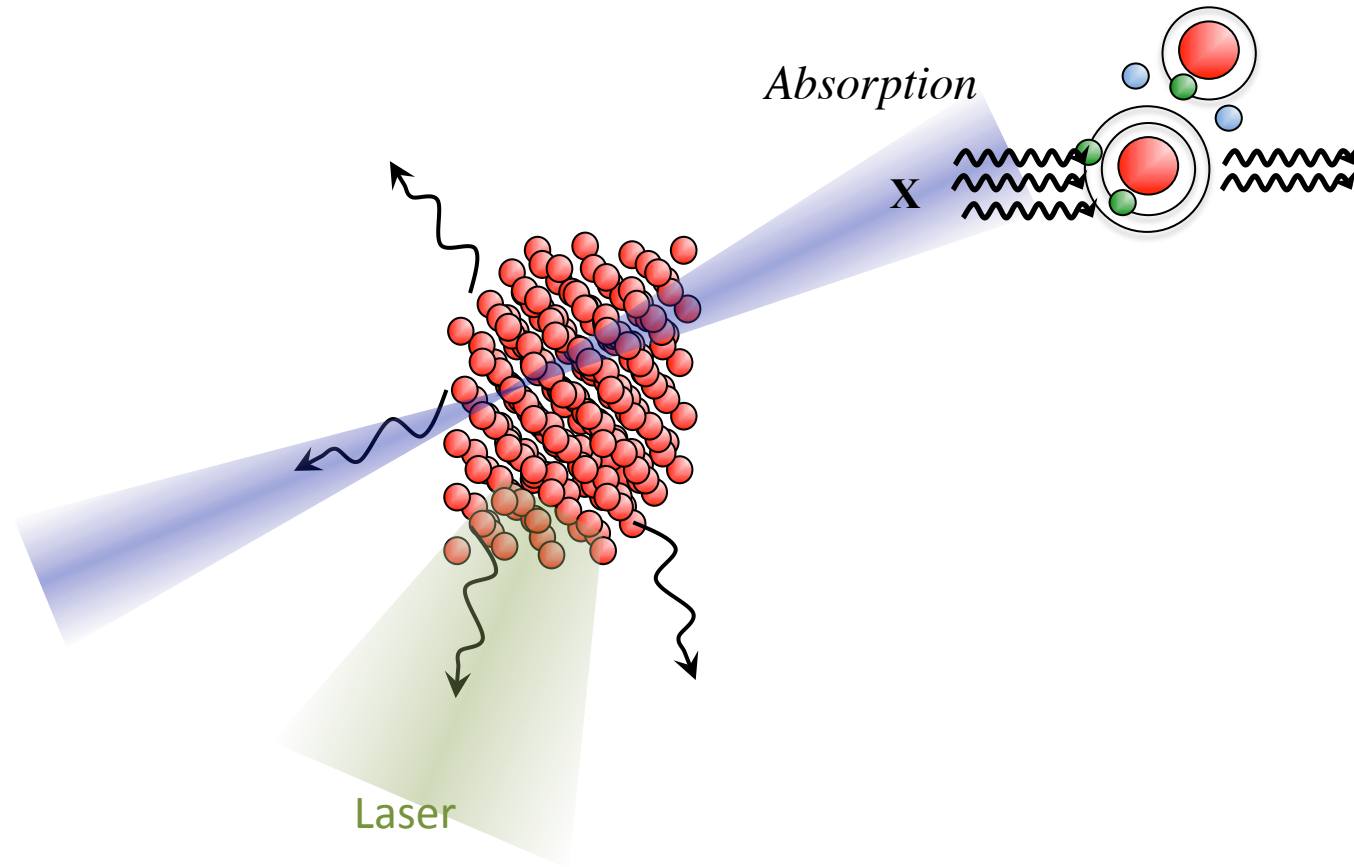
Hard X-ray Scattering for liquids and amorphs



HPG glass



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

X-ray_Elements

X-ray Properties of the Elements

Click on an element to see its properties

1
H
Hydrogen

3
Li
Lithium

11
Na
Sodium

19
K
Potassium

37
Rb
Rubidium

55
Cs
Cesium

7
Fr
Francium

4
Be
Beryllium

12
Mg
Magnesium

20
Ca
Calcium

38
Sr
Strontium

56
Ba
Barium

88
Ra
Radium

5
B
Boron

13
Al
Aluminum

31
Ga
Gallium

49
In
Indium

81
Tl
Thallium

6
C
Carbon

14
Si
Silicon

32
Ge
Germanium

50
Sn
Tin

82
Pb
Lead

7
N
Nitrogen

15
P
Phosphorus

33
As
Arsenic

51
Sb
Antimony

83
Bi
Bismuth

8
O
Oxygen

16
S
Sulfur

34
Se
Selenium

52
Te
Tellurium

84
Po
Polonium

9
F
Fluorine

17
Cl
Chlorine

35
Br
Bromine

53
I
Iodine

85
At
Astatine

10
Ne
Neon

18
Ar
Argon

36
Kr
Krypton

54
Xe
Xenon

86
Rn
Radon

21
Sc
Scandium

29
Cu
Copper

47
Ag
Silver

65
Tb
Terbium

83
Bi
Bismuth

22
Ti
Titanium

30
Zn
Zinc

48
Cd
Cadmium

66
Dy
Dysprosium

84
Po
Polonium

23
V
Vanadium

31
Ga
Gallium

49
In
Indium

67
Ho
Holmium

85
At
Astatine

24
Cr
Chromium

32
Ge
Germanium

50
Sn
Tin

68
Er
Erbium

86
Rn
Radon

25
Mn
Manganese

33
As
Arsenic

51
Sb
Antimony

69
Tm
Thulium

87
Fr
Francium

26
Fe
Iron

34
Se
Selenium

52
Te
Tellurium

70
Yb
Ytterbium

88
Ra
Radium

27
Co
Cobalt

35
Br
Bromine

53
I
Iodine

71
Lu
Lutetium

28
Ni
Nickel

36
Kr
Krypton

54
Xe
Xenon

29
Cu
Copper

37
Rb
Rubidium

55
Cs
Cesium

30
Zn
Zinc

38
Sr
Strontium

56
Ba
Barium

31
Ga
Gallium

39
Y
Yttrium

57
La
Lanthanum

32
Ge
Germanium

40
Zr
Zirconium

58
Ce
Cerium

33
As
Arsenic

41
Nb
Niobium

59
Pr
Praseodymium

34
Se
Selenium

42
Mo
Molybdenum

60
Nd
Neodymium

35
Br
Bromine

43
Tc
Technetium

61
Pm
Promethium

36
Kr
Krypton

44
Ru
Ruthenium

62
Sm
Samarium

37
Rb
Rubidium

45
Rh
Rhodium

63
Eu
Europium

38
Sr
Strontium

46
Pd
Palladium

64
Gd
Gadolinium

39
Y
Yttrium

47
Ag
Silver

65
Tb
Terbium

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Zr
Zirconium

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Cd
Cadmium

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Dysprosium

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Antimony

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Thulium

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67
Ho
Holmium

68
Er
Erbium

69
Tm
Thulium

70
Yb
Ytterbium

71
Lu
Lutetium

14
Si
Silicon

28.09

14

Si

Silicon

atomic number

atomic weight

symbol

name

black solid

blue liquid

red gas

white synthetically prepared

most stable isotope

alkali metals

alkaline earth metals

transitional metals

other metals

nonmetals

noble gases

1
H
Hydrogen

2
He
Helium

3
Li
Lithium

4
Be
Beryllium

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Boron

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Carbon

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Lu
Lutetium

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Hf
Hafnium

73
Ta
Tantalum

74
W
Tungsten

75
Re
Rhenium

76
Os
Osmium

77
Ir
Iridium

78
Pt
Platinum

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Au
Gold

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Hg
Mercury

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Tl
Thallium

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Pb
Lead

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Bismuth

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Polonium

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Astatine

86
Rn
Radon

87
Fr
Francium

88
Ra
Radium

89
Ac
Actinium

90
Th
Thorium

91
Pa
Protactinium

92
U
Uranium

93
Np
Neptunium

94
Pu
Plutonium

95
Am
Americium

96
Cm
Curium

97
Bk
Berkelium

98
Cf
Californium

99
Es
Einsteinium

100
Fm
Fermium

101
Md
Mendelevium

102
No
Nobelium

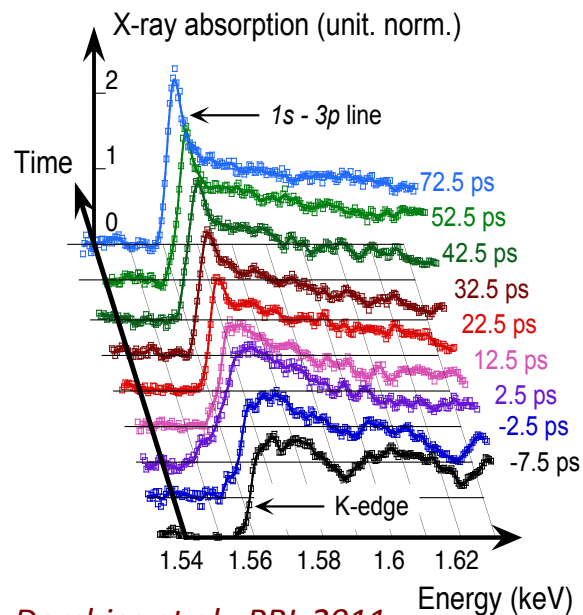
103
Lr
Lawrencium

© 2001 Lawrence Berkeley National Laboratory

K-edges above 24keV

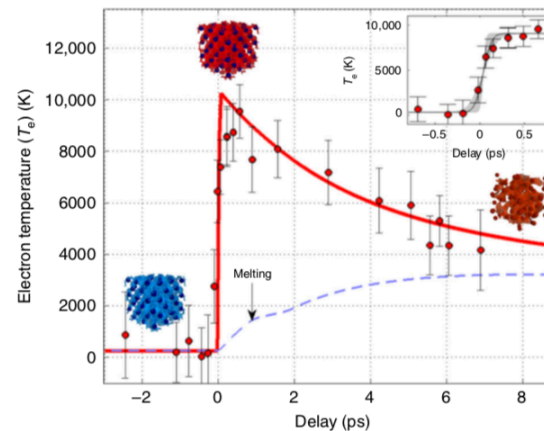
XAS for ultrafast laser heating on Higher Z-elements

Solid-liquid-vapor transition with ultrafast laser heating



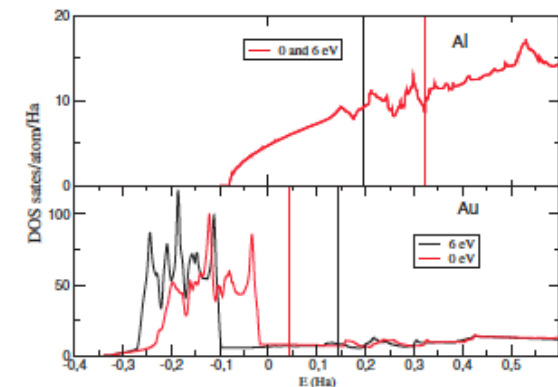
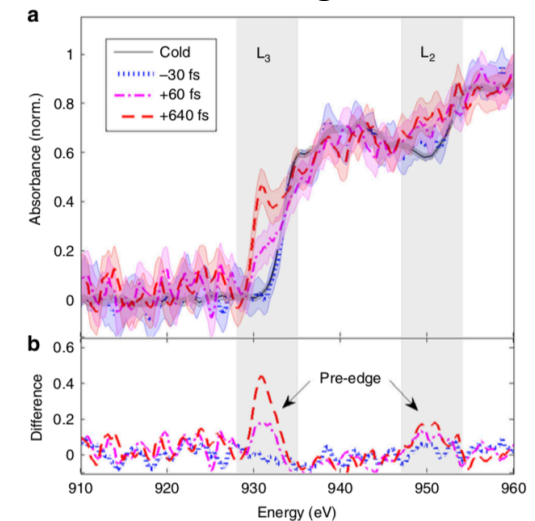
Dorchies et al., PRL 2011

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



Recoules et al, PRL 2006

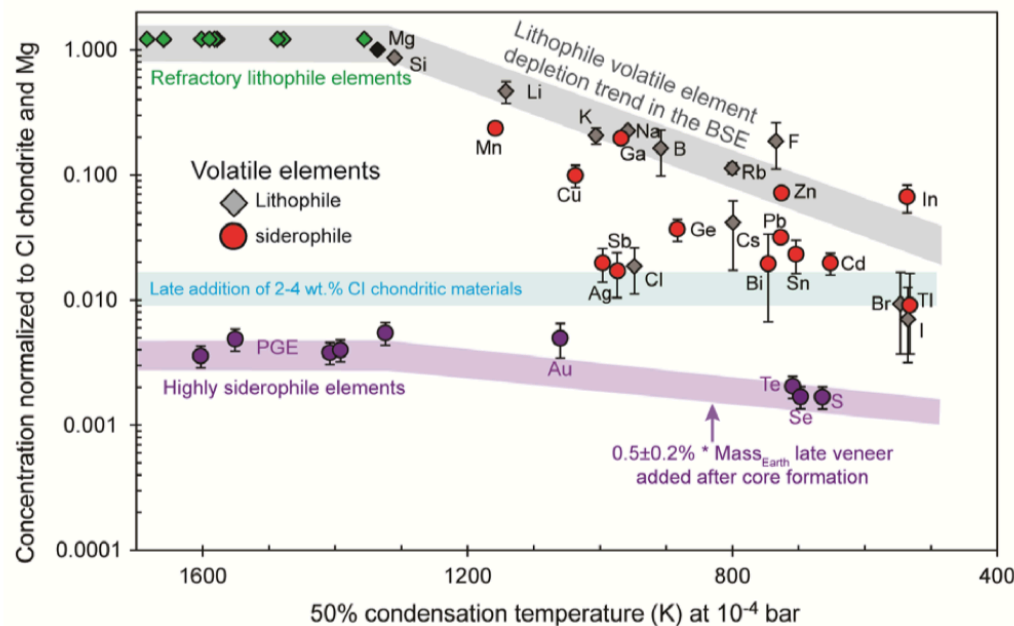
Mahieu et al. 2018



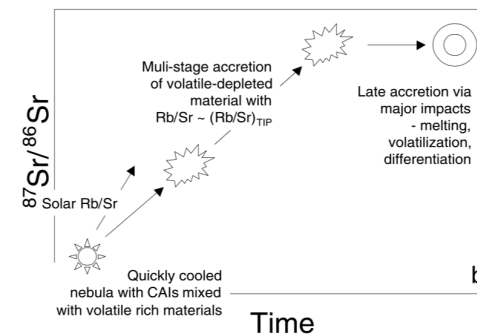
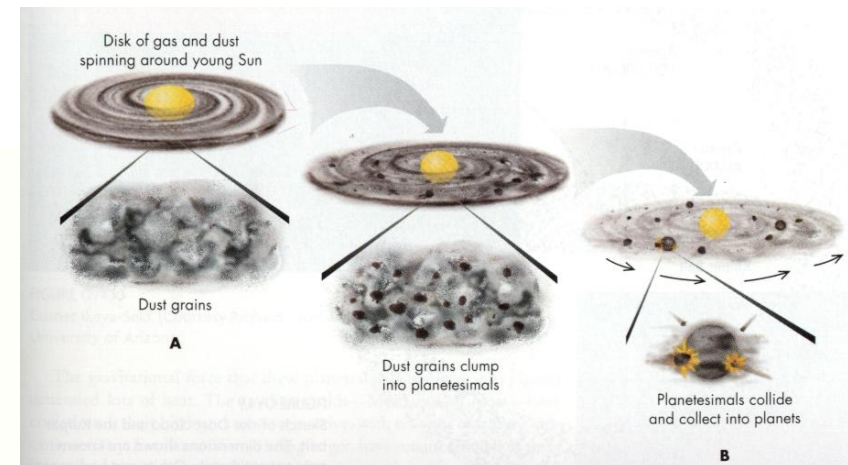
- Understanding how electron structure affect the melting under ultrafast heating
- Reconstruct the full DOS (p, d) at the L-edge and K-edges of Sn, Au, Ta, Bi
- Access fs temporal resolution and go further than actual limitations of secondary X-ray sources

Trace Elements for understanding the Earth and Moon formations

- The Earth Bulk Silicate has a slightly 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



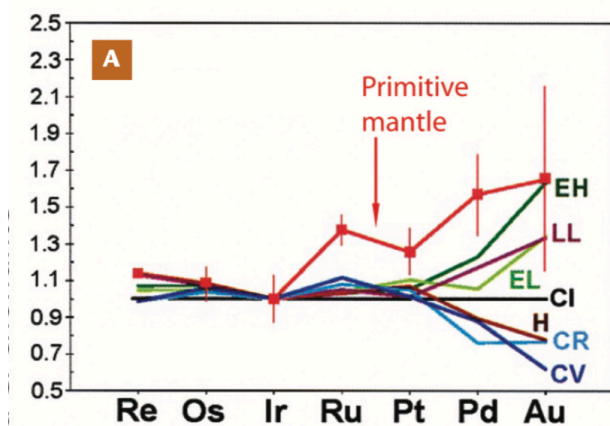
Wang et al



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)

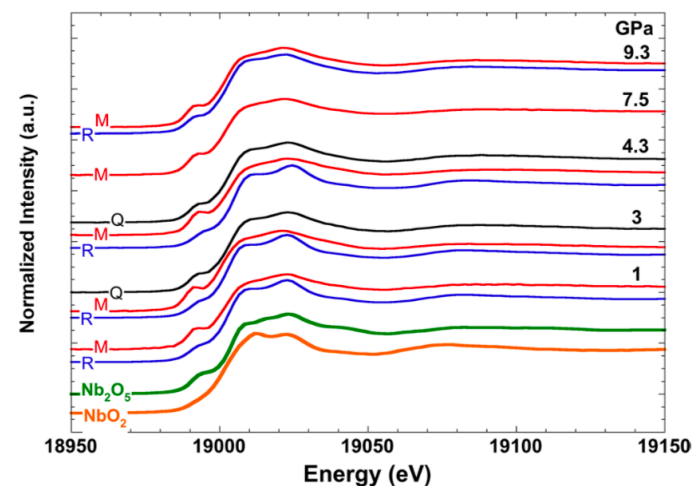
Siderophile K-edges

- 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