Scientific opportunities with very hard x-ray SR/FEL radiation

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Non Collider Science Opportunities at FCC-ee kickoff, August 23, 2024

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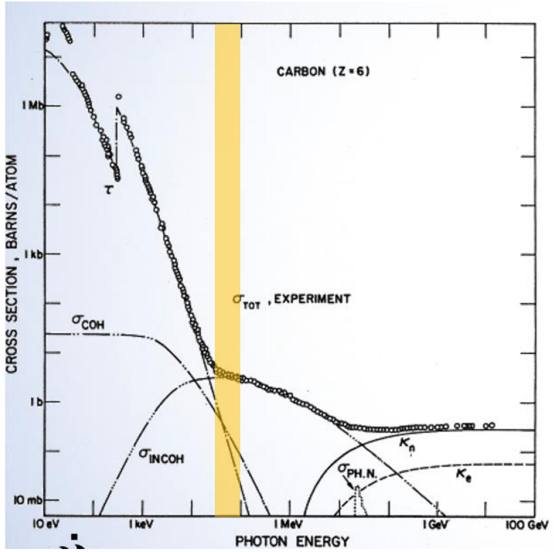
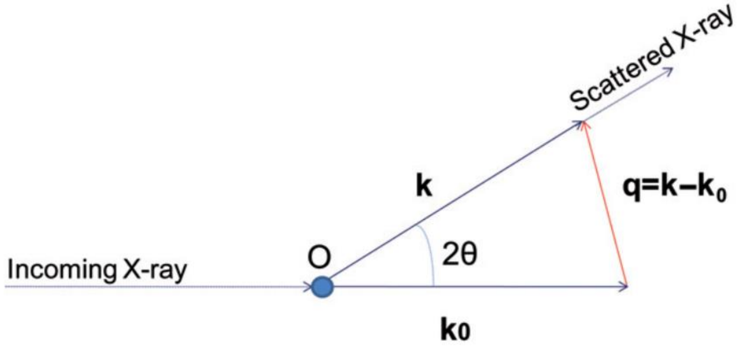
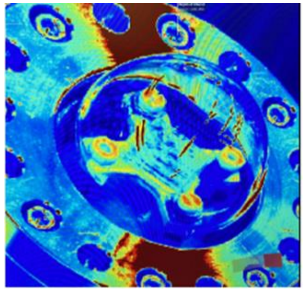
Definition & advantages: Very hard X-ray FEL radiation

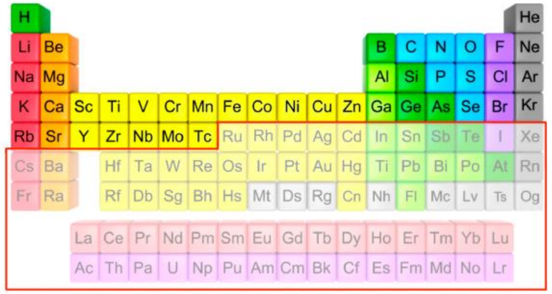




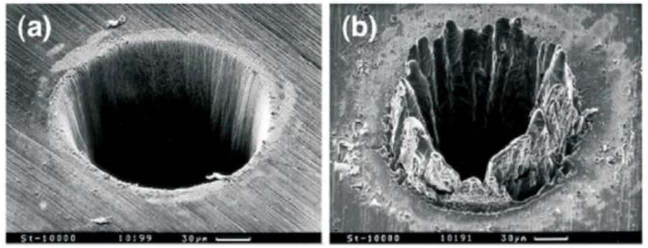
- Photon energies ~ 30 – 100 keV

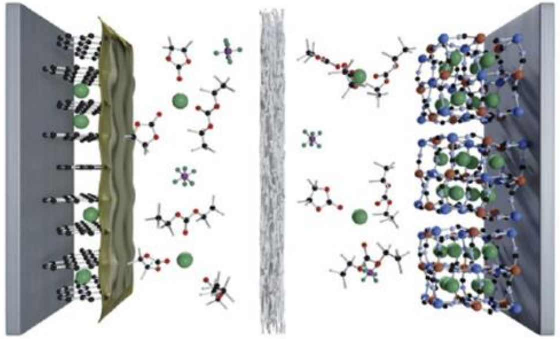


- Instrumentation & method advantages
  - **Larger penetration depth** for bulk sensitivity, and access to complex sample environments
  - **Larger momentum transfer** at moderate scattering angles for improved accuracy in modelling, for inverse analysis schemes, and for crystallography of small unit cell materials
  - Access to **core-level** spectroscopy of **heavier elements** and nuclear resonances
  - **Reduced radiation damage** for high repetition rate tracking of induced (pumped) dynamics and stochastic phenomena in heterogeneous samples
  - New techniques (e.g. Compton scattering)

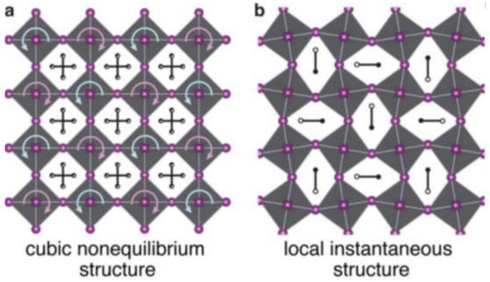


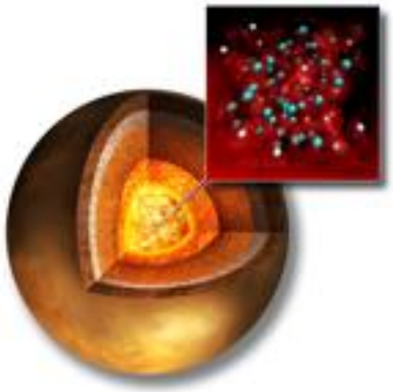
Broad Scientific Areas of Application of Hard X-rays





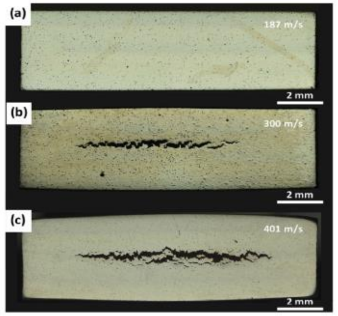
- Applied Materials and Industrial Applications
- Structural Dynamics in Disordered Materials
- Dynamics of Functional Materials
- High Pressure, Planetary Science, Warm Dense Matter, Relativistic Laser Plasma, Strong Field Science

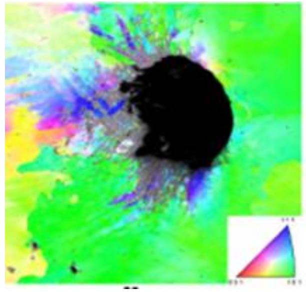




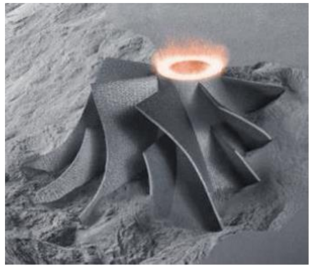
I. Applied Materials and Industrial Applications

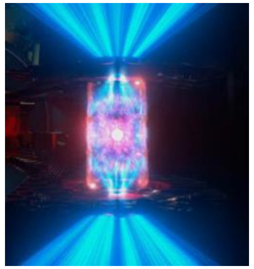
- Real time control of irreversible processes at the relevant timescales, across length scales
  - many materials are hierarchically organized, all length scales must be investigated (from atomic to macroscopic scale 3-D dislocations, cracks)
  - random events (spontaneous failure) require large sample areas/volume, high res in space and time, timescales down to ps (high T diffusionless transformations, nano-scale phase formation)
  - from reference materials (Al, Si) to relevant materials (3d metals, metallic glasses, ceramics, composites, rocks)

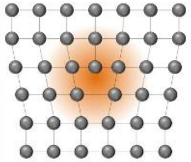


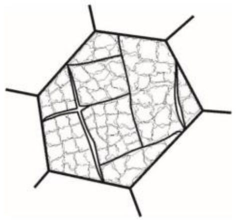


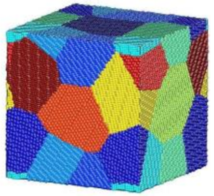
- Examples :
  - ► crack propagation in semiconductors
  - ► plastic deformation or martensitic phase transformation in metals
  - ► switching of domains in ferroelectrics
  - ► flux lattices in superconductors
  - ► fuel instabilities in inertial fusion
  - ► biomineralization in bones
  - ► flow in geomaterials
  - ► 3D printing



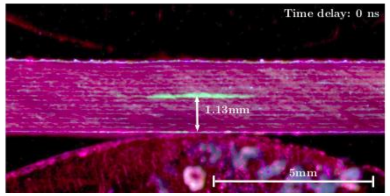








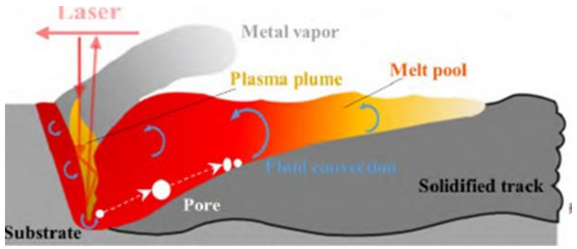
I. Technical Limitations



Lack of diagnostics with sufficient bulk sensitivity, spatial and temporal resolution

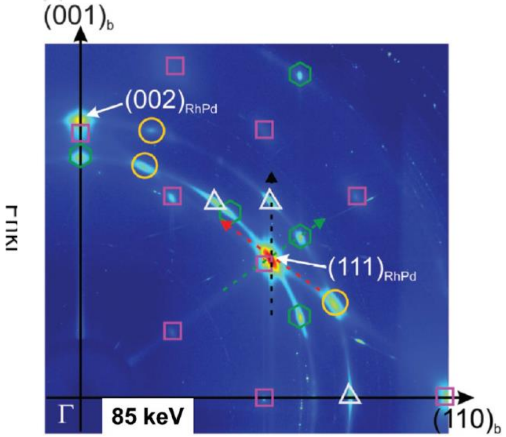
Materials for planetary security and spacecraft protection against debris

- Understand structural changes induced by High Velocity Impacts (7-30 Km/s)
- Laser shocks can reproduce pressure loadings of such impacts (~ 100 GPa in 100ns)
- Observe shock wave propagation, crater formation (~mm depths, mm^3 volumes)
- Simulations available, but no experimental data



Design and manufacture more sustainable, lighter, and longer lifetime materials and structures

- Measure residual stress fields
- Delamination, fissure propagation in carbon fiber-reinforced polymers, semiconductors, metals

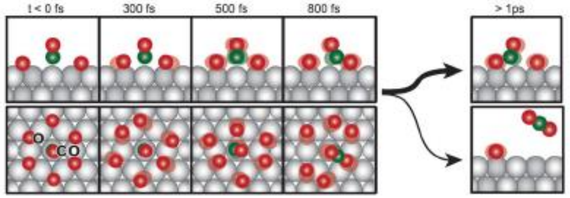


Real time control of processes in additive manufacturing, laser peening, cavitation

- Melting, solidification
- Understand origin of defects that lead to failure: distortions, strain, porosity, cracking

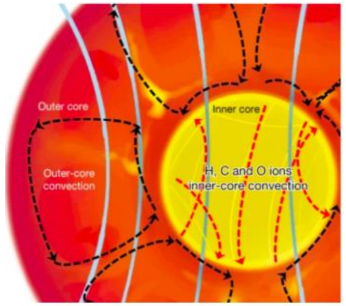
Operando and industrial scale catalysts for cleaner energy production, pollution control

- Steel production: improve energy efficiency and lowering CO_2 emission
- Penetration of reactor walls for operando investigations
- Sub-ns structural changes on surfaces and nanoparticles

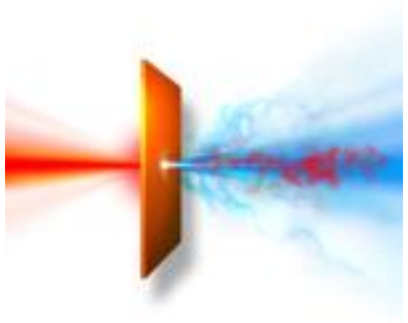


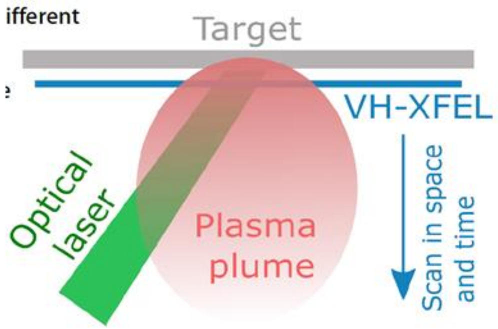
II. Matter at extreme conditions of Pressure, Temperature, EM Fields

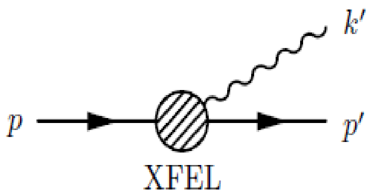
High Pressure, Planetary Science and Geology, Electron Dynamics, Warm Dense Matter, Relativistic Laser Plasma, Strong Field Science

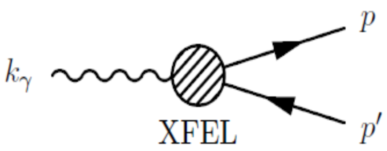


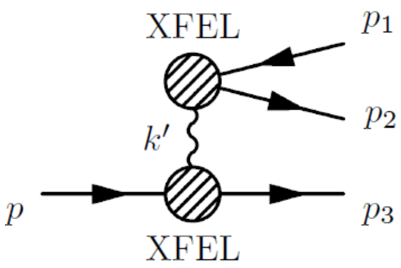
- Structure and chemistry at extreme P/T conditions: geoscience (planetary interiors, formation), new materials
- Inertial Confinement Fusion diagnostics of implosion symmetry, convergent geometries
- High Z materials in High Energy Density Physics (atomic physics, warm dense matter): Collisional-radiative behavior of plasmas, non-LTE, ionization dynamics and radiation transport in stellar atmospheres
- Strong-Field Science: Trident process to test models for dark matter





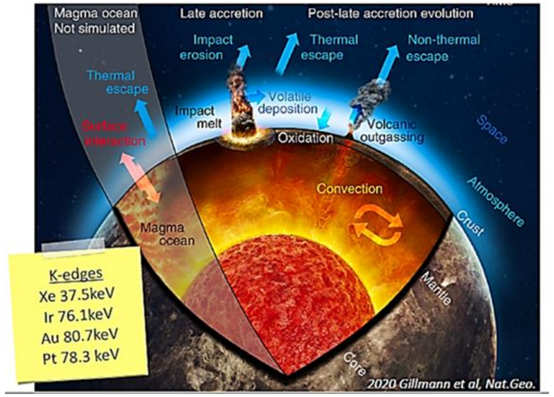






European XFEL

II. Technical Limitations



HIGHER

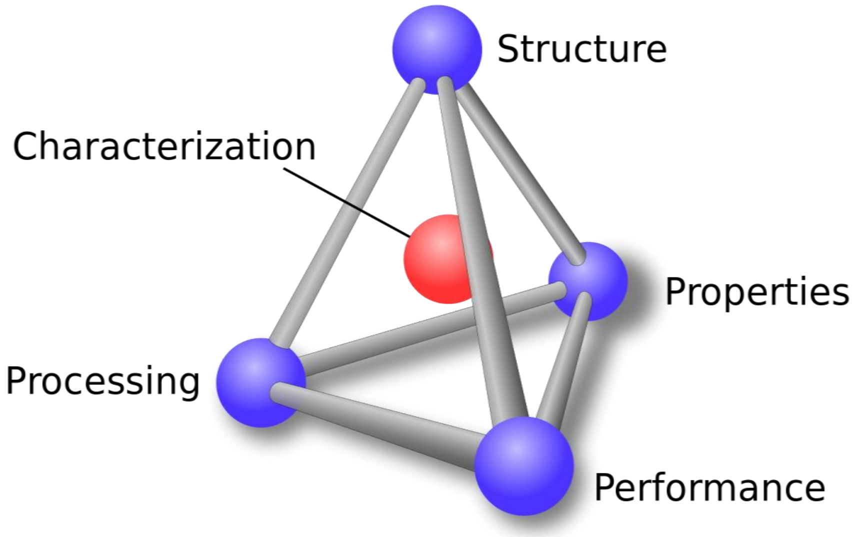
Volumes
Imaging resolution
Compressed matter
Energy spectroscopy
Q-range diffraction

- Structure of liquids and melts: structure determination, higher resolution → high-Q scattering
- Element selective probes for local structure, valence state → access absorption edges
- Chemistry of low Z elements during impacts (rocky planets) → photon hungry inelastic scattering (X-ray Raman)
- Strong Field Science (Trident process) → high photon energy to reduce e- beam energy required for threshold
- Diagnostics of large sample volumes and/or extreme densities and/or in absorbing environment → high penetration

III. Structural dynamics in disordered materials, advanced tailor-made functional materials & innovative devices

Understanding photo-dynamics, out-of-equilibrium transient states

- enhanced performance
  - light-emitting devices, solar cells
  - quantum technology materials
  - stronger magnets
- lower energy consumption during operation
  - non-volatile memory concepts
  - photo-switches
- efficiency-optimized and sustainable synthesis
  - increased efficiency of catalytic processes e.g. for green H_2
  - fully controlled solidification *e.g.* freeze-in of liquid melts
- use of non-toxic and abundant elements
  - rare-earth-free magnetic materials



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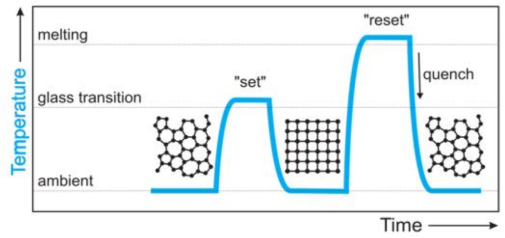
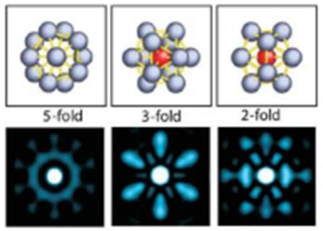
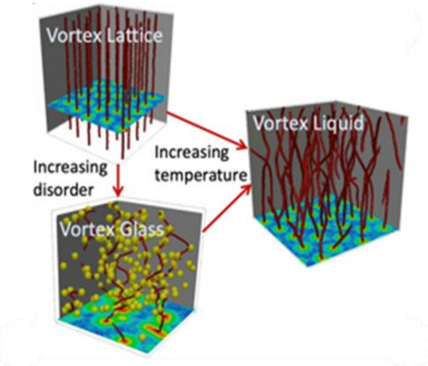
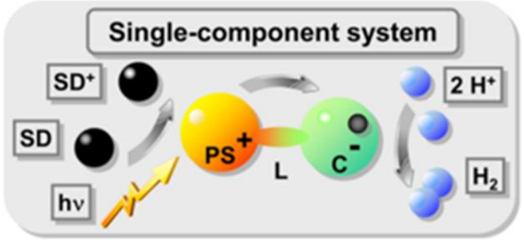
III: Open questions

- How are diffusivity and atomic short- to medium-range order in glass-forming phase-change materials? What is the structure-kinetics relationship during their solidification?
- What structural rearrangements cause the slowdown of atomic motions in supercooled metallic liquids? What is the microscopic origin of the compositional dependence of the glass-forming ability of metals?
- How do high-temperature superconductors respond to strong pulsed magnetic fields? What are the structural foundations and field-dependent dynamics of trapped field magnets and piezomagnets?
- What is the energy flow in a photocatalyst upon wave-packet excitation? What ultrafast inter-system crossings and couplings to the environment generate the energy-rich catalytically active state?
- How do electronic states and symmetry reorganize upon photo-, IR or THz excitation? What are the multiscale dynamics of photo-induced phase transitions in compounds with electronic bistability?



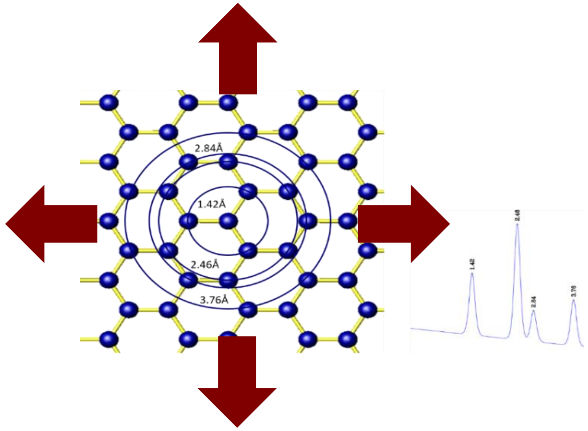




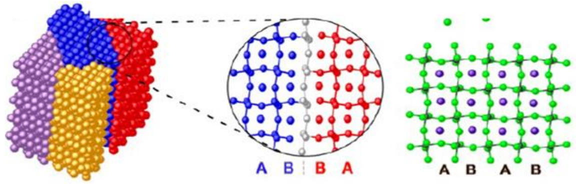


III. Technical Limitations

- Limited Q-range: resolutions obtainable on sub-ps timescale (out-of-equilibrium) too coarse for any detailed structure determination
  - Phase change materials: subtle structural changes in different liquid, amorphous, solid phases
  - Metallic glasses: kinetics of glass forming, from equilibrium to supercooled melt to glass
  - High Tc superconductors: strong pulsed fields restrict access
  - Photocatalysts: unambiguously discern subtle differences in models of solute/solvent response
  - Photo-switching: small molecule high–Q serial Xtallography



- ultra-fast Pair Distribution Function (PDF) methods non existing
  - local structure in nano-, amorphous-, molecular materials, liquids, local symmetry-breaking in solids
  - track phase transitions in situ, high P,T liquid structures, recrystallization, gas-separation, molecular transport in porous materials, charge-discharge process in batteries, nucleation of nanoparticles
  - follow local bonding state/atomic coordination changes, how they propagates out with time from the location where photoexcitation occurred
  - reconstruct 3D-ΔPDF from randomly oriented images of nanocrystals (formation & relaxation polarons, defects in very small objects < 10A)
  - flux limited at ultra fast timescales



Conclusions

- A lot of exciting new science
- Wide range of science questions, out of experimental reach today, from catalysis to the steel industry, from planetary to strong field science.
- Very hard XFEL radiation @ EuXFEL
  - A tool to understand how materials behave under a large range of conditions
  - Key for providing a 'reality check' on theoretical models & rational path towards development of new materials
  - Attraction of new (wider) XFEL user communities, in particular in:
    - Chemistry
    - Materials science
    - Extreme Fields science

"New directions in science are launched by new tools much more often than by new concepts. The effect of a concept-driven revolution is to explain old things in new ways. The effect of a tool-driven revolution is to discover new things that have to be explained."

— Freeman Dyson