Opportunities for UK-XFEL:

Intelligent design of materials for dynamic environments

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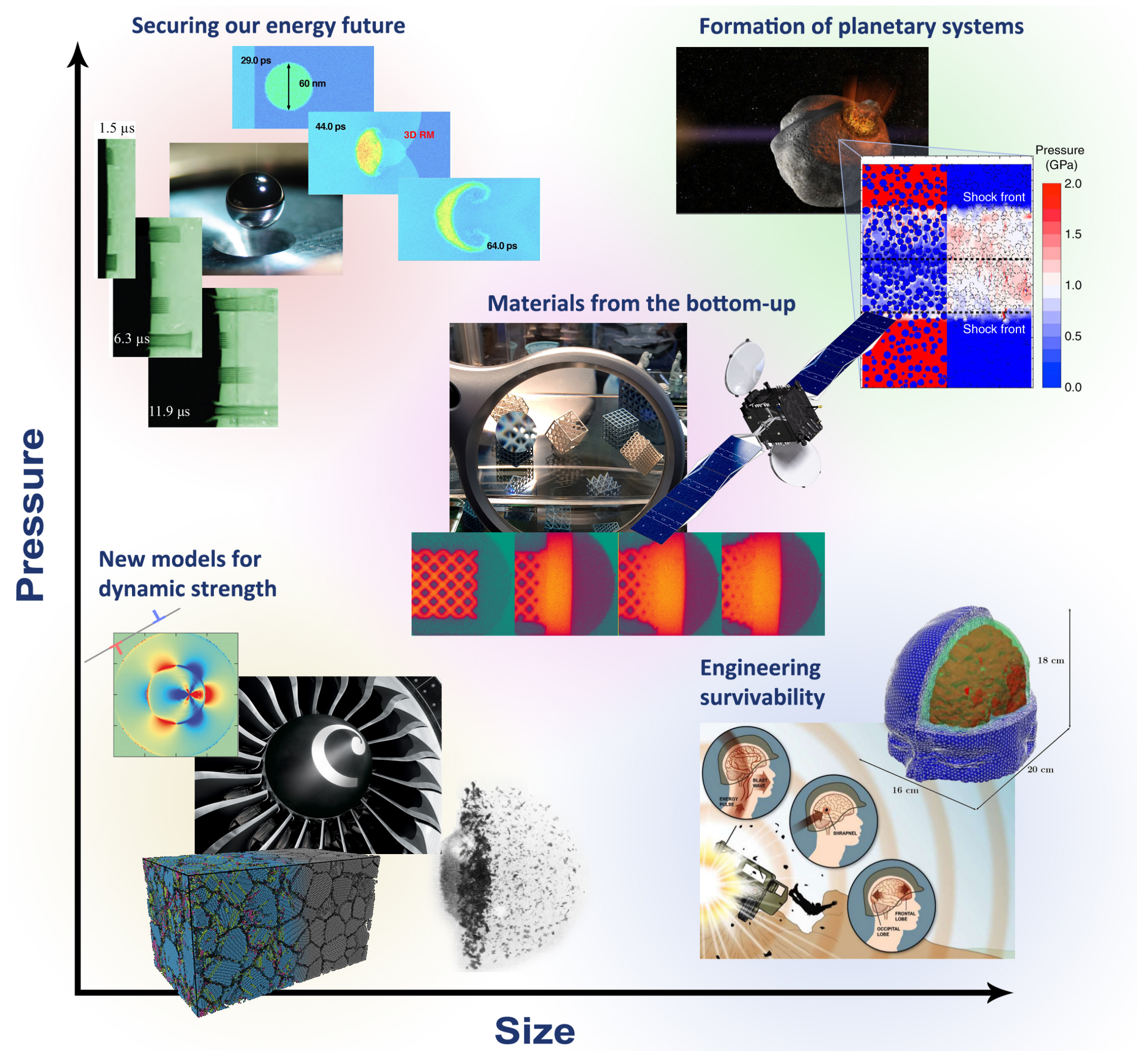
UK-XFEL Event
Royal Society
16 July 2019

Mechanical integrity is a multiscale problem



- Engineering resilience and reliability of systems in dynamic environments.
- Complex material systems: novel textures/processing, multi-component, composites
- Strength, plasticity, damage, failure relevant over decades of stress, size- and time-scales

An Engineering Grand Challenge

Intelligent design of multifunctional materials

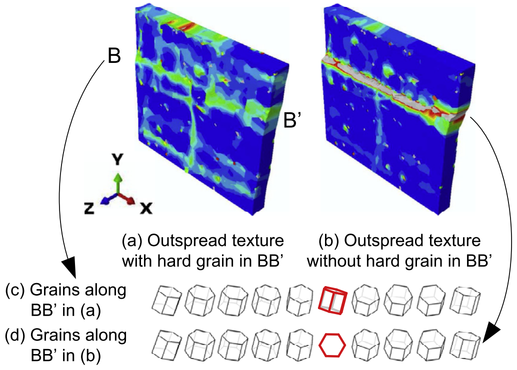
- Materials with predefined properties to meet specific application needs.
  - Engineering length scales permit complex material combinations, performance can be tuned through judicious selection of materials, their respective macro-/micro-structural configurations.

- Requires understanding of the material responses to external stimuli, which may come in different forms (e.g. amplitude/rate of application/release, etc.).

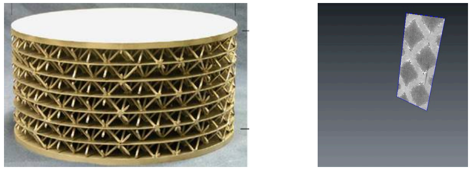
- Also requires direct control over the fabrication of materials at the microstructural scale.

We can influence the behaviour of materials…

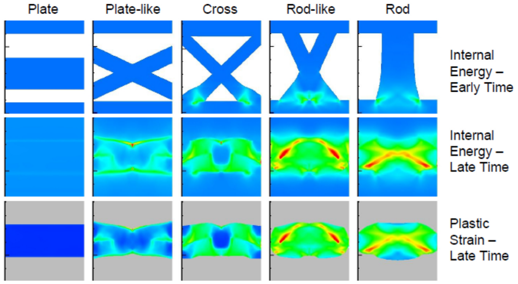
Textured lightweight alloys



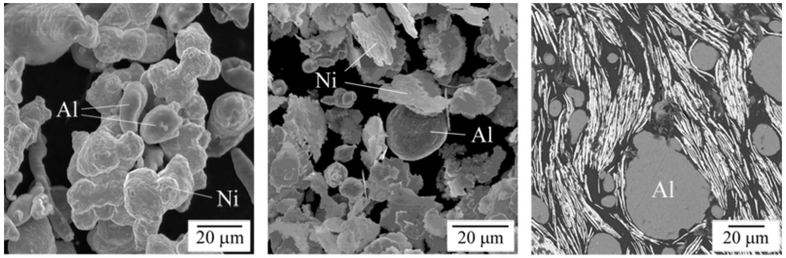
Additively manufactured lattice materials



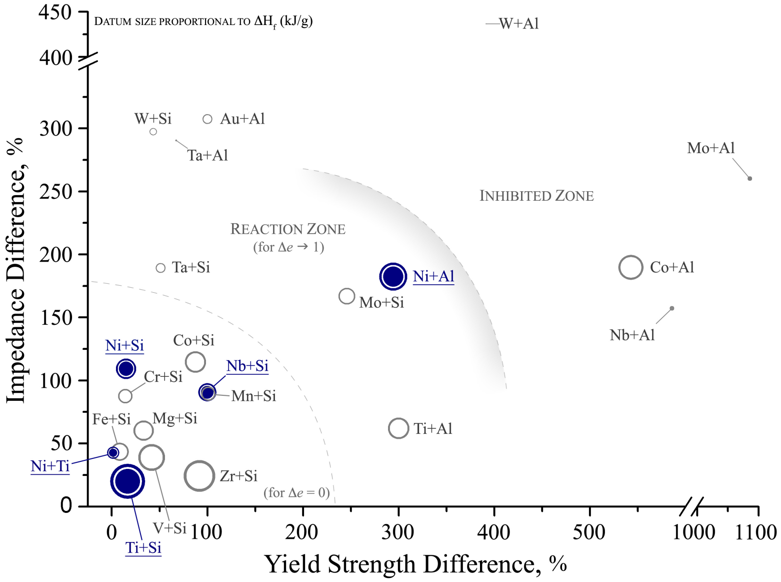
$$X^0 = f(d, \alpha, \phi, \ldots Y, \rho, \ldots)$$



Reactive powder mixtures



$$X^0 = f(d_n, \sigma_n^d, V_n, e_n, \sigma^{NND}, \ldots, Y_n, \rho_n, \ldots)$$



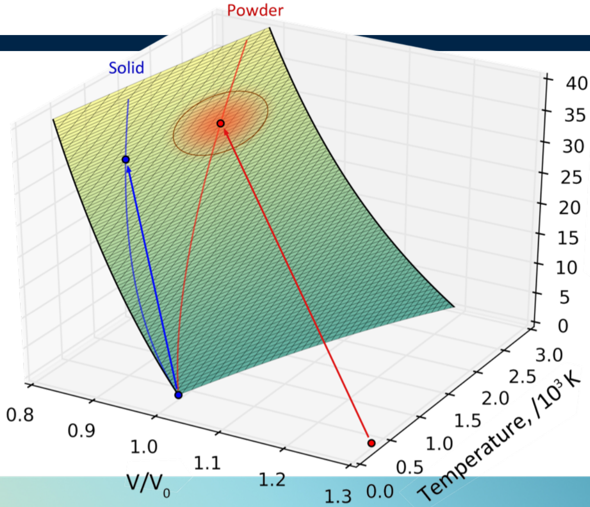
Z. Zhang et al., *Int J Plast* 79, 196 (2016); R.E. Winter et al., *Mod Sim Mat Sci Eng*, 22, 5021 (2014); D.E. Eakins et al., *Int Mat Rev* 54, 181 (2009).

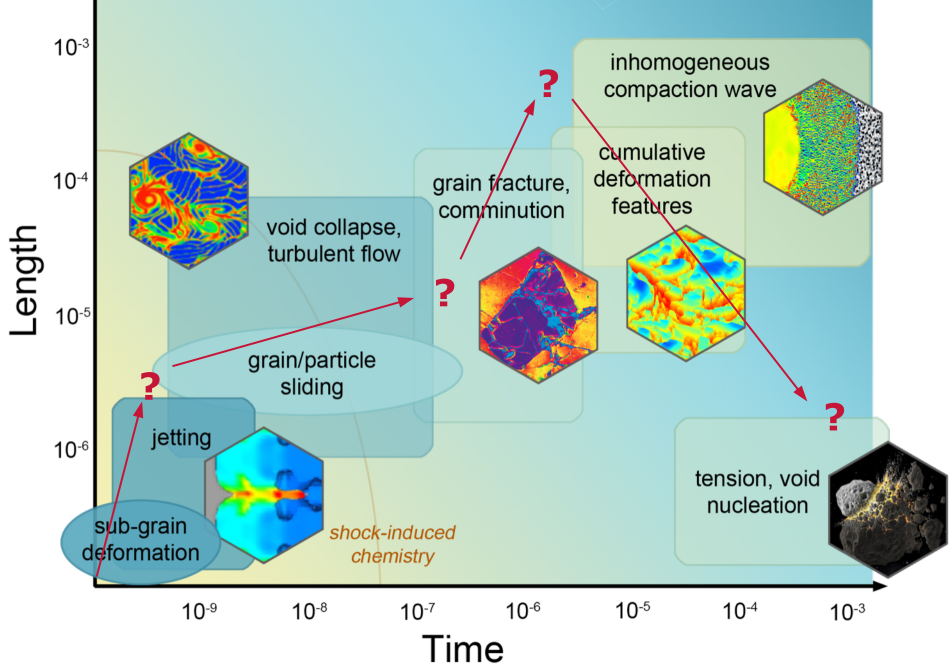
…but can we control?

- We cannot predict the correlation between applied loading/configuration and dissipative mechanisms.
- We don't know sequence of hierarchical processes that link the meso- to macro-scale.
- We lack techniques to directly interrogate the microstructure at sufficient x,t resolution.
- Loss of dimensionality. It's a 4D problem diagnosed in 2D to fit into a 1D model. Upscaling…

➢ We cannot intelligently control response if we don't understand the trajectory of behaviour.

➢ We require new techniques to reveal key stages of deformation/failure





Towards sub-surface probing

Synchrotron light sources offer:

- High flux, high energy, **high spatial resolution (μm – mm),** spatial coherence.

Synchrotron Radiation Facilities

- Energies: 10 – 150 keV.
- Flexible spectrum (mono, pink, white…)
- $10^{7\text{-}9}$ photons bunch^{-1} mm^{-2}.
- Variable beam size (1 x 1, 12 x 12 mm).
- Single bunch (100 – 140 ps).
- Partial spatial coherence.
- Repetition rate, ~150 ns (sparse modes)

- ~10 mm Al, 2 mm Ti, 15 mm SiO_2
- Diffraction, spectroscopy, etc.
- Single-bunch measurements
- Meso/macroscopic specimens
- No motion blur at 1:1 magnification
- Phase contrast enhancement
- ~1 mm wave motion in Al

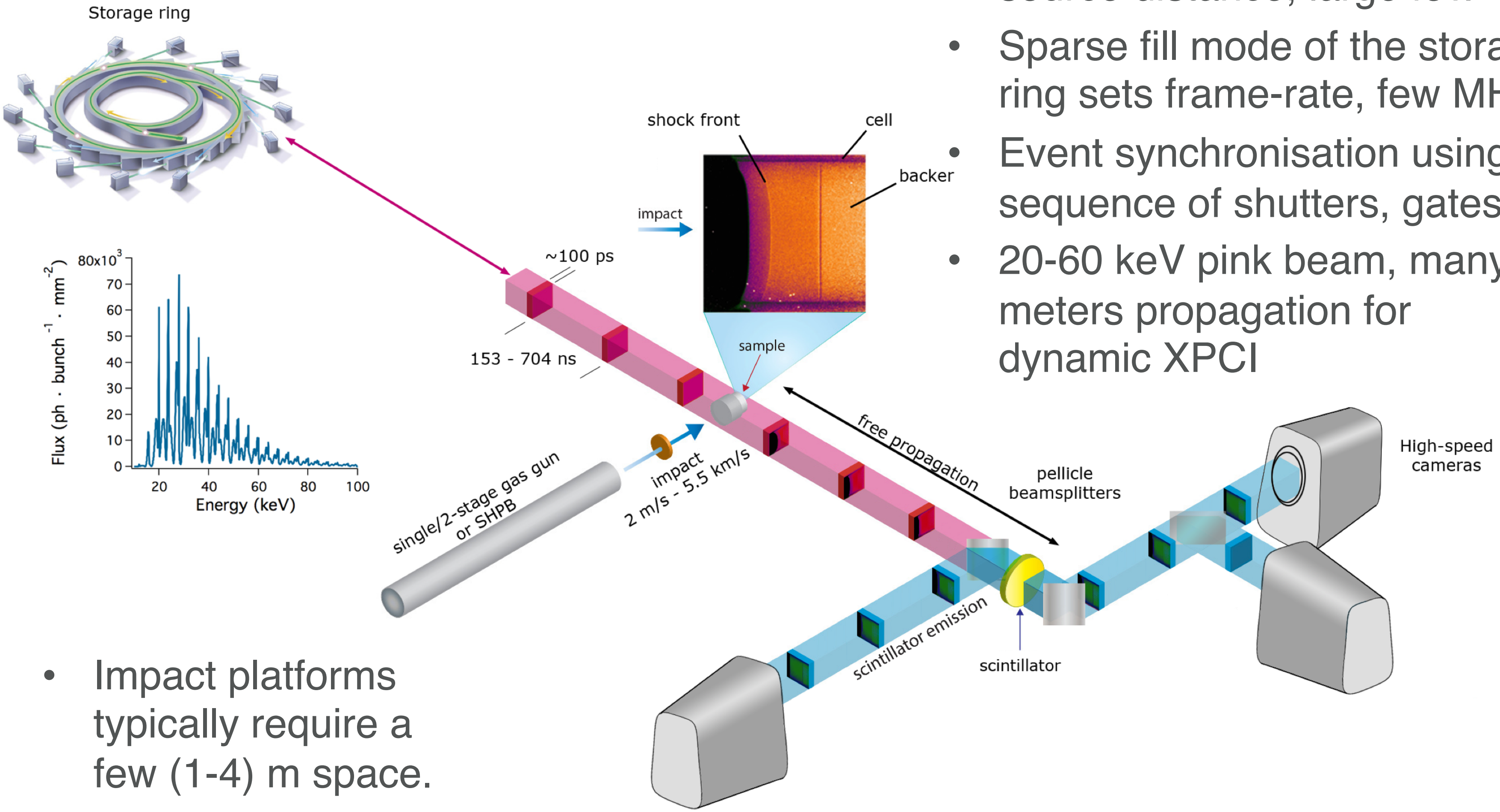
Focus:

- Sample volumes: single grain - 0.5 cm^3.
- *Long-lived* phenomena (> 500 ns).

- Metals, powders, natural matl’s
- **Single-shot X-ray sequences**

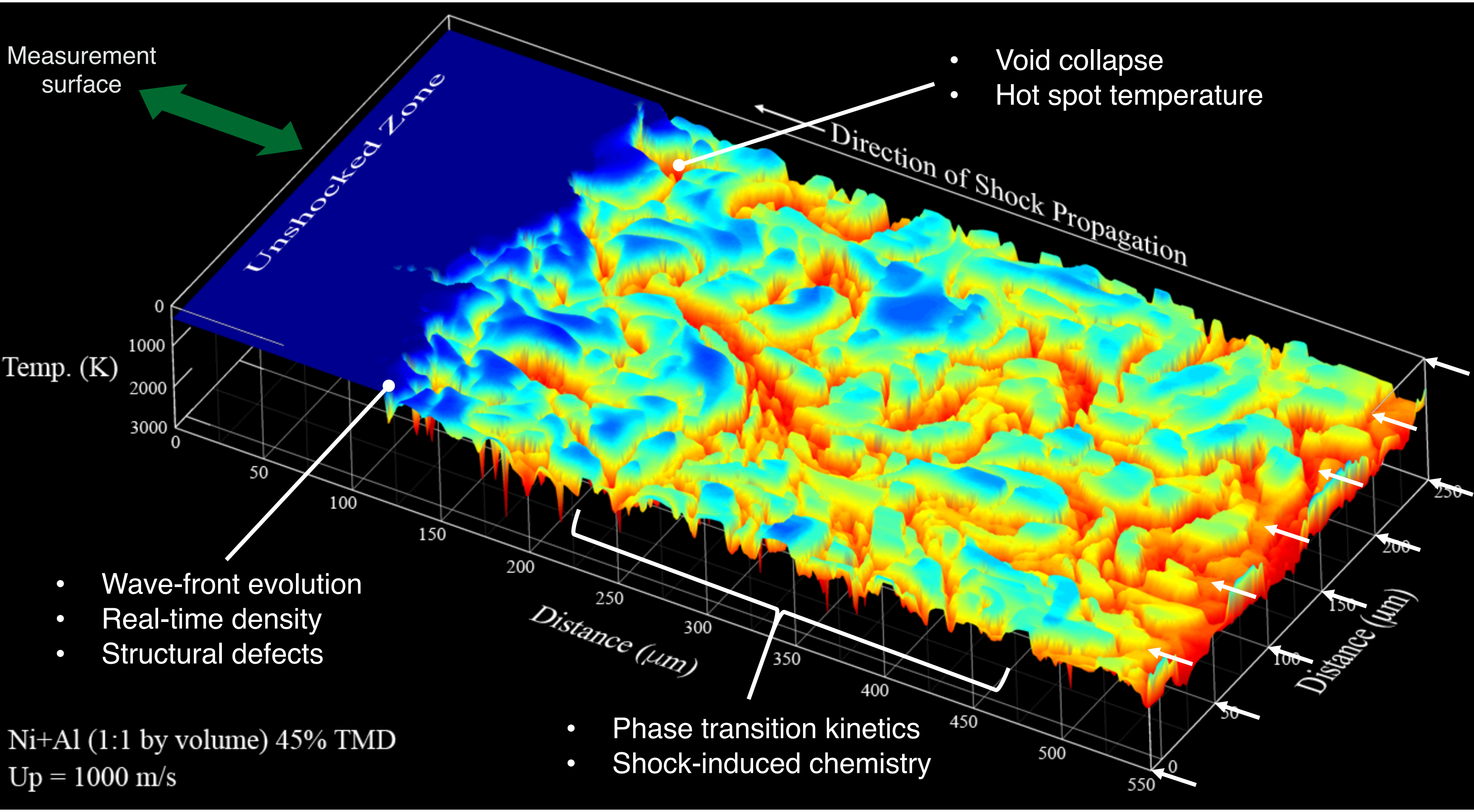
Dynamic experimentation at light sources

- Coherent imaging beamline – source distance, large fov.
- Sparse fill mode of the storage ring sets frame-rate, few MHz
- Event synchronisation using sequence of shutters, gates
- 20-60 keV pink beam, many meters propagation for dynamic XPCI



- Impact platforms typically require a few (1-4) m space.

Peeking behind the curtain



Measurement surface

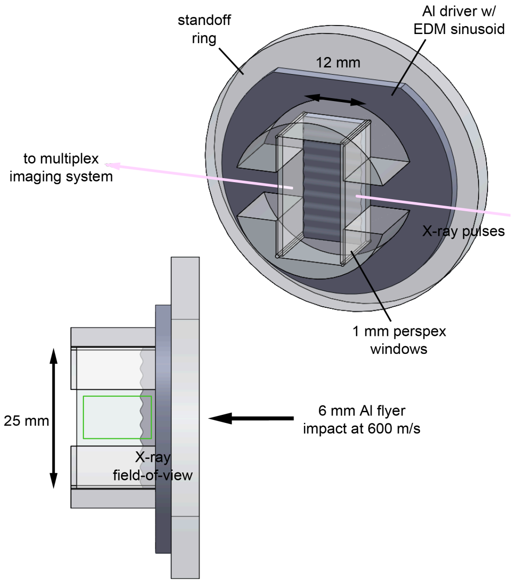
- Void collapse
- Hot spot temperature

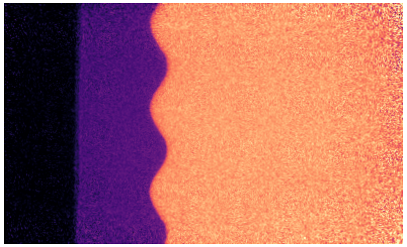
- Wave-front evolution
- Real-time density
- Structural defects

- Phase transition kinetics
- Shock-induced chemistry

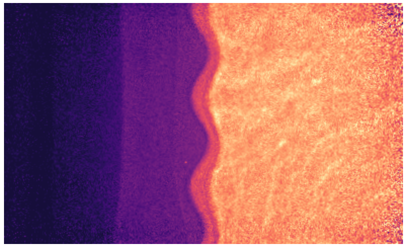
Ni+Al (1:1 by volume) 45% TMD
Up = 1000 m/s

In-situ wave front evolution

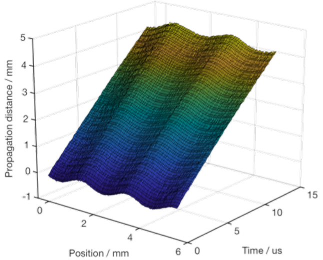


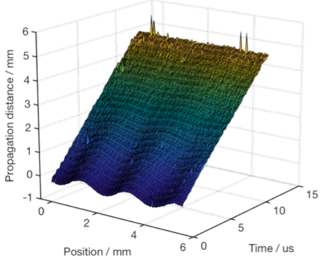


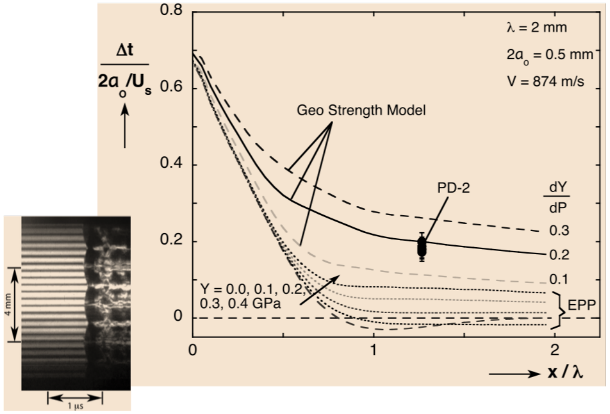
7% TMD sipernat

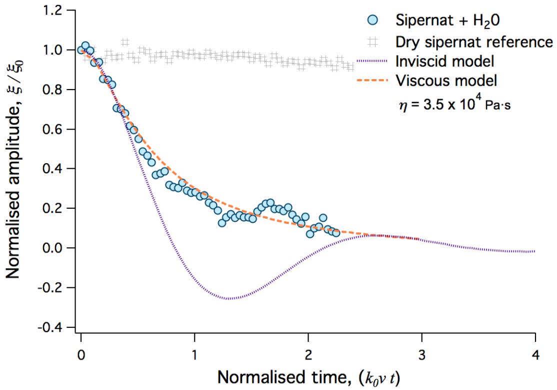


7% sipernat + 15% water





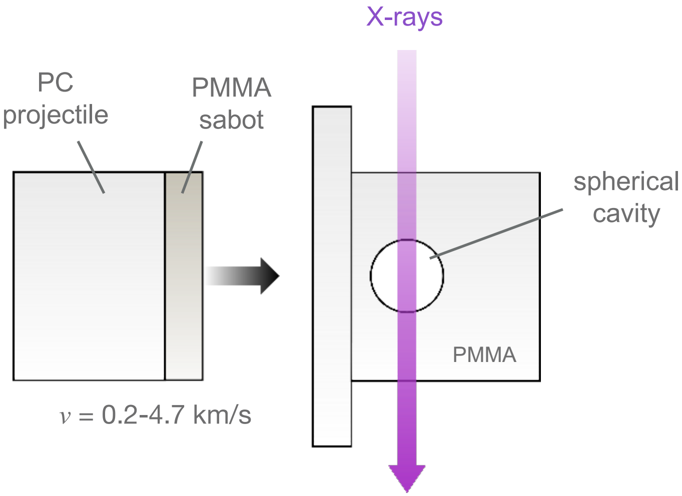


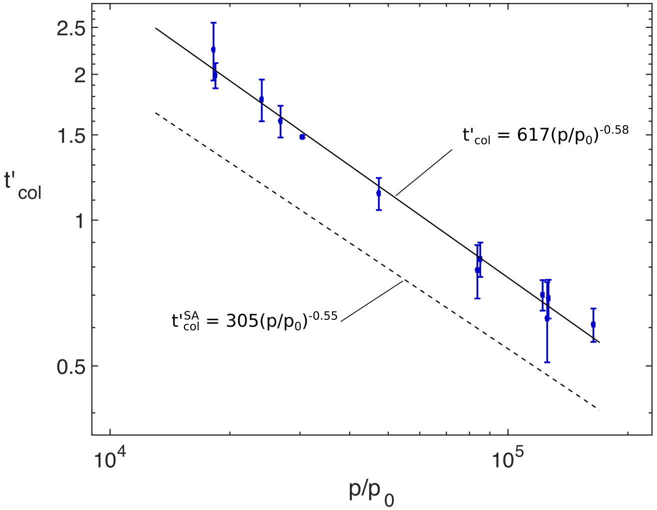


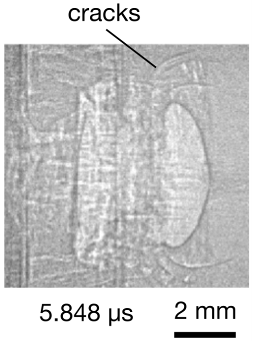
- Continuous tracking of sub-surface wave-front structure.
- Strength/viscosity details relevant to blast loading of natural materials.
- Phase transitions?

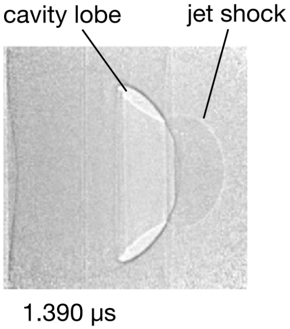
A. D. Sakharov et al., *Soviet Phys. Doklady* 9, 1091 (1965); T.J. Vogler, *J Dyn Behav Mat* 1, 370 (2015).

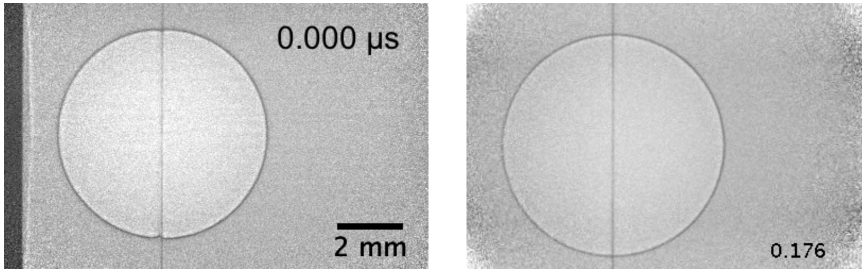
Mesoscopic effects: Void collapse in solids









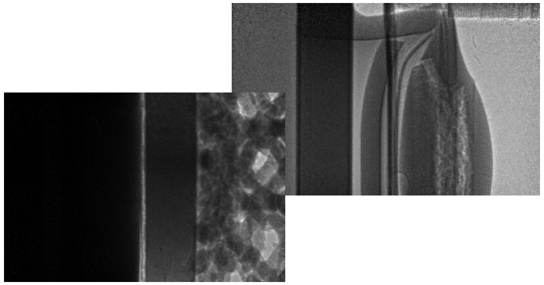


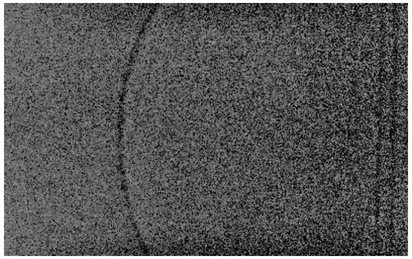
- Transition in collapse mechanisms with impact stress.
- Collapse time metric obscures mechanism of collapse.
- Temperatures in the cracks? Jet?
- State of matter upon release?

Anderson et al., *Proc Meet Acoust* 19, (2013)

Limitations of synchrotron facilities

Current 3rd generation synchrotron sources enable us to peer under the surface of dynamic compressed matter to get closer to origins of damage and failure.





4X PCI image of cavity

Accessing the grain scale will be met be several key challenges…

- Imaging resolution

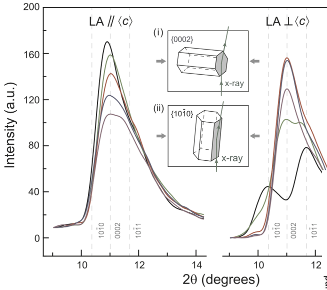
  ~few to 10s um, limited by bunch flux

- Scattering

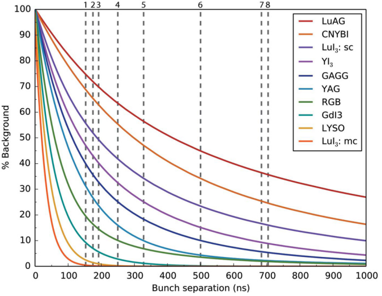
  low signals require intensified detectors based on noisy MCP tech

- Bunch frequency

  Forced to use sparse fill modes (detection)



1 μs exposure



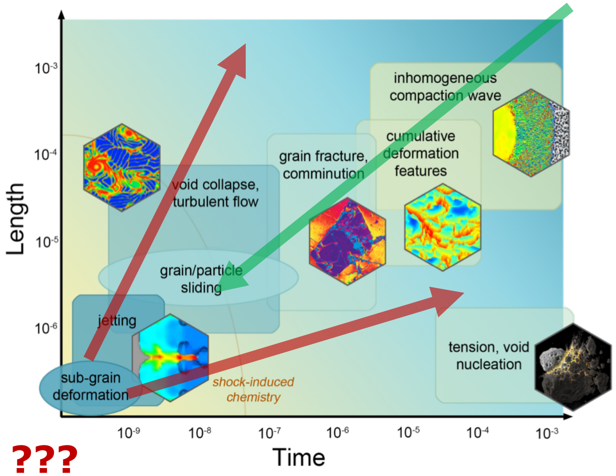
Gates > 100 ns

Opportunities for UK-XFEL

I. Targeted experiments studying the mechanisms of deformation under controlled dynamic loading conditions, which inform macroscopic behavior.

Deformation mechanisms

- Dislocation dynamics
- Slip/twin interplay
- Phase transitions



???

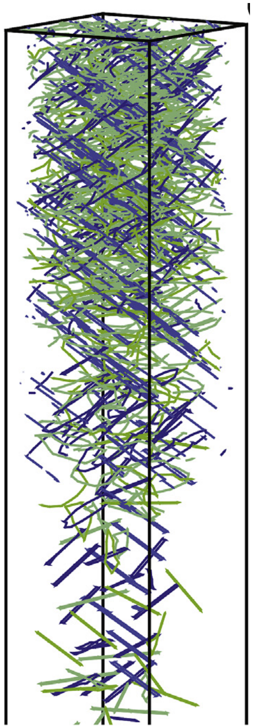
II. Material properties during materials synthesis through real-time scattering

Ultrafast processes

- Additive manufacturing
- Laser-shock peening

Origins of plasticity

- Dislocations, as the agents of plasticity, govern the slip-mediated deformation of materials.
- Models rely upon mobile dislocation density, and details of nucleation, motion and interaction.



J. Taylor, J. Gilman and others:

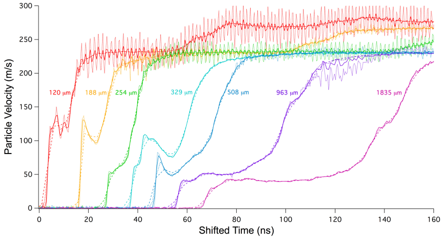
$$\dot{\epsilon}^p = \Phi b(\boldsymbol{\rho_0} + \boldsymbol{\alpha}\epsilon^p)v_0 \exp(-D/\tau)$$

$$\frac{dP}{dx} = -2G\dot{\epsilon}_0^p/c$$

J. Clayton and J. Lloyd:

$$\frac{dP}{dt} = \frac{-\hat{\alpha}G}{t_0\left[\frac{3}{2} - \frac{1}{2}\frac{c_l^2}{U^2}\right]}\bar{P} \cdot \left[1 + f_t \cdot \left(1 - \frac{U}{c_l}\right) \cdot \frac{\boldsymbol{M}}{\rho_{D0}}\frac{t}{t_0}\bar{P}\right]$$

- Estimated from bulk experiments, inferred from wave profiles, molecular dynamics – never observed *in situ*!



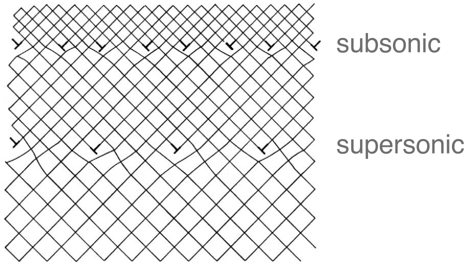
J. Taylor, J. Appl. Phys. 36, 3146 (1965); J. J. Gilman, J. Appl. Phys. 36, 3195 (1965); J D Clayton and J T Lloyd 2018 J. Phys. Commun. 2 045032

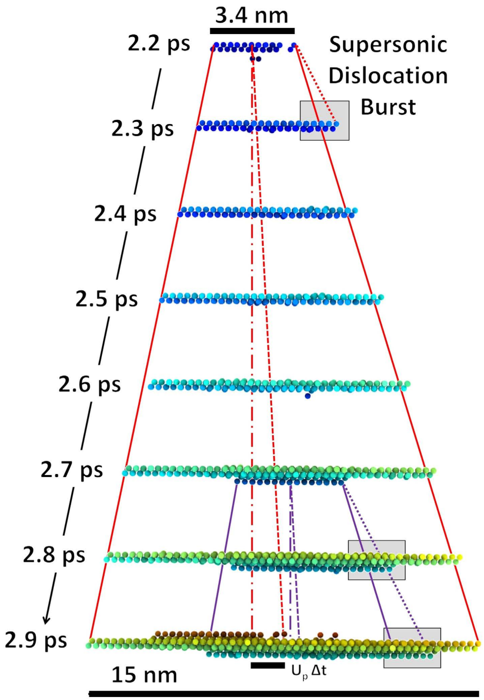
Supersonic dislocation motion?

- First theorized by Eshelby in 1949, and has been a topic of frequent speculation over the years.
- Models/theory have shown that under certain conditions, supersonic motion is possible.
- Motion has implications for dislocation density evolution, and thus underpins the strength of materials under shock loading.

- Length-/time-scales only matched to an XFEL:
  - Measure dislocation density *in-situ*
  - Measure individual dislocation motion
  - Validate/define new mobility and drag laws

J. Weertman (1981)

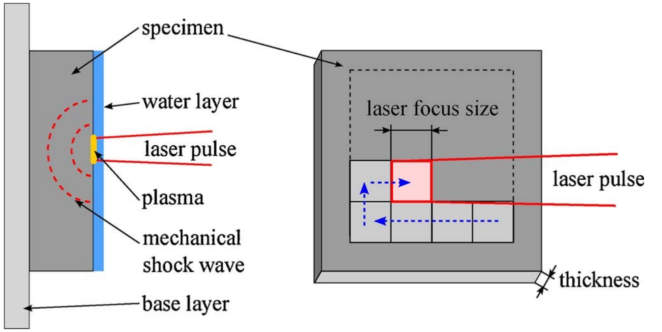


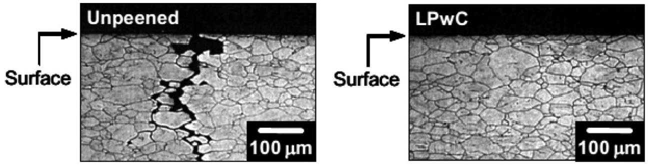


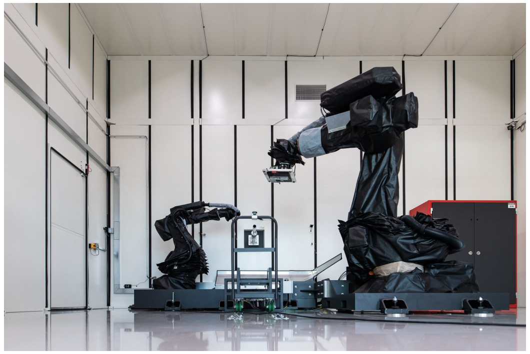
P. Gumbsch et al., *Science* 283, 965–968 (1999); E. Hahn et al., *Scientific Reports* 6, (2016); S. Peng et al., *Physical Review Letters* 122, (2019).

Laser-shock peening

- Surface processing technique to improve the fatigue life and resiliency of components.
- Laser-driven shock waves drive damage and even phase transformations few mm depth, surface in compression limiting growth of fatigue cracks.
- Can even return cracked component to original life!
- Processing involves selection of pulse energy, spot size, overlap, coating, etc.
- Commercial systems utilize high-power lasers, requiring transport of components to bespoke facilities.





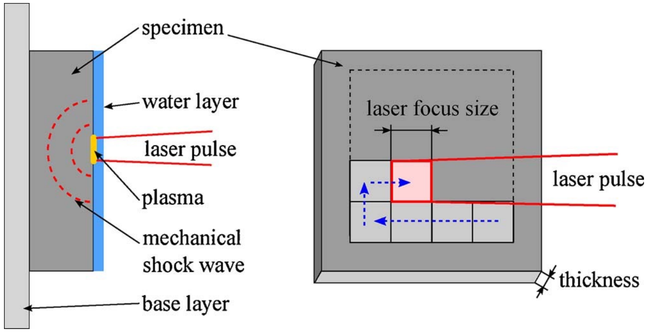


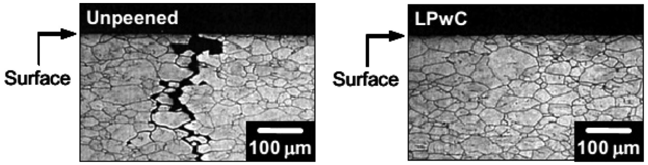
2.6 M€ facility in Hamburg

S. Keller et al., *J Mat. Proc. Tech*. 255, 294-307 (2018); S. Kalainathan et al., *Opt & Laser Tech*., 81, 137 (2016).

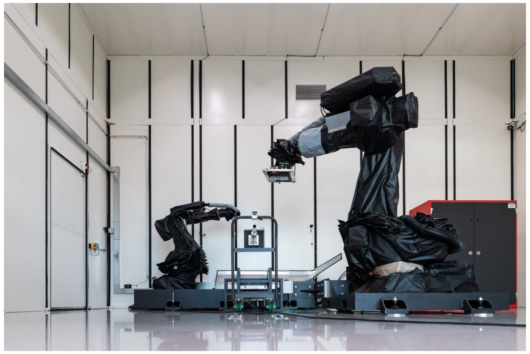
Laser-shock peening

- Low power LPwC technique could let LSP move from an at-manufacture approach (or at best, lengthy service) to an in-place service, leading to less down-time.
- Historically lengthy iterative optimisation for different materials, shapes, etc.
- Modelling laser-target interaction in complex geometries: progressive evolution of defect structures/temp, link to residual stress.





- N-dim space requires high rep-rate XFEL
  - Track the interaction of new defects with pre-existing and evolving defect substructure.
  - Real-time residual stress imaging?
  - Improved models to optimise LSP to achieve desired defect state, depth, performance.



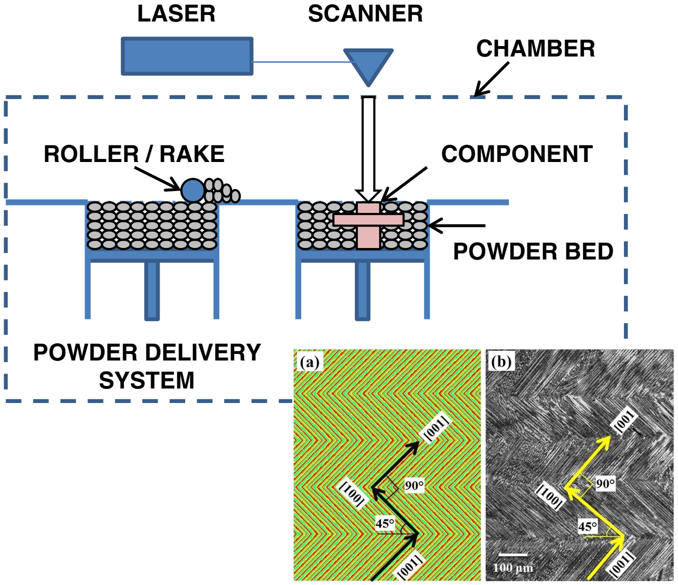
2.6 M€ facility in Hamburg

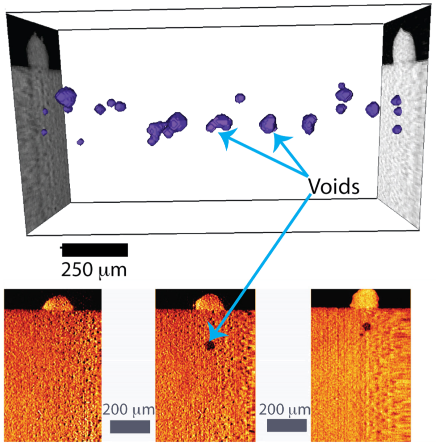
S. Keller et al., *J Mat. Proc. Tech*. 255, 294-307 (2018); S. Prabhakaran et al., *Mat. & Des.* 107, 98 (2016).

Additive manufacturing

- Bottom-up layer-by-layer fabrication of prototypes and end-use parts.
- Ability to fabricate complex or “impossible” parts (from a CM perspective)
- Potential for direct control of mechanical properties at grain scale, leading to new bulk shape optimisations – weight savings, etc.

- Market value of over $7B in 2017.
- Take-up limited by print time, and uncontrolled mechanical properties (texture, processing defects).
- E.g. conditions for keyhole mode melting influenced by complex parameter space: power, spot size, velocity, layer height, etc.

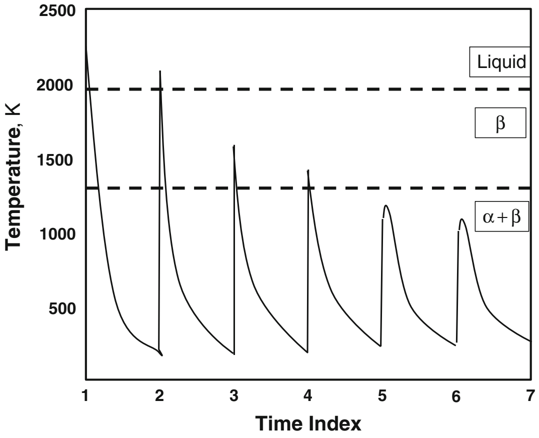




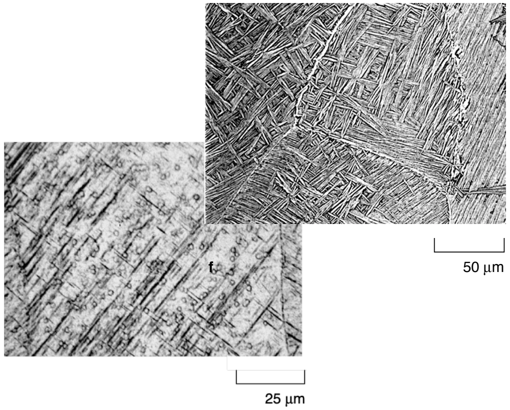
W.E. Frazier, *J Mat Eng Perf* 23, 1917 (2014); W.E. King et al., *J Mat Proc Tech* 214, 2915 (2014); H.L. Wei et al., *Scientific Reports* 5, (2015);

Materials by design from the bottom-up

- Optimum parameters found by modelling the powder bed fusion process.
- Prediction of grain-size, texture, and chemistry challenged by complex temperature history.
- Mechanical properties thus affected by build plate content.



- Opportunities for a high rep-rate XFEL
  - Use potential for single-bunch X-ray probing to monitor phase formation during melting, solidification cycles.
  - Link thermal history to phase fractions, morphology (e.g. lath width) – predict mechanical properties.

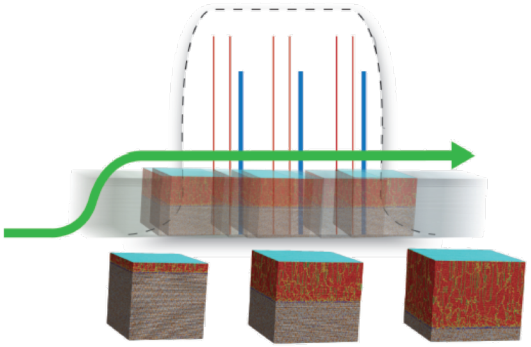


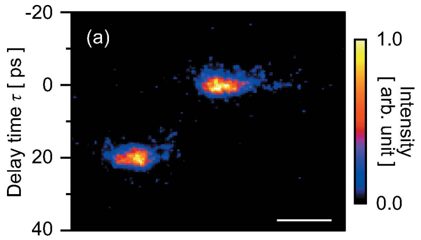
W.E. Frazier, *J Mat Eng Perf* 23, 1917 (2014); J. Irwin, et al., *J Manuf Sci Eng* 138, 111007 (2016).

Wish-list for UK-XFEL

Key facility desirables

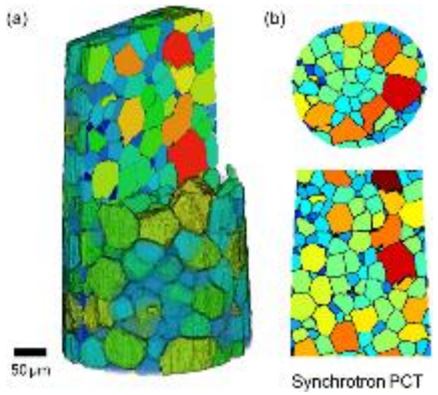
- Flexible energy range, harder the better.
- Multi-pulse capability (arbitrary macro/micro-bunch spacing, split/delay), spanning ps to ns.
- Pulse spectral chirping, to facilitate separation through scattering?
- High repetition rate.
- Variable beam sizes to tailor interaction volume – imaging to diffraction.
- Large experimental halls to permit bulky apparatus.





Support

- Access to lasers with fully customisable pulse length, shape, spot size, etc. (and the staff to run them!) – Integration with Central Laser Facility?
- Access to pre/post characterisation techniques (X-ray tomography, neutron diffraction) – proximity to Diamond/ISIS?



S.A. McDonald et al., *Scientific Reports* 5, (2015); T. Hirano et al., *J Synch Rad* 25, 20 (2018).

Final thoughts

- The intelligent design of materials depends upon a hierarchy of behaviour with its origins at the microscale; across a diagnostic gap.

- Also a gap between theory and practice – realization of architectured materials over engineering length-scales.

- A UK hard X-ray free electron laser can help close these gaps, by providing fundamental information on,
  - Mechanisms of dynamic stress relaxation in materials,
  - Kinetics/pathways of shock-induced chemistry,
  - Processing/structure/property correlations in additive manufacturing,
  - Real-time defect structure evolution in laser shock peening

➢ Opportunity to influence direction of UK manufacturing towards a new materials revolution.