leoradm@stanford.edu

Operando Science Enabled by the Linac Coherent Lightsource (LCLS)

Leora E. Dresselhaus-Marais
Assistant Professor
Materials Science & Engineering,
Mechanical Engineering (Courtesy)
Photon Science (Term)

Stanford University

SLAC

Precourt Institute for Energy

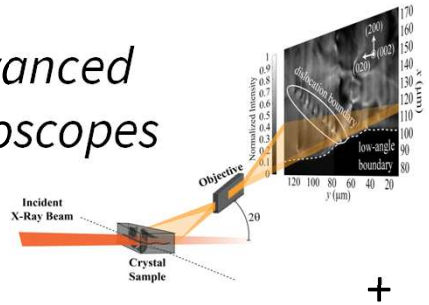
Website

leoradm@stanford.edu

My Perspective: Science Underlying Sustainable Manufacturing

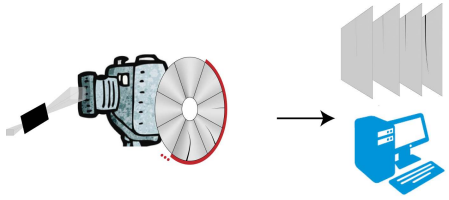
"Modern Toolbox"

Advanced Microscopes

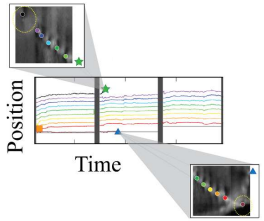


+

"Rare Event" Cameras

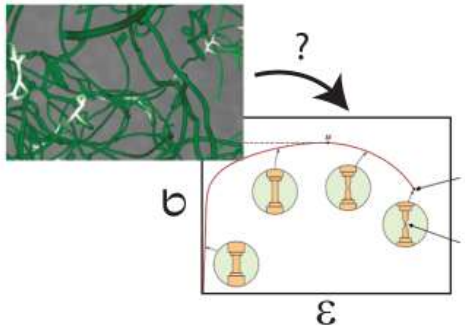


+



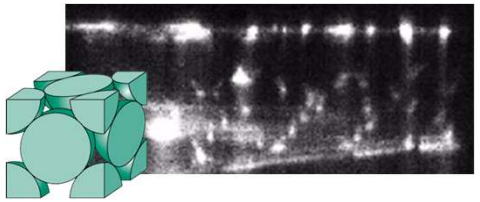
AI for Analysis, Control, Reactor Models

Controlling Strength



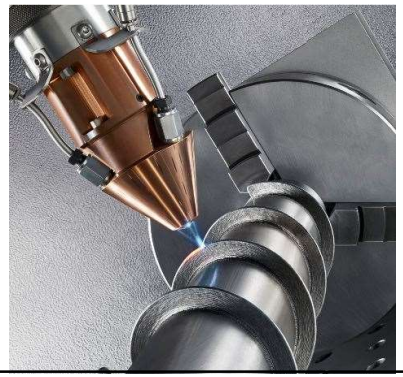
Metals Processing Science

Refining Processing

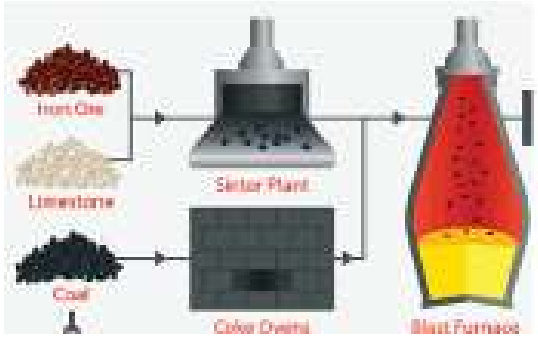


Enable Sustainable Technology

Metal 3D Printing

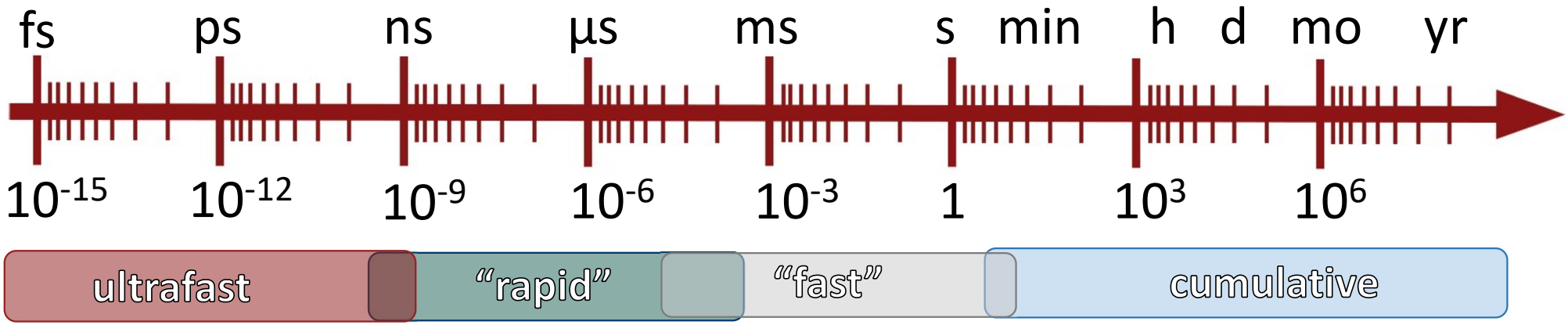


Resource Sustainability



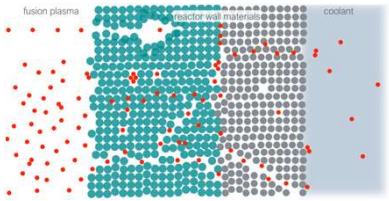
Manufacturing Science Spans Many Timescales

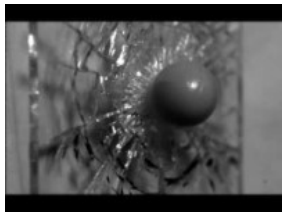
leoradm@stanford.edu



Nano Phenomena:

Electrons, Extreme Dynamics, Photons, Phonons



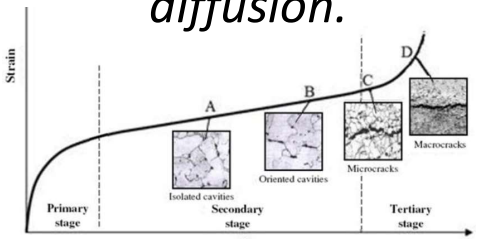


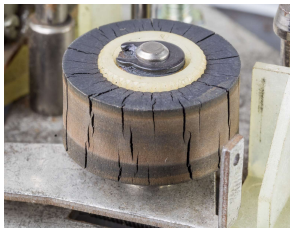
Mesoscale Dynamics:

fracture, phase transitions, chemistry

Meso-Micro:

crystal plasticity, equilibrium processes, diffusion.





Structure-Scale:

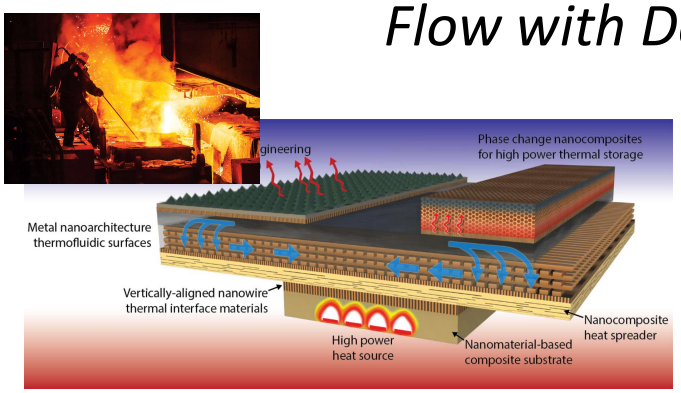
Fatigue, Corrosion, Embrittlement

Lifetime & Performance of Devices Require Science Connecting All Timescales

Thermal Engineering to Control Waste Heat

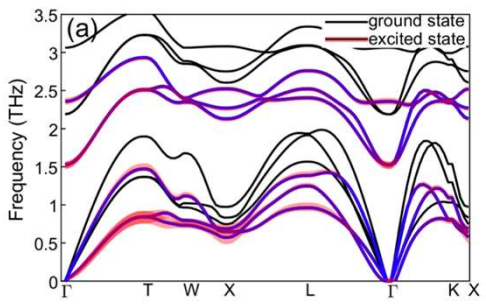
leoradm@stanford.edu

Thermal Engineers Need to Control Heat Flow with Defects



Barako, et al. Nanotechnology, **29**, 154003 (2018).

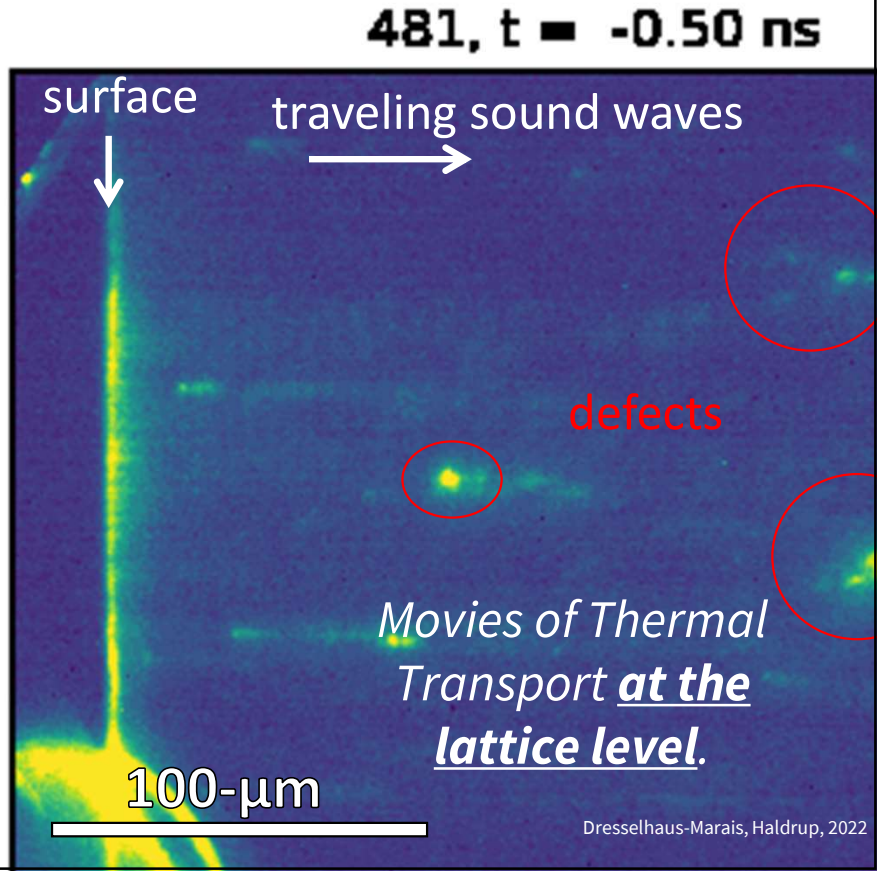
Measured Phonon States



Teitelbaum *et al.* **PRB** 103, L180101 (2021)

Requires control of Phonons at Operating Conditions

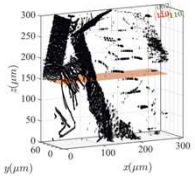
Phonon Interactions with Dislocations

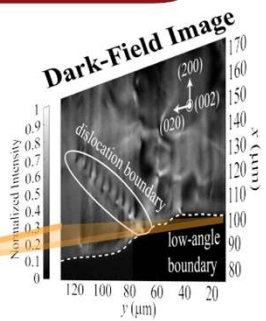


Movies of Thermal Transport ***<u>at the lattice level</u>***.

Dresselhaus-Marais, Haldrup, 2022

New Microscope to Image Strain & Defects in Lattices



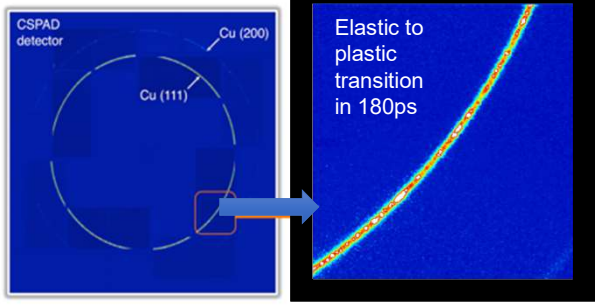


Dresselhaus-Marais, et al. Science Advances, abe8311 (2021)

Incipient Failure & Transformations for Materials Discovery

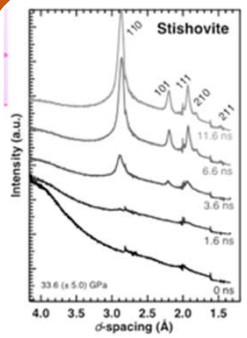
leoradm@stanford.edu

Shock Waves Test Failure for Alloy Design



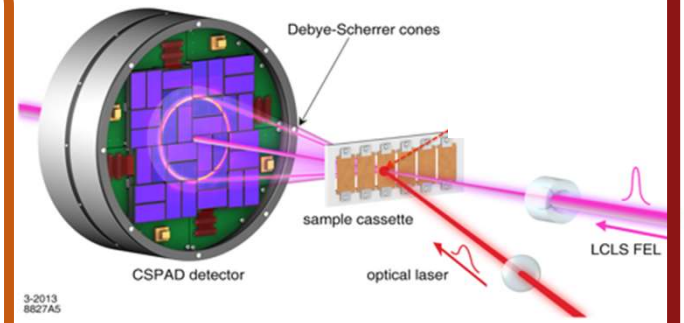
- Ultrafast laser generates shock waves
- Failure studies allowed Rolls-Royce to design Ti alloys

Milathianaki et al, *Science*, 342, 220 (2013)

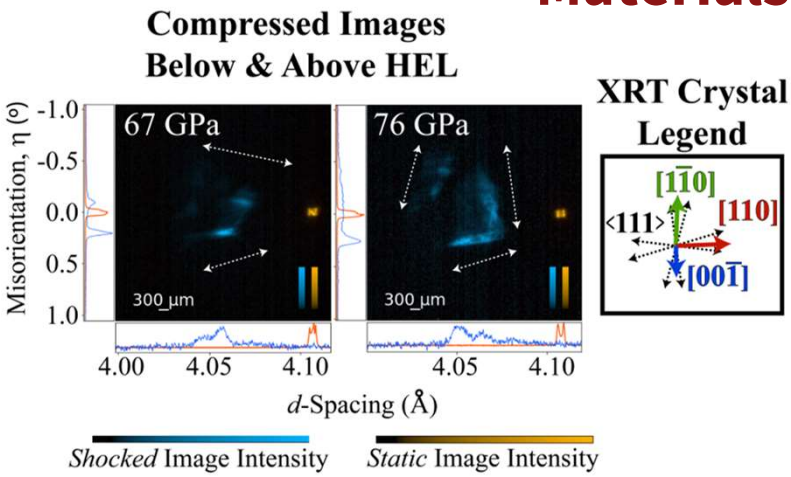


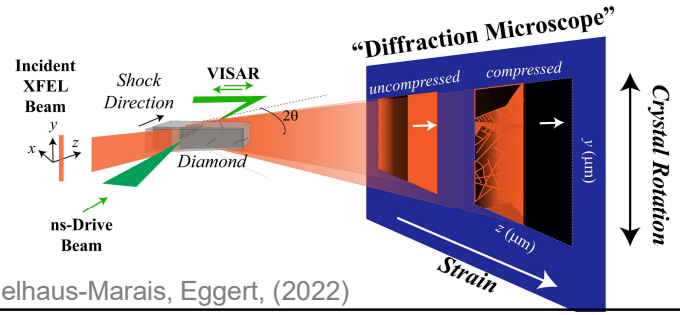
- SiO_2 (stishovite) crystallization in meteorite impact conditions
- Kinetics of phase transformations inform synthesis opportunities

A. Gleason et al, *Nature Comms* (2015).



Imaging Failure Mechanisms to Design New Ultrahard Materials

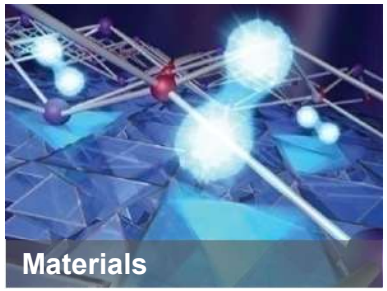


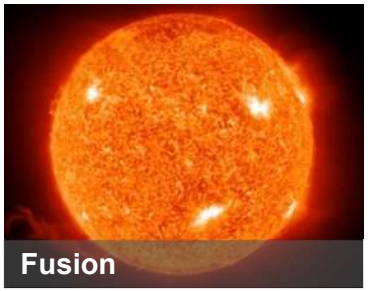


Dresselhaus-Marais, Eggert, (2022)

leoradm@stanford.edu

LCLS's Unique Capabilities enable High-Impact Science & Discovery



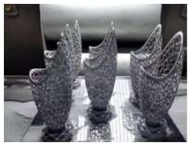


Building New Communities for Operando Science

leoradm@stanford.edu

Accessing the Scales to Enable Control in Metal 3D Printing

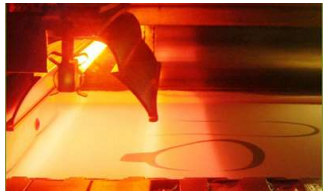
Metal 3D Printing (AM) is transforming manufacturing today.



R. Ye, "3ERP Presents: an Affordable Route into Metal AM" 3DPrint.com.

"Additive Manufacturing: Aviation and aerospace industry" GE Additive.

Printing layer-by-layer to construct unique components.

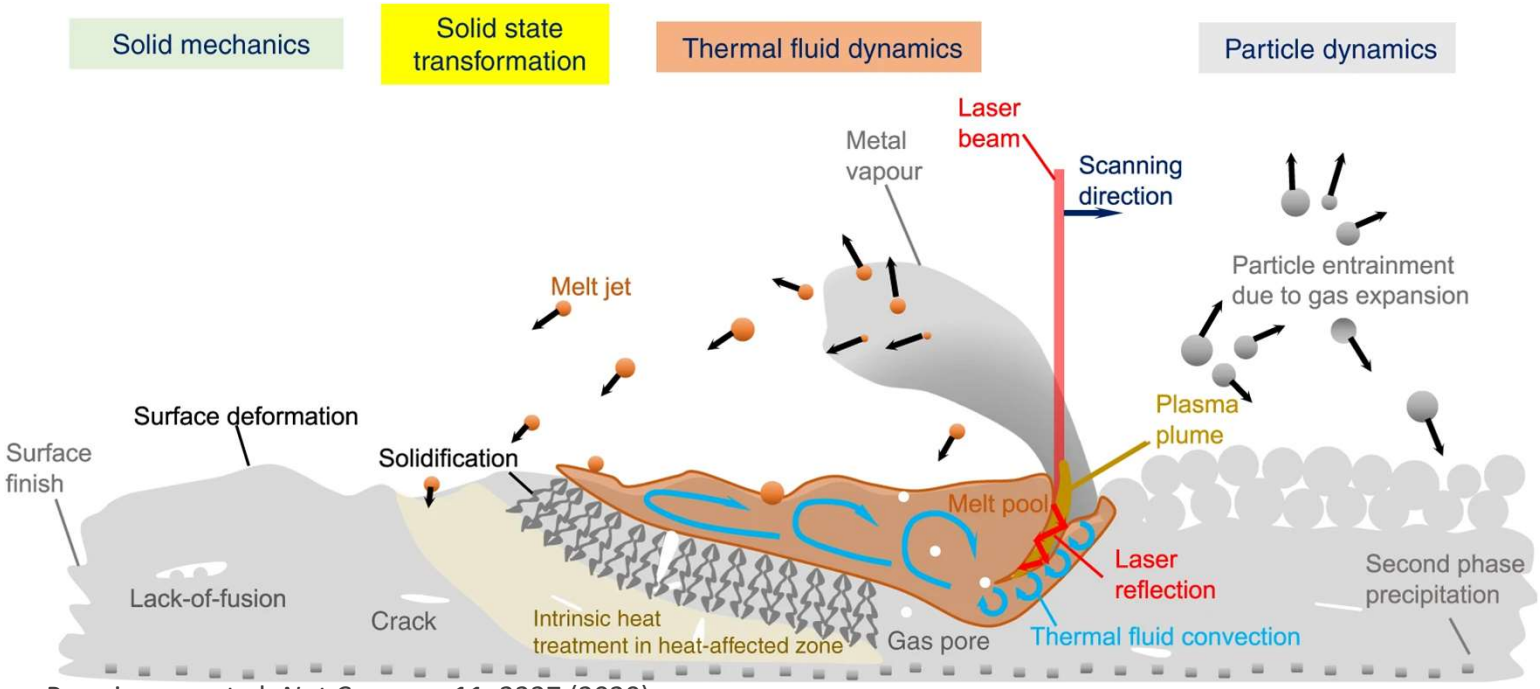


"About Additive Manufacturing – Powder Bed Fusion" Loughborough University, *AMRG.*

For robust metal-AM parts, we need control of the microstructure.

Persistent Fundamental Gaps Inhibit AM Feasibility:

We require robust fundamentals to understand & control the lifetime & performance of printed parts

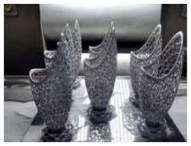


Panwisawas, et al. *Nat Commun* **11,** 2327 (2020).

leoradm@stanford.edu

Accessing the Scales to Enable Control in Metal 3D Printing

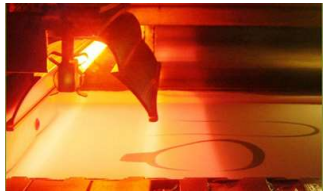
Metal 3D Printing (AM) is transforming manufacturing today.



R. Ye, "3ERP Presents: an Affordable Route into Metal AM" 3DPrint.com.

"Additive Manufacturing: Aviation and aerospace industry" GE Additive.

Printing layer-by-layer to construct unique components.



"About Additive Manufacturing – Powder Bed Fusion" Loughborough University, *AMRG.*

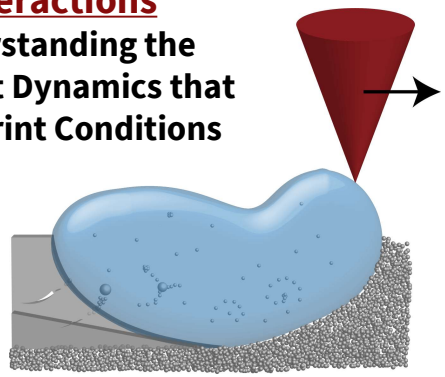
For robust metal-AM parts, we need control of the microstructure.

Persistent Gaps in Fundamental AM Science:

We require robust fundamental models to understand & control the microstructure

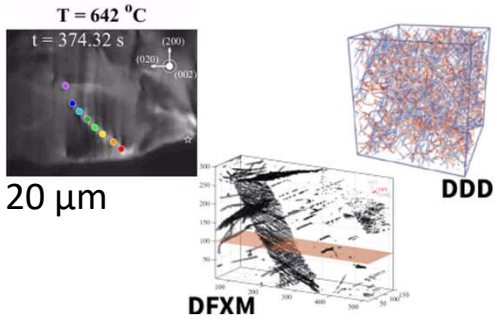
fs-ns: Light-Matter Interactions

Understanding the Incipient Dynamics that Drive Print Conditions



ns-ms: Solid Mechanics

T-Driven Microstructural Dynamics



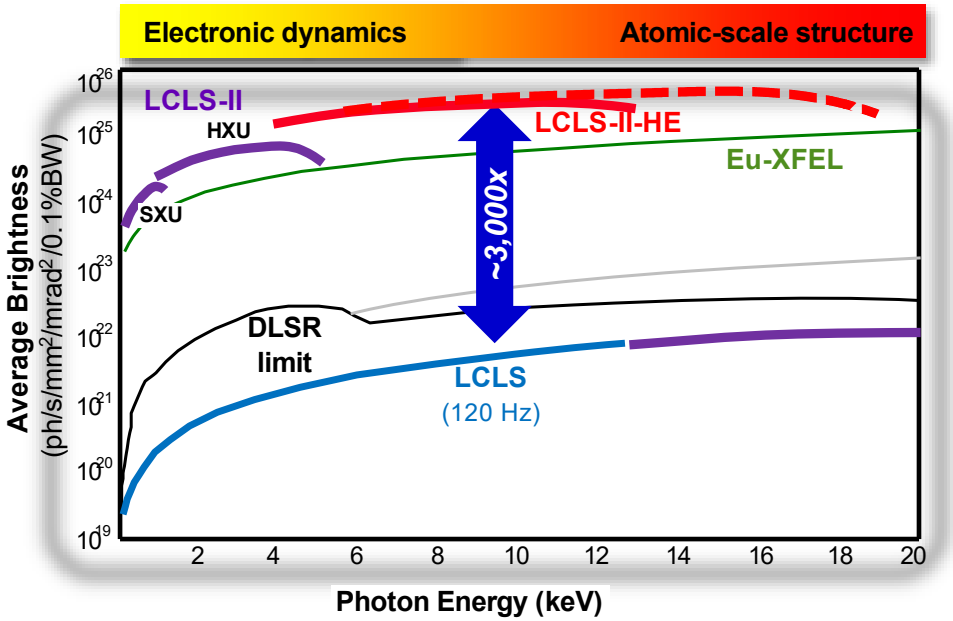
ps-µs: Turbulent Fluid Dynamics

Competing Driving Forces in Melt-Pool Cause Spatter, Segregation, Mixing

XFEL Coherence & Ultrafast Science Required for Range of time- & length-scales

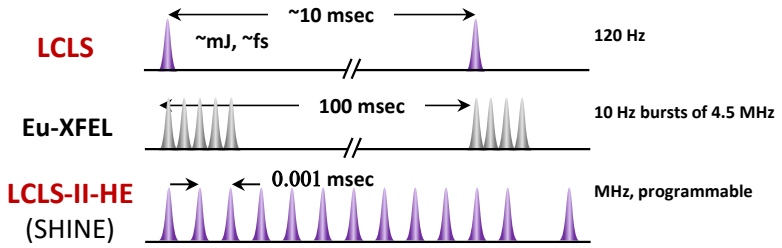
leoradm@stanford.edu

Looking Forward: LCLS-II-HE will provide a step-jump in capability



LCLS-II-HE will provide:

- Ultrafast, coherent, hard X-rays
- ~3,000-fold increase in average spectral brightness
- ~8000-fold increase in repetition rate
- Programmable time structure
- Mature experimental basis, and advanced modes of operation

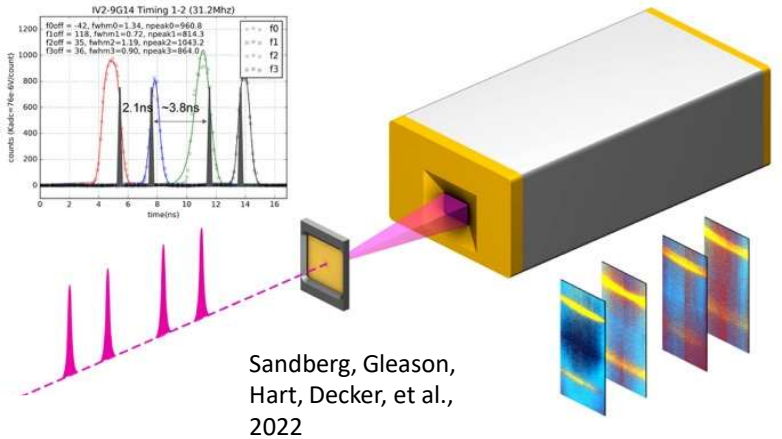


Leaping from 120 Hz to 1 MHz will be transformative:
Enabling Access to Multi-Timescale Science representative of Real-World Systems

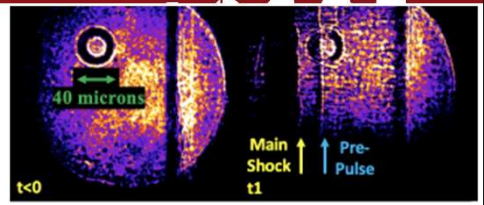
leoradm@stanford.edu

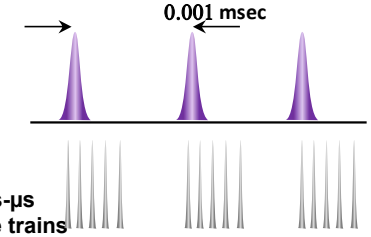
Developing the Detectors & Accelerator for Operando Needs

Developments in Pulse Trains & Detectors Enable Key Science Opportunities

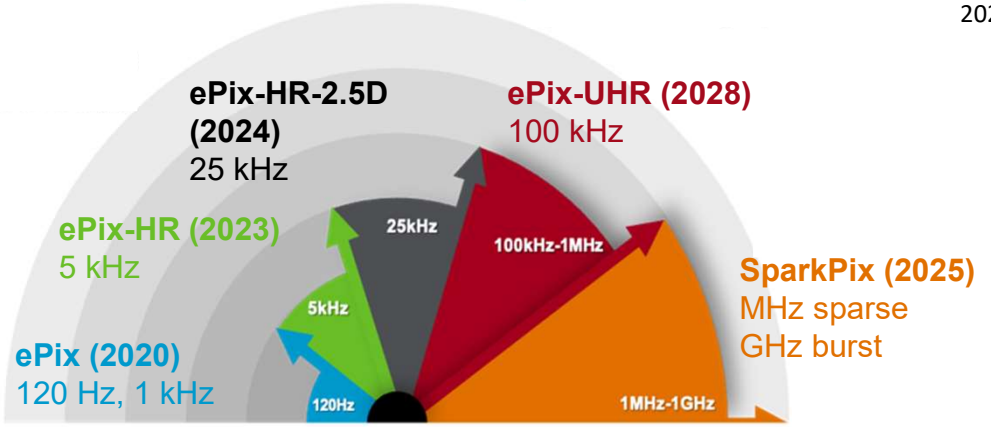


Sandberg, Gleason, Hart, Decker, et al., 2022



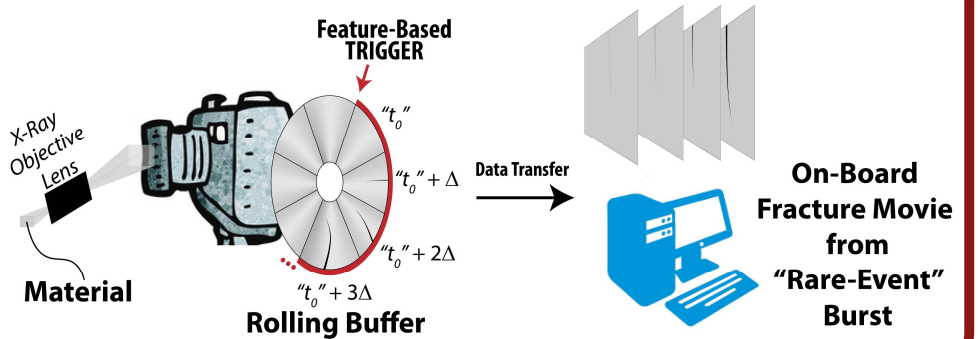


SLAC Technology and Innovation Directorate
(TID: Angelo Dragone et al)



SLAC ePix Development Plan

Rare Event Camera for Stochastic Processes



R. Coffee, L. Dresselhaus-Marais

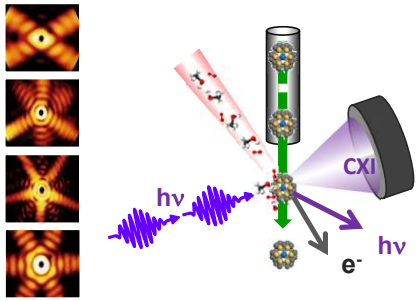
Team Approach Offers Opportunities to Access Multi-Timescale Processes in Real-World Systems

leoradm@stanford.edu

LCLS-II will transform our understanding of dynamics in real-world systems

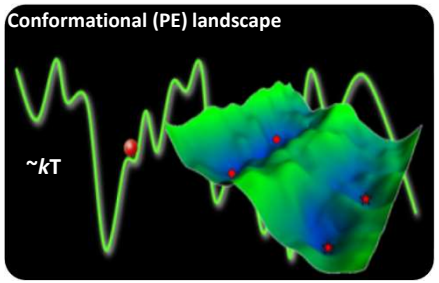
How to accelerate chemical reactions

- Correlate catalytic reactivity and structure
- Real-time evolution with chemical specificity and atomic resolution



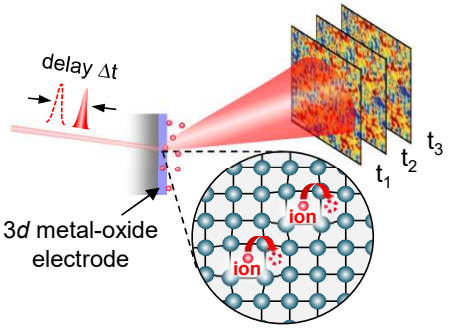
Watching biology in action

- Study large scale conformational changes via solution scattering
- Physiological conditions (room temperature, solution phase)
- Dynamics ties structure to function



Understanding material function and failure

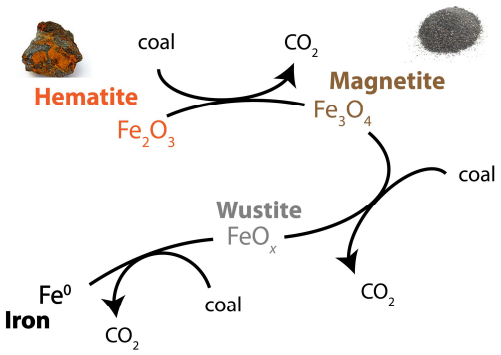
- Characterize dynamic systems without long-range order
- Directed design of energy conversion and storage materials

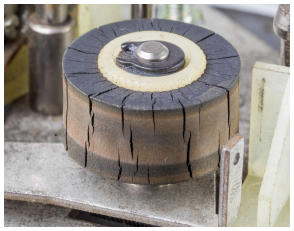


leoradm@stanford.edu

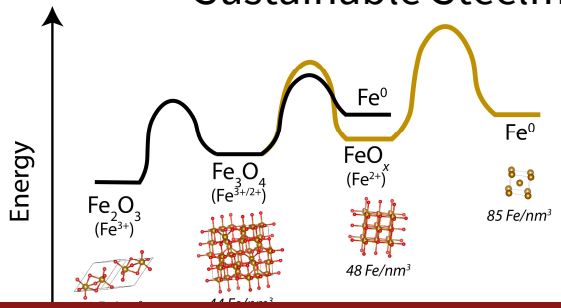
Hydrogen Dynamics in Environmental Ultrafast Electron Diffraction

Material Performance & Chemistry in Hydrogen Environments are Key to Hydrogen Economy

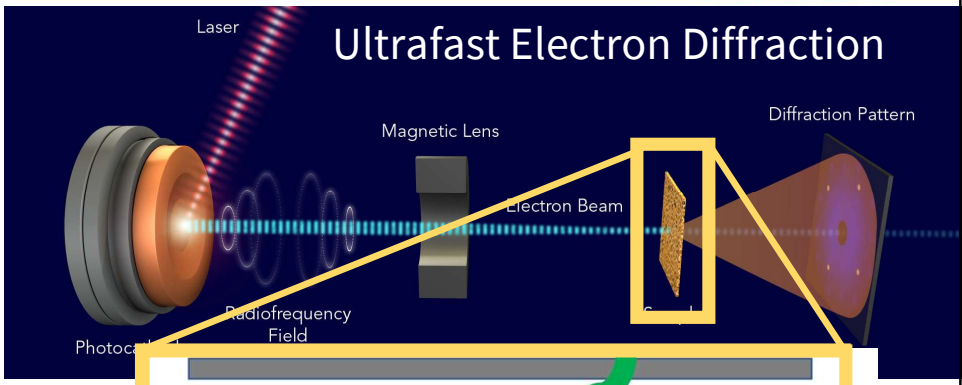


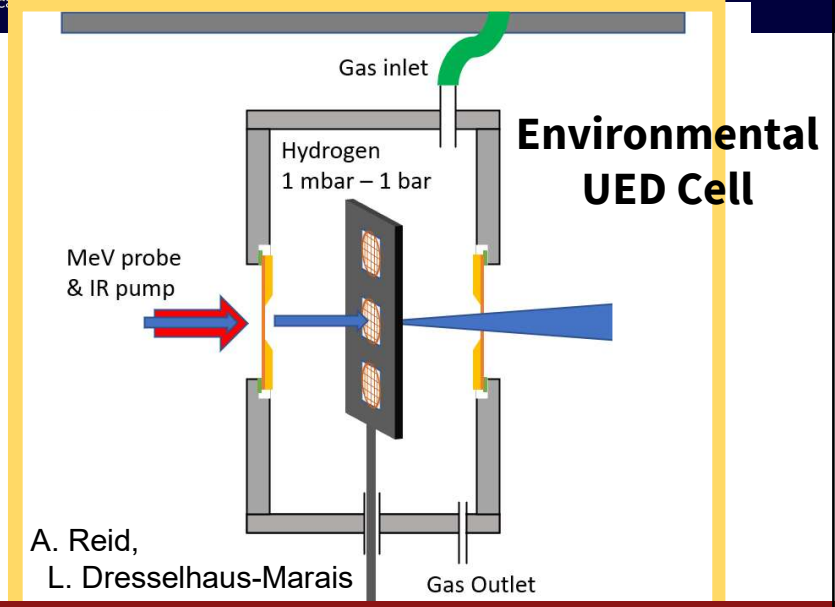


Hydrogen Science Required to Enable Sustainable Steelmaking



Gas-Phase environment to Test the Fundamental "Rare-Event" Science Chemistry of Hydrogen in Engineering Systems





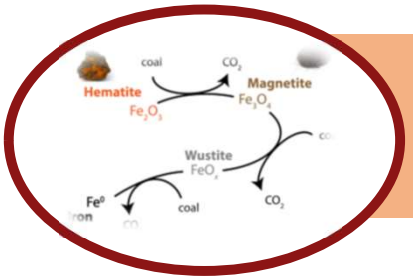
Environmental UED Cell

A. Reid,
L. Dresselhaus-Marais

Measuring Chemistry, Diffusion, Embrittlement at its Native Timescales

leoradm@stanford.edu

Summary: LCLS Opens a Wide Range of Operando Science

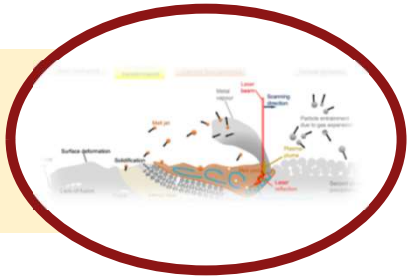


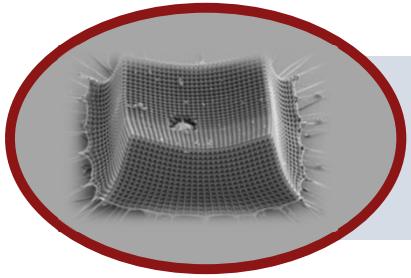
Mapping Reaction Landscapes in Real Environments:

Pyrometallurgical extraction chemistry (Critical Materials), Geochemistry, Upcycling Plastics, Natural & Artificial Photosynthesis, Green Catalysis

Materials Science & Physics:

Physics Underlying Defect Engineering, Thermal Transport, Electronic Designs, & Advanced Materials Discovery





NanoMaterials:

Quantum Information, Architected Materials Dynamics, & Emergent Phenomena

Biological Function & Structural Dynamics

Dynamics in Physiological Environments, Biomass Energy & Waste Management