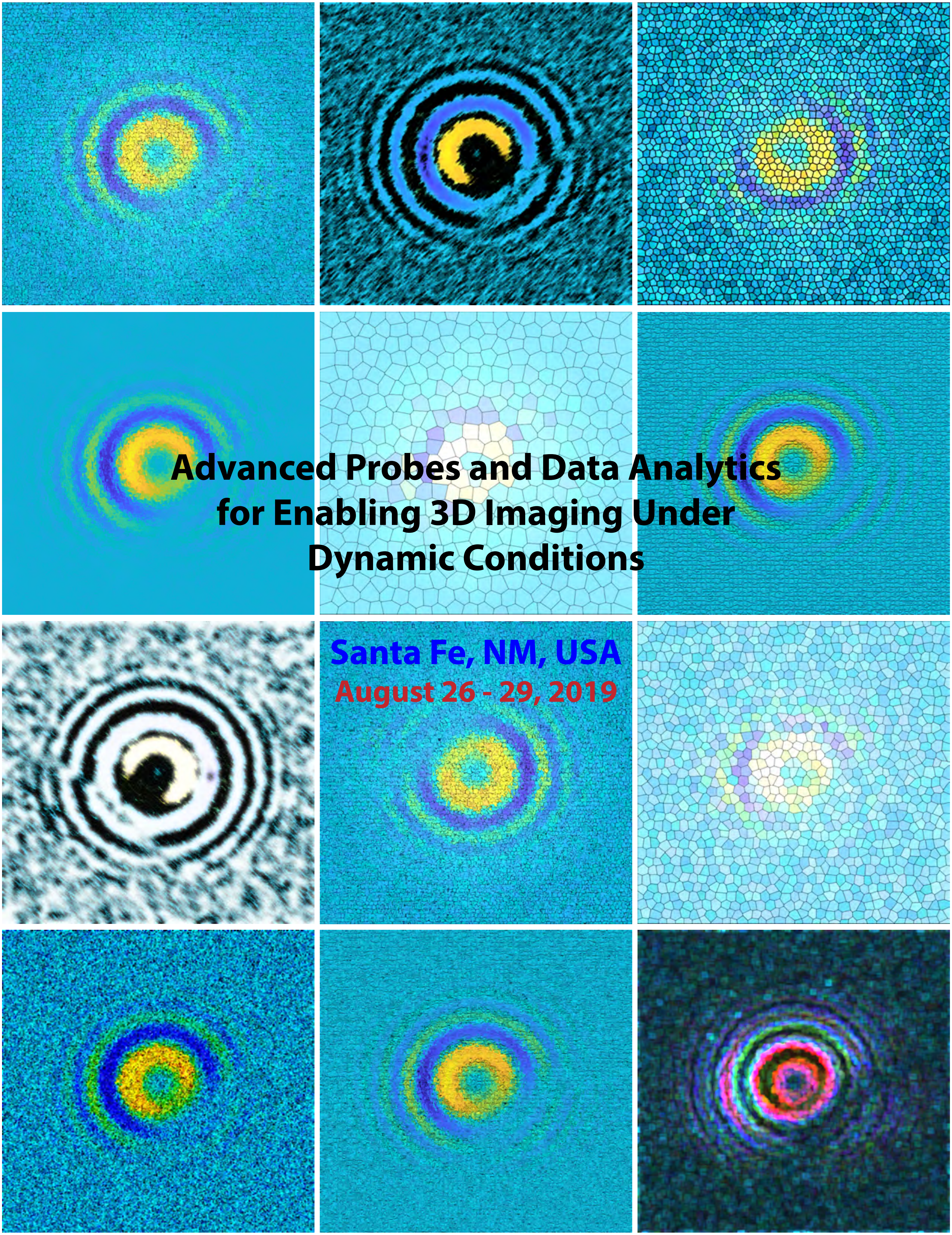

Advanced Probes and Data Analytics for Enabling 3D Imaging Under Dynamic Conditions

Santa Fe, NM, USA

August 26 - 29, 2019

Advanced Probes and Data Analytics for Enabling 3-D Imaging Under Dynamic Conditions

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`http://www.cvent.com/d/lyq756`

LAUR-19-31832

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Participants

Executive Summary

There has been a rapid acceleration in the development of new three-dimensional dynamic materials characterization techniques at synchrotron and free electron laser light sources that enable scientists to access material structures, properties, and performance from nano- to macro-scales at relevant time-scales. The advancement of detector technologies capable of harnessing the full brightness and time structures of these light sources are identified as a critical need for the materials dynamics community. In addition, transformational science is achievable through intimate coupling of modern data analytics with mesoscale modeling capabilities.

Major findings of this workshop are :

1. Moving towards three-dimensional (3-D) characterization at the fastest time scales (ps-μs) will require multi-projection probes/beams.
2. Information retrieved from high-value experiments can be greatly improved through optimized sampling and sophisticated reconstruction algorithms that make the best use of current detector technologies.
3. The material science community focusing on *in situ* 3-D dynamic materials' characterization needs to articulate a fixed set of detector requirements and secure long-term funding to advance the development of the ideal detector(s).
4. A need for better integration between experiments and simulations is identified. The use of simulations/machine learning to inform experimental design and guide the interpretation of experiments is critical to enable a mechanistic insight across length and time-scales.
5. Multi-scale material model predictions need to forward model experiments for uncertainty quantification / sensitivity and interdependence of parameters. From this, reliability metrics can be obtained.
6. The use of machine learning in the materials community is dominated by adaptation of previously developed algorithms. Algorithms need to be developed to directly address materials challenges, particularly the characterization of weakest-link events and material heterogeneity.

Introduction

A fundamental understanding of the dynamic (time-dependent) behavior of heterogeneous material systems at the mesoscale ($< \mu$m, $< \mu$s) is currently lacking. The goals of this workshop were: **1)** To identify the technological gaps that need to be addressed for enabling three-dimensional (3-D) materials imaging at the mesoscale to develop an understanding of properties and performance of materials under dynamic conditions. **2)** Determining the most promising research directions that utilize advanced probes, detector technologies, and data analytics for predictive dynamic material model development. **3)** Design of next generation materials with tailored properties.

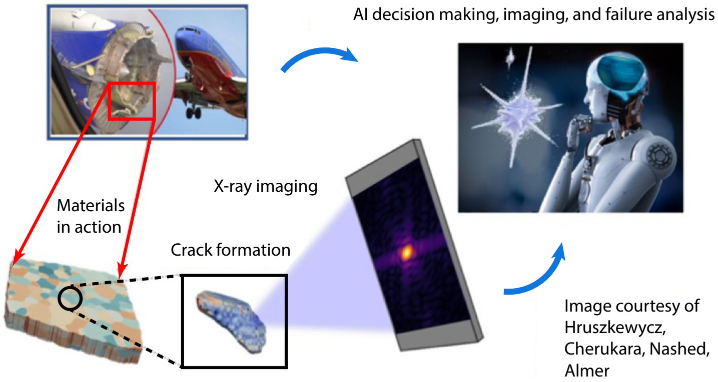

Figure 1: 3-D dynamic imaging, using available capabilities to field the best-possible experiments, and forging a synergic relationship among experimentalists, detector developers, and data scientists.

Workshop focus areas

1. Experimental techniques and sample environments (*in situ*) for single pulse dynamic imaging (high-energy X-rays, electrons, protons, and ions)

2. Detector technology for dynamic imaging using high-energy X-rays and electrons (development, calibration, and characterization)

3. Data analytics and advanced algorithms for real-time feedback during dynamic measurements (machine learning methods for inverting measured data and develop reduced material models)

For each focus area, the workshop participants aimed to identify and articulate the current state of the art, determine promising paths forward, and recommend areas of future investments of talents, resources, and research funding. Summary and findings from each working group are presented in the following sections.

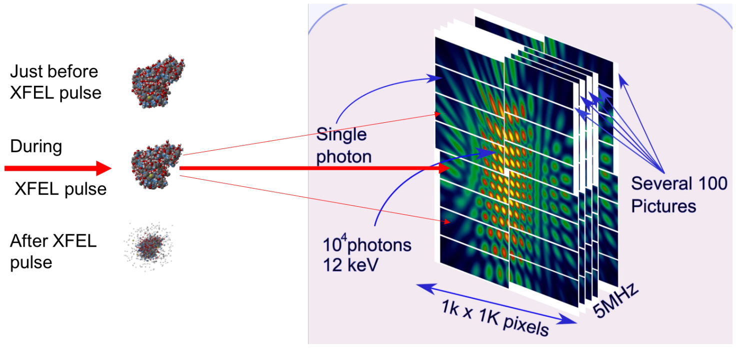

Figure 2: Single pulse imaging requires high-brilliance of Xray free electron lasers and dynamic detector technology. (Image courtesy of Heinz Graafsma.)

Experimental techniques and sample environments

Introduction

This decade has seen a revolution in coupling dynamic loading platforms (gas guns, lasers, Kolsky/Hopkinson bars) with high-energy and highly coherent synchrotron radiation at advanced light sources. These capability developments have allowed us to peer into high rate, dynamic response of materials (structural phase transition, mechanical deformation) *in situ* at micro-to-macro scale in real-time. Applied stress and damage failure modes vary greatly in space and time. Dynamic 3-D imaging is crucial to probe the evolution in structure of these materials during impact events to understand the links between microstructure and properties of materials, for defense and commerce applications. In addition, streamlining transition of experimentally measured validation data will be important for advancing material models, to enable users to focus on material problems driven beamline science.

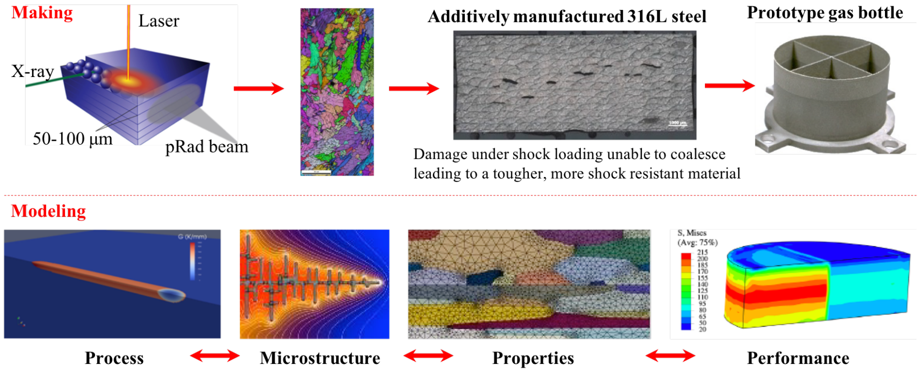

Figure 3: Critical experimental data across multiple length and time scales are required to inform and validate modeling and simulations for designing new materials with tailored properties and performance. (Image courtesy of C. Barnes.)

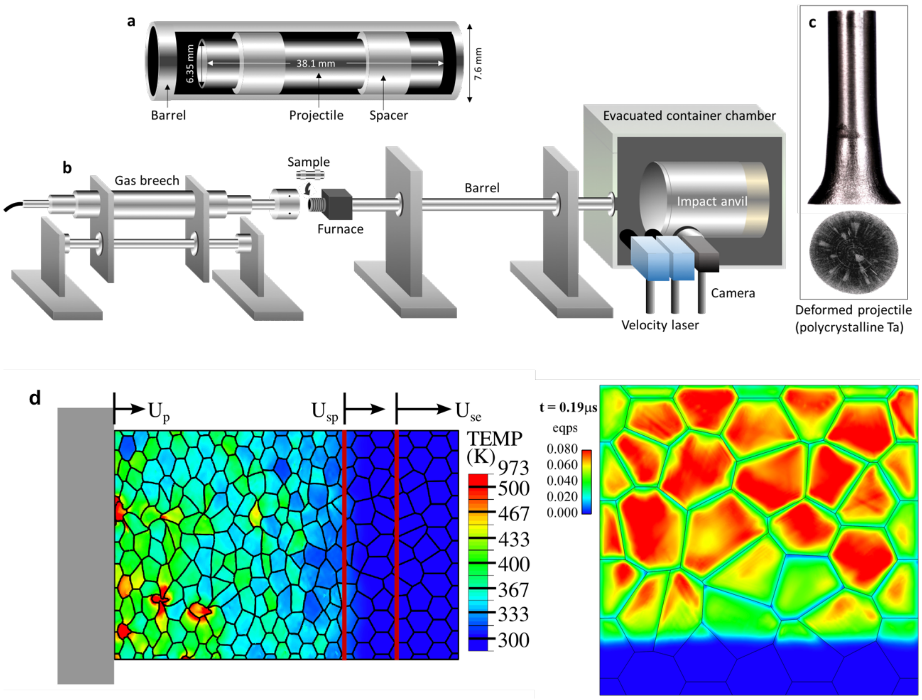

Figure 4: *In situ* measurements at beamlines provide relevant data crucial for validating mesoscale simulation of heterogeneous material fields under dynamic loading conditions (Image courtesy of GT Gray, DJ Luscher). One type of experiment uses a projectile (a) to impact an anvil and observe the interaction (b) as well as study the polycrystalline projectile after impact (c). This data can then be compared to simulations and aid in model development (d).

Current state-of-the-art

Excellent material structure capabilities characterization from nano- to macro-scales:

- Coherent X-ray diffraction (BCDI, CDI, ptychography) [1, 2, 3, 4, 5, 6, 7, 8, 9] and dark-field X-ray microscopy [10] allow characterization of material structures, dislocations, and strain with sub-10 nm 3-D spatial resolution in sub-micron-sized samples. These measurements are reaching some level of maturity for static and quasi-static measurements.

- High Energy X-ray diffraction microscopy (HEDM) allows probing of grain level properties and collective grain-level behavior in polycrystalline materials. HEDM allows investigation of large sample volumes and getting detailed insight during quasi-static experiments [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27].

- Powder diffraction allows macroscopic insight into average grain scale behavior. Feasible for single point interrogation during dynamic/high rate measurements. Significant investments in pairing dynamic compression platforms with high-flux X-ray facilities in the last decade has produced a number of dynamic compression beam lines for user experiments (e.g. DCS at APS [28], LCLS-MEC [29], SACLA, European XFEL-HED, ESRF [30, 31], Diamond [32]).
- Imaging is feasible on sub-second timescales with resolution from 10s of nm to macro-scale [33, 34]. Radiography of strongly absorbing materials has been performed [32, 35], and phase contrast imaging can be effectively used to image feature in weakly scattering materials [36, 37, 38, 39, 40, 41].
- Monitoring transient processes such as crack propagation, explosion during electric arc ignition, laser-induced micro-cavitation and jetting in water, laser-shock-induced compression [31, 42, 43] are made possible, by pushing the limits of time-resolved hard X-ray imaging for materials characterization at ESRF utilizing timing-modes with reduced bunch number but increased electron bunch charge density per singlet [44, 45]. Monitoring stochastic processes at nano to micro-second timescales are further enabled at XFEL sources [46] and process monitoring during additive manufacturing can be achieved with ultra-fast X-ray imaging at APS [47].

Challenges

- Getting 3-D information under dynamic conditions is difficult - High Energy Diffraction Microscopy (HEDM), Bragg Coherent Diffraction Imaging (BCDI), tomographic imaging, etc. are relatively slow techniques due to measurements from multiple projections required for 3D microstructure reconstructions [12].
- Resolving the dynamics of a single high-rate event requires high-energy X-rays and high photon flux in combination with fast high-resolution detectors. XFELs provide high photon flux, but are currently limited in repetition rate. Synchrotrons experiments are often photon-starved.
- Density retrieval through quantitative analysis of phase contrast images can be difficult and non-trivial, due to various factors including limited pre-characterization of the sample, non-ideal experimental geometries, low flux and low coherence of the incident beam.
- Experimental design is critical, but frequently the conditions for dynamic materials experiments are mutually exclusive to the conditions for optimal imaging/probing. Experimental design must include physical necessary compromises.
- Materials experiments that examine stochastic processes, like material failure, need to be able to measure the temporal dynamics of a single event.

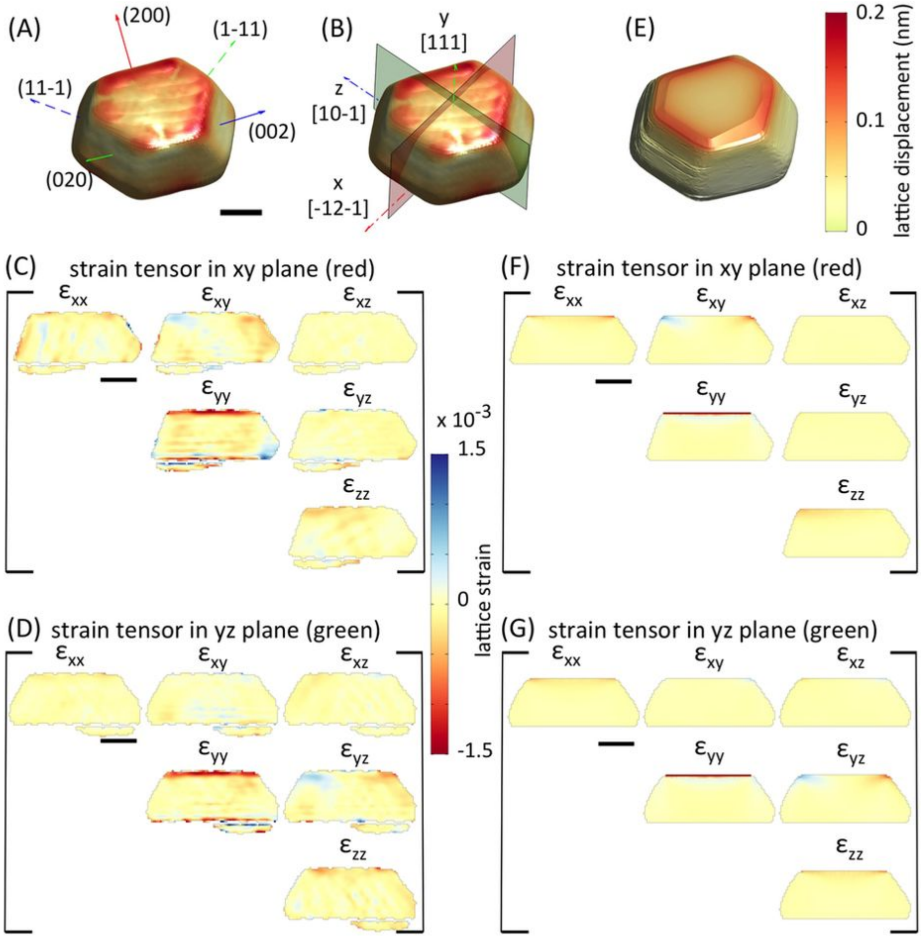

Figure 5: Advanced experimental techniques such as BCDI can reliably probe 3D nano-scale strains associated with complex crystal defect structures and provide fundamental insight into defect formation and evolution. 3D lattice distortions measured using BCDI in ion-implanted nanocrystal is shown [5]. Multiple Bragg reflections are measured to calculate 3D strain tensor from the atomic displacement field (A-D). Complementary crystal plasticity model is performed to compare the predictions (F-G) with experimental observation.

- Sample size: High Z (atomic number) materials are of interest in many cases, but due to strong absorption, the sample dimensions may need to be reduced to the limit in which the sample is no longer representing bulk material behavior.
- Translating local, nano-scale information to macro-scale and bulk-scale response is often difficult.

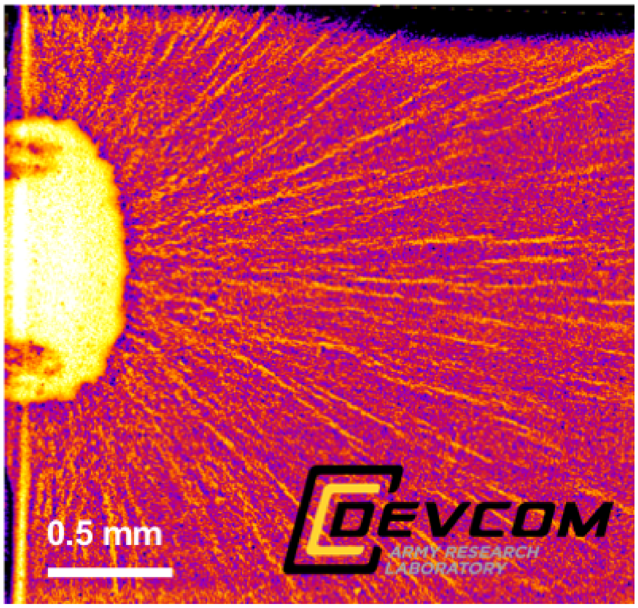

Figure 6: Radiographic imaging aids in probing irreproducible stochastic response of materials as shown here. (Image courtesy of B. Schuster).

- Containment systems for hazardous materials are a challenge, especially for dynamic experiments that can disperse or aerosolize the materials.

Opportunities

- Light source upgrades (e.g. multi-bend achromat storage rings at synchrotrons) and exotic accelerator operating modes (e.g. customized temporal pulse trains or multiple output photon energies) are improving beam parameters for dynamic materials experiments. Tools for automatic beam conditioning are becoming available, which can assist experimenters in optimizing the beam for their measurements.

- Thorough pre-characterization of specimens can be used to analyze and interpret dynamic experiments where the materials cannot be fully characterized.

- Multiple beams are needed for 3-D imaging under dynamic loading. Some multiple beam techniques are already available or could become available in the near future.

- Detector technology advancements will enable experiments to be performed on higher rate dynamics.

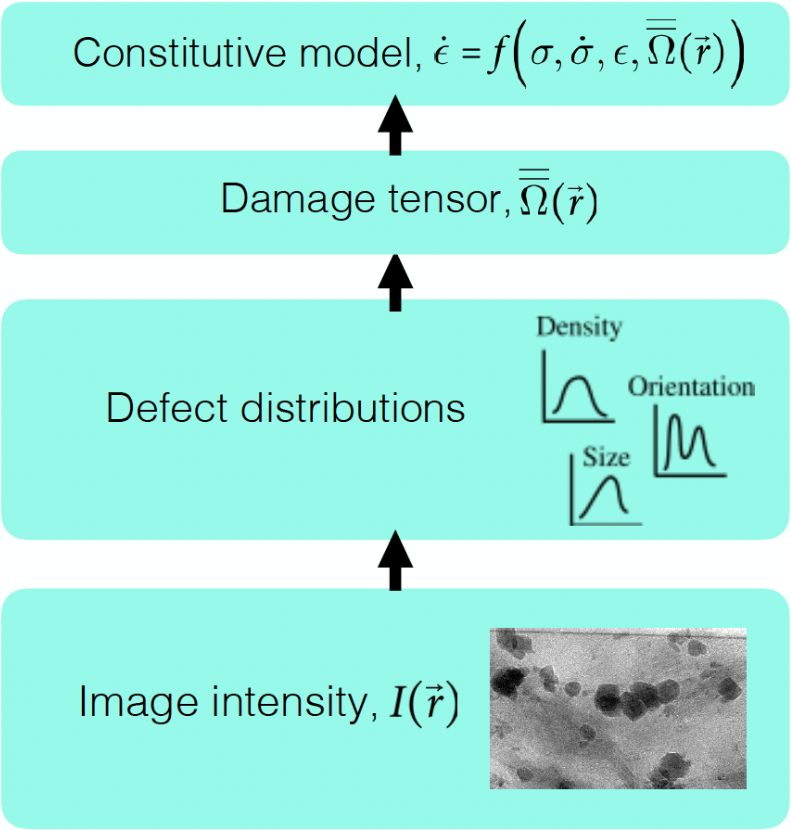

Figure 7: Imaging and diffraction experiments can provide crucial data for microstructure informed model development. (Image courtesy of T. Hufnagel).

- Forward modeling with coupled simulations of the materials and the diagnostics can guide optimal experimental design.
- Experiments can be designed to selective probe specific information, such as dislocation density near grain boundaries.
- Availability of state-of-the-art multiscale modeling capabilities will allow comparison between data and physical models - a necessity for improved understanding of different phenomena and predictive capability [9, 16, 20, 23, 22, 48]

Highest priority investment areas

The experimental techniques and sample environments working group, in consultation with the full group of workshop attendees, recommends that the highest priority investments for experimental challenges include:

1. Using slower 3-D X-ray techniques for pre-characterization of samples for dynamic loading. *In situ* information gathered from the 3-D techniques (BCDI, HEDM, ptychography) used under static/quasi-static loading and X-ray techniques (XRD, SAXS, PCI) used under dynamic loading will be combined to construct an as complete a picture as possible.

2. Determining the best possible sample environment and/or experimental configuration to get the best out of fielded experiments using the available capabilities and resources. This goal would be enabled by further development of computational capabilities that could simulate the experiment and the diagnostics.

3. Using or developing multiple beam techniques that can provide 3-D characterization of materials during dynamic conditions.

4. Communicating detector needs to researchers working on detector development, and forging relationships with data scientists to guide future experimental designs.

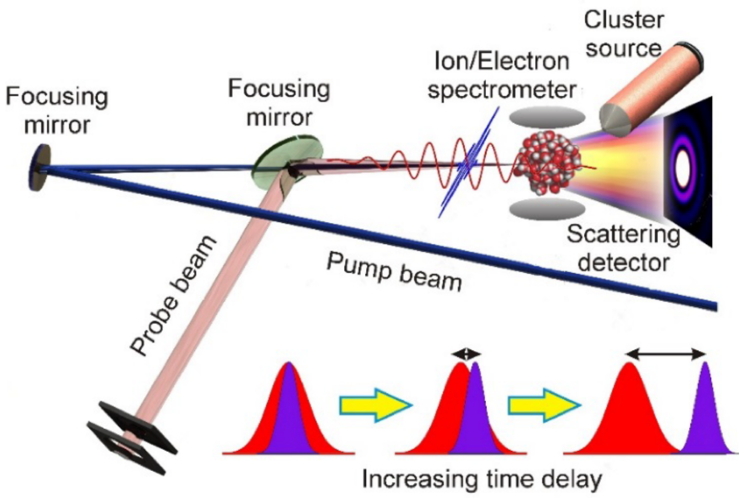

Figure 8: Envisioning dynamic multimodal imaging experiments at 3^{rd} and 4^{th} generation light sources. (Image courtesy of N. Parab).

Detectors and beams

Introduction

Advances in modern accelerator and detector technologies (in conjunction with access to dynamic drivers for *in situ* measurements) continue to open up new opportunities for dynamic materials science experiments [49]. There is great interest in the community to direct these advances towards access to beam parameters and detector capabilities that enable single pulse 3D imaging. Relevant beam requirements explored included use of multiple simultaneous beams, increasing the charge per-pulse, enabling flexibility in pulse structure, and increasing the available energy range. In addition, matching detector properties to beamline capabilities is critical for improving the efficiency of beamline science. Developing new scintillators or direct detection materials that are tailored for the specific energy, pulse conditions, and sample environment can enhance the detection limit and resolution of these techniques. Coupling scintillator materials with detectors that have increased frame rate, sensitivity, and data output and processing at meaningful rates is critical for both high speed experiments as well as sample throughput. With the required increases in the speed of data collection for these advances, mechanisms to efficiently process, transport and analyze this data will also need to be developed. Solutions may range from on-board data reduction and/or processing to simplify storage to running advanced machine learning algorithms and inclusion of meta-data directly into the imaging to address the challenge of connecting experimental data to relevant scientific questions.

Current state-of-the-art

- There are a multitude of detectors, using both direct and indirect detection schemes.
- Indirect direction allows for tailoring a scintillator for use with fast optical cameras. A large variety of scintillator materials are available that are sensitive to various X-ray energies; these can have dramatically different efficiencies and decay rates. An example of this type of detection is the DCS multiplexed fast camera, which essentially has detector-gated acquisition of consecutive scintillator frames on different cameras. This is

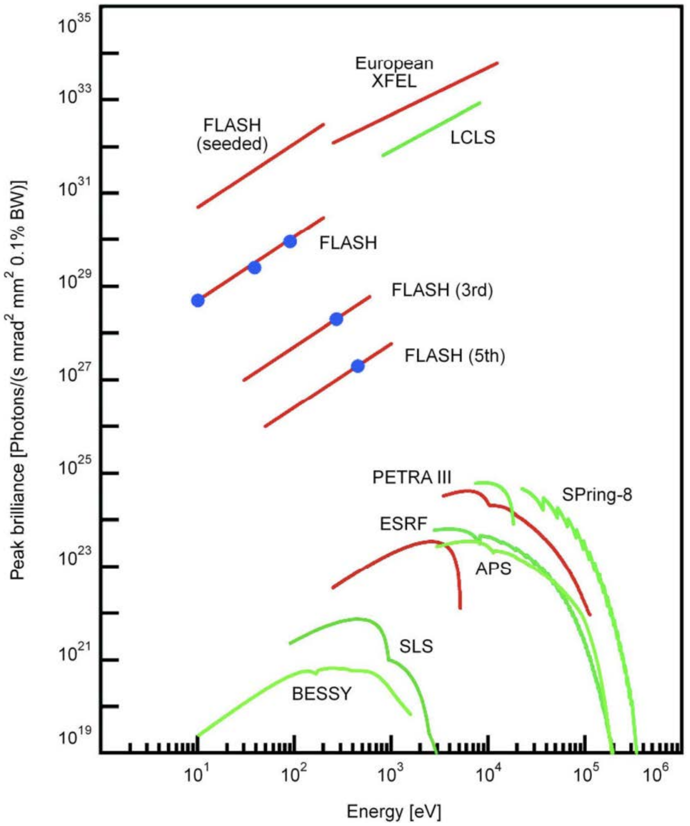

Figure 9: X-ray free electron lasers (XFEL) are sources of extremely intense X-ray pulses. A factor of 10^9 increase in peak brialliance was achieved by the XFEL in comparison to 3^{rd} generation synchrotron sources (Image courtesy of Heinz Graafsma).

the premier detector available at the APS DCS facility, however the current scintillators used are light inefficient and exhibit "ghosting" effects. Development is required for increased framerate, reduced decay time and improved sensitivity.

- Solid state direct detection is most commonly performed via silicon, however germanium, CdZnTe, and CdTe have also been exploited for efficiency at high energies; the optimal detector for a given application depends on required active area, speed and photon energy (Examples: Eiger, CSPAD, ePIX, AGIPD). Direct transmission with diffraction imaging can be combined to reveal stress and strain in single-crystalline materials [50].

- Orthogonal data collection from dual beam instruments exist at LCLS and DARHT, but generally single beam facilities are used. Dual beam would allow for the probing of various processes simultaneously, or for possible 3-D experiments at much higher frame rates.
- Current XFELs operate at a few keV; there are XFELs that are planning to provide x-rays up to 25 keV. In order to examine the material properties of high-Z materials (including the actinides), much higher energies will be required.
- Upgrades are planned at a variety of synchrotron facilities that will increase x-ray brightness and coherence. A current high-energy high-flux synchrotron beamline is sector 1 at APS, which provides 9 x 10^{11} photons per second at 10 keV (the flux drops with increased energy).
- Available pulse structures (widths and spacing) are generally pre-defined by the design of the facility and include either a single or a few options (with the exception of CHESS, which advertises flexibility in pulse structure, and pRad, which can customize pulse structure).

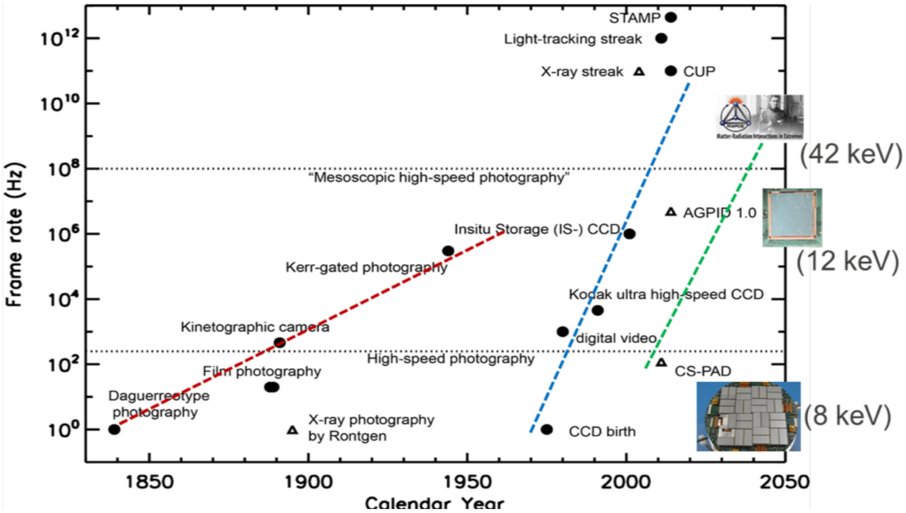

Figure 10: Evolution of high-speed imaging technologies. (Image courtesy of Zhehui Wang)

Challenges

- Matching the number of photons (or protons) per pulse (with broadband available for some techniques) to the experimental needs (lifetime of the experiment), and frame-rate of the detector (in some cases also the scintillator speed) must all be considered.

- Many experiments are photon/proton starved (and/or the detectors are not sensitive enough) and pulse durations and spacings are most commonly not adjustable to experimental needs. Flexibility in pulse structure, duration (ps to ms), and intensity need to be tailorable to the experimental needs.
- High brightness, high energy, high repetition rate, short pulse length sources are needed.
- Increased field of view is desirable for some imaging techniques.
- There are limitations on gradients that can be sustained in current materials for accelerators; improvements in gradient can result in more compact and less expensive accelerators.
- Frame rates for currently available detectors at best enable a few images to be recorded during a dynamic event.
- Detector active areas and pixel sizes often require tiling of multiple detectors to obtain required data.
- Detection is needed over dramatically different timescales (sub-ns to ms).
- Dead areas on detectors cause loss of data for rare events, especially during *in situ* dynamic measurements.
- Scintillator challenges include: afterglow and bloom, which reduce speed and resolution, as well as susceptibility to damage.
- Fast scintillators (rapid response with little "afterglow") tend to emit at shorter wavelengths (below 400 nm) with reduced light yield. This presents a challenge for indirect detectors due to limited efficiency of available sensors and visible light optics in this range. Funding for detector development is typically not long-term enough to complete the work adequately.
- There is little to no communication between the experimenters, beamline scientists, and scintillator/detector scientists so that development needs can be optimized.
- Experimental set-up and detector calibration can be a challenge, especially when using multiple or tiled detectors.
- Depending upon the complexity and utility of the experiment, access to facilities can be a challenge. Some types of experiments (e.g. HEDM) are only practiced at a few locations but have a large number of users.
- Many beamlines reside outside of the United States, and those that are in the United States have historically shown little willingness to handle high hazard samples and/or classified experiments. The overall throughput of 'easier' samples means that these high effort experiments may take years to complete.

- ‘Simple experiments’ may collect 10’s of terabytes in a single trip. Often the data storage is not overly difficult, but data handling (analysis, reduction prior to storage, streaming) can be very difficult. A few-second experiment may take months to determine if it worked.

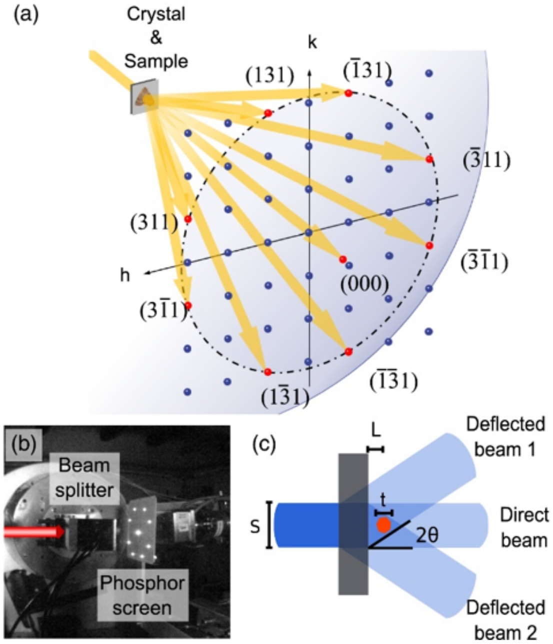

Figure 11: A crystal beamsplitter is used upstream of the sample to generate multiple simultaneous projections [51].

Opportunities

- Advanced detector technologies (microelectronics [52], development of CMOS image sensors, interconnect technologies, heterogeneous integration, new semiconductor and scintillator materials [53], wide-band fast data-link) are being pursued in many separate efforts. A concerted and sustained effort toward a specific goal could produce an experiment-ready detector technology.

- There is an opportunity for the community to come together to define priorities and relay detector specifications to developers.

- A joint approach from the community could target development of a sensor which can digest the short wavelengths emitted by fast scintillators. Sensor development for a single facility is often too costly, however an approach involving many institutions could provide a solution.

- Improvements in and incorporation of alternative (to Si) semiconductor materials (Ge, CdTe, CZT, CZTS [54], GaAs, diamond) can enable fast direct detection of high energy photons.

- Adaptive gain switching can increase detector dynamic range, but requires implementation to enable smooth integration for data analysis [55].

- On-board processing, advanced modeling and machine learning techniques can be used to reduce the processing workload and data storage needs for next-generation detectors.

- Machine learning can be employed for a variety of relevant applications, including, but not limited to, improvement of scintillator material development, accelerator tuning, detector calibration, and data processing and analysis.

- Expanding facility capabilities to enable the use of multiple simultaneous beams can enable single-pulse 3-D imaging; this can include expansion to dual axis, split beams [51, 56], (may require more charge per pulse), or development of compact accelerators.

- Materials development for RF cavities (including control of microstructure of currently used materials) can result in improved accelerator performance and/or more compact and less expensive accelerators.

- Access to experimental facilities can be improved through facility upgrades, administrative mechanisms, increased staffing, and increased experimental throughput (e.g. pRad could expand into additional areas or offer multiple experimental platforms for rapid exchange to enable higher user throughput).

Highest priority investment areas

The highest priorities identified by the community in need of significant investment were development of advanced detector technologies, and a mechanism for relaying the requirements for these next-generation technologies to the developers. Specifically, a sustained long-term effort will be required, with a set of clearly defined key parameters, to effectively develop and implement a transformative instrument or set of instruments. Opportunities were identified in detector materials research, sensor and electronics architecture, and on-board data handling to improve sensitivity, dynamic range, frame rate, and data output. Although access to multi-beam imaging is critical for moving to single pulse 3-D imaging, detection capability to take advantage of this will need to be addressed.

Data analytics and advanced algorithms

Introduction

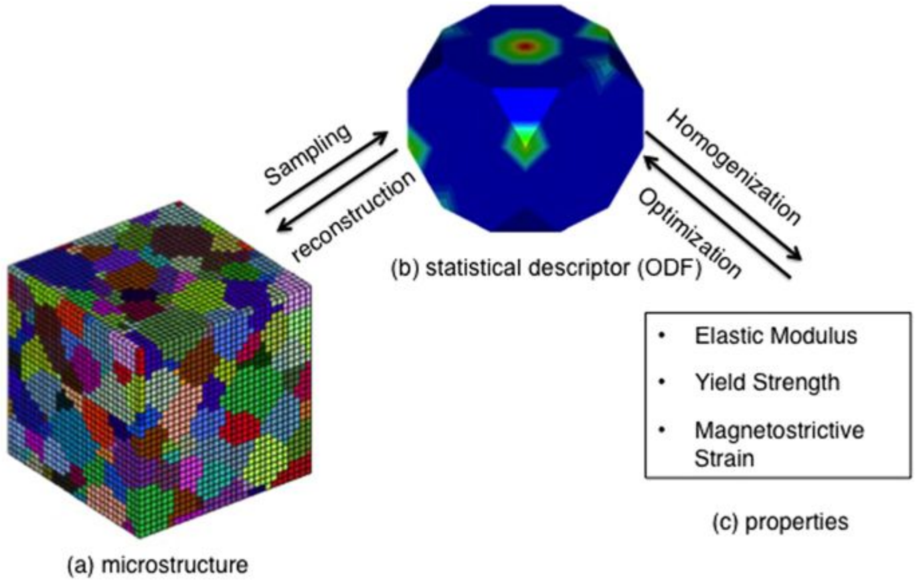

Figure 12: Machine learning for sampling vast material space for optimal property prediction [57]

Materials informatics and data science are powerful tools that can have significant impact towards accelerated materials discovery and design [58]. As we move towards faster data acquisition, real-time data analysis becomes crucial for providing feedback to researchers and guide beamline experiments. Currently such real-time feedback is not possible, especially for detailed 3D imaging, where researchers typically spend hours collecting individual sample state data and then weeks or months utilizing high performance computing resources to perform the reconstructions. One of the most promising applications of advanced machine learning and adaptive feedback algorithms is enabling faster microstructure reconstructions, based on sparse but high-dimensional imaging and diffraction data.

Another major challenge associated with modern dynamic imaging and diffraction experiments is the distillation of raw data (images) from multiple modalities down to material understanding. A path forward for overcoming this challenge is the development and use of novel data analytics tools, tailored for materials science applications. Beyond data analysis, dissemination of the data to the broader material and computer science communities requires that agreed upon standards be developed to allow the data to be searchable and easily interpreted by researchers who did not necessarily collect the data. Data collected using multiple modalities and facilities has challenges and is multifaceted that can be as broad as the inclusion of onboard data reduction that can simplify storage, to simply getting beamline scientists to use common formats. These challenges also provide opportunities for dynamic imaging and diffraction researchers to come together and build teams to address pressing data challenges. Running advanced algorithms such as machine learning, data compression, and including meta-data directly into the imaging can all simplify the challenge of connecting the experimental data to answer the real world scientific questions.

Current state-of-the-art

- Incorporation of deep neural networks [59, 60] and adaptive feedback [61] in data reconstruction algorithms to reduce computation time and increase reconstruction accuracy.

- Data processing and analysis infrastructures that utilize distributed computing available to the wider materials community which reduce the computational burden on individual research groups [62].

- Flexible experimental data (image) processing routes (‘Plug and Play’) that allow researchers to take advantage of the wide array of tools that have been developed by the computer science community for model based data reconstructions [63, 64].

- Application of statistical, unsupervised learning, and data-driven techniques for building structure-property relationships of materials in order to accelerate the material design process [65, 66].

Challenges

- The materials community lacks tools that can be used to analyze large microstructural data sets (particularly *in situ*) to automate the process of finding low frequency failure nucleation events.

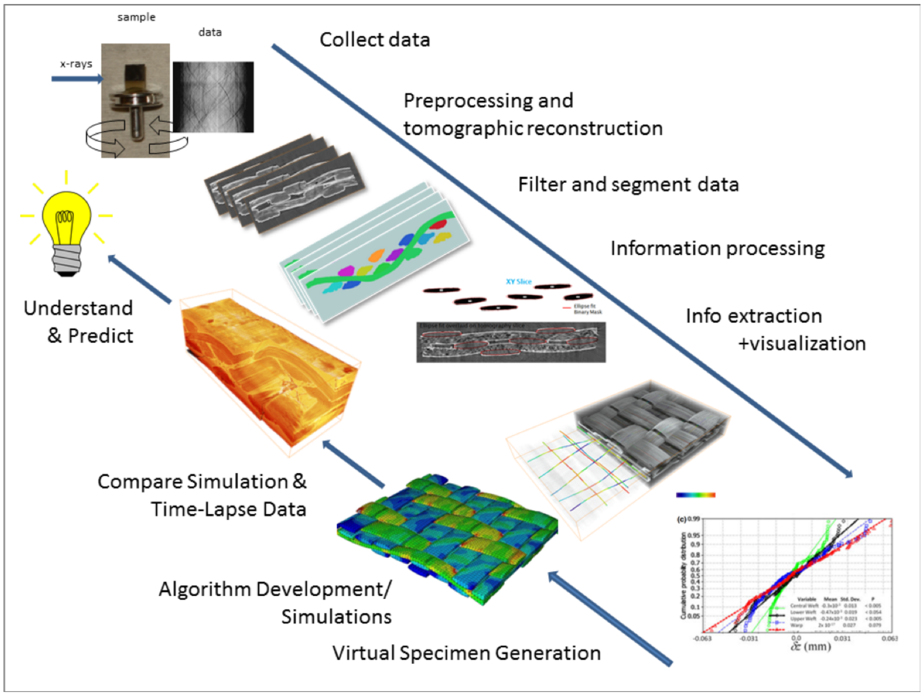

Figure 13: Roadmap for integrated approach with strong connections between experiments, data-science, modeling for intelligent material design with tailored properties (Image courtesy of H. Krishnan).

- There is currently no community wide standard for tagging data sets and associating metadata with them so that the data can be readily used by future researchers.
- Raw data volumes being collected are rapidly becoming so large that they will not be able to be permanently stored and new methods will be required to rapidly reduce the dimensionality of the data and only save data of interest.
- The metrics for which different reconstruction and forward modeling algorithms are judged generally revolve around rate of convergence. Uncertainty metrics need to be developed from which reconstruction fidelity can be judged.
- Metrics for comparison between algorithms are not determined.
- Signal processing methods used to 'clean' and analyze data are generally physics agnostic. The development novel, physics-aware algorithms [60, 67, 68], for signal detection and processing is currently a work in progress, particularly those poised to exploit enhanced beam coherence at upcoming

fourth-generation light sources. Such computational efforts will require continued innovation and development, to allow dimensionality reduction on larger and more complicated data sets without fear of losing critical microstructural or micromechanical information.

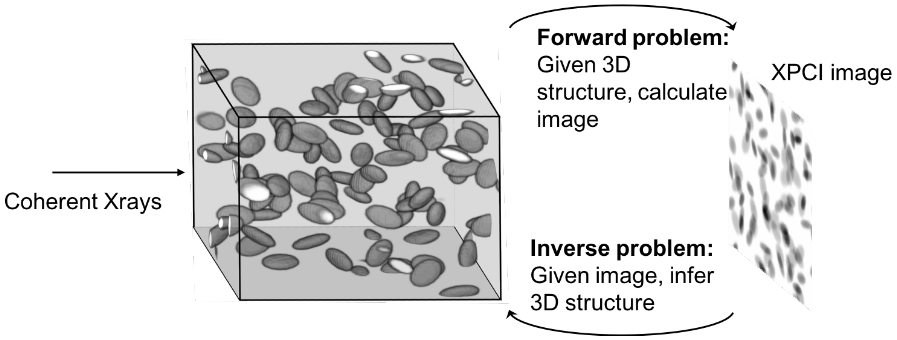

Figure 14: 3D microstructure reconstruction from 2D projections is an extremely ill-posed inverse problem [69]. For high-fidelity 3D reconstructions, multiple angle projections are required by rotating the sample, which is not feasible during dynamic measurements. Combination of multi-beams and/or full initial state characterization might be required to extract 3D dynamic information from experiments.

Opportunities

- Building multimodal X-ray characterization capabilities that can be used to inform one another to accelerate the data collection process [25].

- Automatic Differentiation (AD) is a powerful method for evaluating derivatives relative to complex systems which is much faster and more accurate than standard finite-difference-based approximations [70]. AD presents a great opportunity for material science dynamics and imaging reconstruction problems if their simulations were written in available AD languages such as tensorflow. The resulting AD models would allow for extremely fast optimization and iterative reconstruction studies by automatically providing partial derivatives relative to all variable of interest. This idea can also be used for general data-based neural network training which can provide differentiable models of complex input-output maps (such as recorded diffraction images being mapped to 3D crystal structures and their electron densities. A simple example of an AD setup is shown in Figure [70].

- Further, exploit powerful computational techniques like AD not only to simulate and develop characterization experiments of increasing complex-

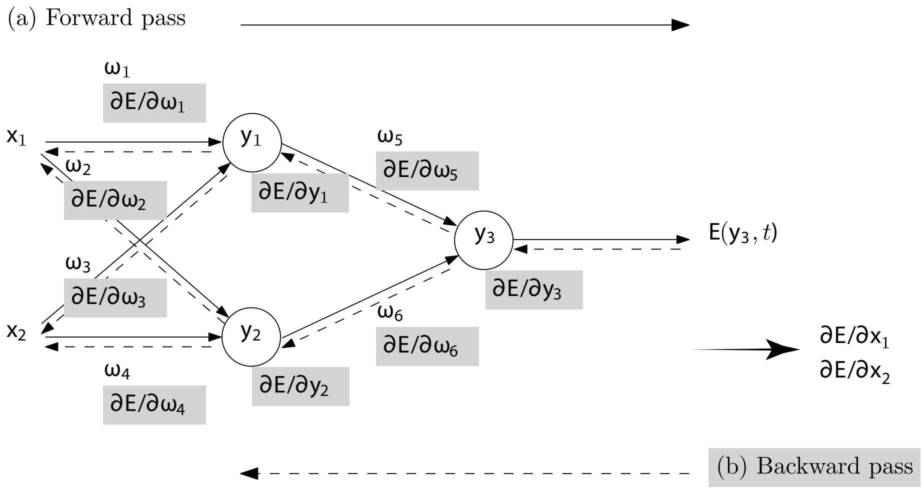

Figure 15: In a neural network (NN) setup taking advantage of AD, training inputs, x_i, are fed forward, generating activations y_i and a prediction of some function, $E(x_1, x_2)$. As the NN is trained to correctly predict $E(x_1, x_2)$ based on data, weights, ω_i, and other parameters of the NN are adjusted and partial derivatives of them with respect to E are learned, from which the partial derivatives relative to the parameters, $\partial E/\partial x_1$ and $\partial E/\partial x_2$ are also learned (This figure is a slightly modified version of Figure 1 in [70]).

ity [71] but also to address the complex error and uncertainty models that follow from such simulations.

- Development of testing standards that can be used to compare reconstruction algorithms to 'ground-truth' in order to evaluate measurement uncertainties.
- Continued development of data processing infrastructure and improving ease-of-use (particularly deploying containerized software) in order to accelerate time to discover [57, 72, 73, 74, 75].
- Building specialized data processing teams at light-sources to produce tools tailored to materials specific applications.
- Creating on-the-fly data processing capabilities to reduce the amount of raw data stored.
- Collecting support from funding agencies to build community wide teams to address data challenges.
- *Developing algorithms directly tailored to materials challenges, particularly tools for identifying low frequency events / features that ultimately dictate material response.

- *Adopting standard data archiving procedures across light sources capable of recording material, experimental, and processing provenance

Highest priority investment areas

The data analytics and advanced algorithms working group, in consultation with the full group of workshop attendees, has determined that the highest priority investments for data challenges include:

1. Funding the development of data analysis algorithms directly tailored to solving pressing materials challenges, including finding 'weakest-link' events and features which dictate mechanical properties.
2. Develop easy-to-use software that can be readily deployed across facilities to tag and add provenance information to data collected using multiple modalities.
3. Perform studies to quantify uncertainties in data reconstruction (inversion) algorithms.

Appendix A

List of acronyms

AM	additive manufacturing
ANL	Argonne National Laboratory
APS	Advanced Photon Source (synchrotron at ANL)
ARL	Army Research Laboratory
BCDI	Bragg coherent diffraction imaging
BNL	Brookhaven National Laboratory
CCD	charge-coupled device
CDI	coherent diffraction imaging
CHESS	Cornell High Energy Synchrotron Source
CMOS	Complementary metal-oxide-semiconductor
CRL	compound refractive lenses
CSpad	Cornell-SLAC Pixel Array Detector
CXDI	coherent X-ray diffractive imaging
CZT	Cadmium zinc telluride
DARHT	Dual-Axis Radiographic Hydrodynamic Test Facility at LANL
DCS	Dynamic Compression Sector (at APS)
DESY	Deutsches Elektronen-Synchrotron (Hamburg, Germany)
DFTB	density functional tight binding
DLS	Diamond Light Source (Didcot, UK)
DOE	Department of Energy
EOS	equation of state
ESRF	European Synchrotron Radiation Facility (Grenoble, France)
EXFEL	European X-ray FEL (Schenefeld, Germany)
EXAFS	extended X-ray absorption fine structure
FEL	free electron laser

FERMI	FEL Radiation for Multidisciplinary Investigations (Trieste, Italy)
FOV	field of view
HEDM	High-energy X-ray diffraction microscopy
LANL	Los Alamos National Laboratory
LCLS	Linac Coherent Light Source (XFEL at SLAC)
LLNL	Lawrence Livermore National Laboratory
MEC	Matter in Extreme Condition end station (at LCLS)
NNSA	National Nuclear Security Administration
NSLS	National Synchrotron Light Source (at BNL)
PAL-XFEL	Pohang Accelerator Laboratory XFEL (Pohang, Korea)
PCI	phase contrast imaging
pRad	proton radiography
RF	radio frequency
SACLA	XFEL in Hyogo, Japan
SANS	small angle neutron scattering
SASE	self amplified spontaneous emission
SAXS	small angle X-ray scattering
SBI	scatter beam imaging
SHPB	split Hopkinson pressure bar
SLAC	Stanford Linear Accelerator Center
SPring-8	Super Photon ring-8 GeV in Hyogo, Japan
USAXS	ultra small angle X-ray scattering
WAXS	wide-angle X-ray scattering
XAS	X-ray absorption spectroscopy
XFEL	X-ray free electron laser
XRD	X-ray diffraction

Appendix B

Workshop Participants

1. Samrachana Adhikari (New York University School of Medicine)
2. Ankit Agrawal (Northwestern University)
3. Jonathan Almer (Argonne National Laboratory)
4. Daniel Banco (Tufts University)
5. Joel Bernier (Lawrence Livermore National Laboratory)
6. Jen Bohon (Los Alamos National Laboratory)
7. Charles Bouman (Purdue University)
8. Don Brown (Los Alamos National Laboratory)
9. Nicolas Burdet (Los Alamos National Laboratory)
10. Gabriella Carini (Brookhaven National Laboratory)
11. Adra Carr (Los Alamos National Laboratory)
12. Jie Chen (Los Alamos National Laboratory)
13. Wayne Chen (Purdue University)
14. Mathew Cherukara (Argonne National Laboratory)
15. Cindy Bolme (Los Alamos National Laboratory)
16. Dana Dattelbaum (Los Alamos National Laboratory)
17. Saryu Fensin (Los Alamos National Laboratory)
18. Diana Gamzina (SLAC National Accelerator Laboratory)
19. Arianna Gleason (SLAC National Accelerator Laboratory/Stanford)
20. Heinz Graafsma (Deutsches Elektronen-Synchrotron (DESY))
21. George (Rusty) Gray (Los Alamos National Laboratory)
22. Ross Harder (Argonne National Laboratory)
23. Felix Hofmann (University of Oxford)
24. Todd Hufnagel (Johns Hopkins University)
25. David Jones (Los Alamos National Laboratory)

26. Harinarayan Krishnan (Lawrence Berkeley National Lab)
27. Ricardo Lebensohn (Los Alamos National Laboratory)
28. Richard LeSar (Iowa State University)
29. Anna Llobet Megias (Los Alamos National Laboratory)
30. Alexander Long (Los Alamos National Laboratory)
31. Darby J Luscher (Los Alamos National Laboratory)
32. Siddharth Maddali Vivekanand (Argonne National Laboratory)
33. Anirban Mandal (Los Alamos National Laboratory)
34. Kevin Mertes (Los Alamos National Laboratory)
35. Eric Miller (Tufts University)
36. Ben Morrow (Los Alamos National Laboratory)
37. Will Neal (Los Alamos National Laboratory)
38. Jeffrey Nguyen (Los Alamos National Laboratory)
39. Darren Pagan (Cornell University)
40. Anup Pandey (Los Alamos National Laboratory)
41. Niranjan Parab (Argonne National Laboratory)
42. Anastasios Pateras (Los Alamos National Laboratory)
43. Brian Patterson (Los Alamos National Laboratory)
44. Reeju Pokharel (Los Alamos National Laboratory)
45. Alexander Rack (European Synchrotron Radiation Facility)
46. Anthony Rollett (Carnegie Mellon University)
47. Richard Sandberg (Brigham Young University)
48. Alexander Scheinker (Los Alamos National Laboratory)
49. Brian Schuster (US Army Research Laboratory)
50. Yancey Sechrest (Los Alamos National Laboratory)
51. Saransh Singh (Lawrence Livermore National Laboratory)
52. Robert Suter (Carnegie Mellon University)
53. Christine Sweeney (Los Alamos National Laboratory)
54. Anjana Talapatra (Los Alamos National Laboratory)
55. Garth Williams (Brookhaven National Laboratory)

Full Program

MONDAY (08/26/2019)

6:00 PM - 8:00 PM Welcome Reception/Registration

TUESDAY (08/27/2019)

7:30 - 8:30 AM Breakfast/Registration

8:30 - 8:40 AM Welcome/Logistics
Reeju Pokharel, Los Alamos National Laboratory

8:40 AM - 9:10 AM
Mesoscale materials science
Dana Dattelbaum, Los Alamos National Laboratory

9:10 AM - 10:00 AM
Tracking Microstructures with High-Energy X-rays
Jonathan Almer[1] , Peter Kenesei[1], Jun-Sang-Park[1], Hemant Sharma[1], Meimei Li[2], Robert Suter[3], and Paul Shade[4]
1) X-ray Science Division, Argonne National Lab, Lemont, IL, USA
2) Nuclear Science Division, Argonne National Lab, Lemont, IL, USA
3) Carnegie Mellon University, Pittsburg, PA, USA
4) Air Force Research Laboratory, Wright-Patterson AFB, Dayton, OH, USA

High-energy x-rays from 3rd generation synchrotron sources, including the Advanced Photon Source (APS), possess a unique combination of high penetration power and spatial, reciprocal space, and temporal resolution. These characteristics, coupled with extensive worldwide efforts over the past two decades, have produced a variety of 3D imaging techniques using both density and diffraction/scattering contrast. I will describe our efforts to combine several of these techniques to study material microstructure through (i) absorption-based tomography, (ii) high-energy diffraction microscopy (HEDM or 3DXRD) and (iii) scattering tomography. The latter two approaches are complementary, as HEDM provides diffraction information (strain, orientation, shape and size) of individual grains in polycrystalline aggregates while scattering tomography yields spatially resolved but grain-averaged information, particularly relevant for fine-grained materials below HEDM limits as well as non-crystalline/amorphous materials. These techniques operate in air with large working distances between optics, samples and detectors. This has enabled development and use of a variety of *in situ* equipment, with an overarching goal to best emulate the service conditions of a given material. I will describe particular equipment including thermomechanical loading systems and additive manufacturing platforms. Limitations as well as planned developments of these techniques will be discussed, both prior to and after the upcoming APS upgrade to a diffraction-limited source.

10:00 AM - 10:20 AM Coffee Break

10:20 AM - 11:10 AM

Current capabilities and limitations in high-speed imaging for studying dynamic mesoscale materials response using high-energy X-rays

Wayne Chen, Purdue University, West Lafayette, IN, USA

For many composite materials under impact loading, the meso-scale deformation, damage, and failure processes are critical factors affecting the impact responses of the materials. To physically understand these transient processes, it is desired to track the damage initiation and evolution in real time during the dynamic deformation of the specimens at this scale. To achieve this goal, we have integrated the high-speed X-ray imaging capabilities present at the Advanced Photon Source beamline 32 ID-B (Argonne National Laboratory) with the high-rate loading offered by the Kolsky compression/tension bars and light gas guns. High-speed X-ray images and X-ray diffraction can be obtained simultaneously. In addition, we explored experimental techniques to capture instant 3-D damage state inside the specimen under impact loading using flash X-ray. These new experimental capabilities were applied to study the impact damage of a variety of materials including geomaterials, energetic materials, fiber-reinforced polymer composites, turbine engine blades with thermal barrier coatings, additively manufactured metals, and biological tissues. To record the initial microstructure and defect distribution, the specimens were characterized with X-ray computed tomography before impact experiments. This presentation illustrates the capabilities that allow real-time visualization of the time sequence of damaging processes in various materials. Limitations in each type of methods are also outlined.

11:10 AM - 12:00 PM

Materials Image Informatics Using Deep Learning: Challenges and Opportunities

Ankit Agrawal, Department of Electrical and Computer Engineering, McCormick

School of Engineering and Applied Science, Northwestern University, 2145 Sheridan Road, Evanston IL USA; ankitag@eecs.northwestern.edu

In this age of “big data”, large-scale experimental and simulation data are increasingly becoming available in all fields of science, and materials science is no exception. Our ability to collect and store this data has greatly surpassed our capability to analyze it, underscoring the emergence of the fourth paradigm of science, which is data-driven discovery. The need to use of advanced data science approaches in materials science is also recognized by the Materials Genome Initiative (MGI), further promoting the emerging field of materials informatics. Of the many types of available data in materials science, image data is quite common and heterogeneous in itself, thanks to the advances in various materials imaging technologies. Within the arena of data analytics techniques, deep learning has led to groundbreaking advances in numerous fields in recent years, such as computer vision, and has become the method of choice for analyzing large amounts of image data, motivating its application in materials science as well. In this talk, I would present some of the recent works from our group employing state-of-the-art data analytics techniques on materials images and microstructure datasets. In particular, we would look at a deep learning solution for indexing electron backscatter diffraction (EBSD) images using 2-D convolutional neural networks (CNNs), and another deep learning based methodology for understanding multiscale localization/homogenization relationships in high-contrast two-phase composites using 2-D/3-D CNNs. Together, the rapid advances in both materials imaging as well as data analytics techniques provide unprecedented opportunities for such materials image informatics to enable better and faster microstructure characterization, reconstruction, and design.

Keywords
Materials informatics, big data, deep learning, structure characterization, electron backscatter diffraction, multiscale localization and homogenization

Funding
NIST Awards 70NANB19H005, 70NANB14H012; AFOSR Award No. FA9550-12-1-0458, DARPA Award No. N66001-15-C-4036, Northwestern Data Science Initiative.

Reference

Ankit Agrawal and Alok Choudhary, “Deep materials informatics: Applications of deep learning in materials science,” MRS Communications, pp. 1-14, 2019. https://doi.org/10.1557/mrc.2019.73

12:00 PM - 12:30 PM

Building a Science Based Understanding of the Process / Structure / Property / Performance of Materials Fabricated with Advanced Manufacturing Techniques

Donald W. Brown[1], J. Carpenter[1], B. Clausen[1], J. Cooley[1], P. Kenesei[2], J-S Park[2],
(1) Los Alamos National Laboratory, (2) Argonne National Laboratory

The last decade has seen tremendous advances in the ability of X-rays and neutrons at large scale facilities to probe microstructure at unprecedented length and time scales under unique environments that simulate manufacturing conditions. Concurrently, manufacturing is undergoing a revolution as investments are made in advanced manufacturing techniques, such as additive manufacture. It is natural that advanced manufacturing techniques should couple with advanced *in situ* characterization techniques in order to accelerate the process of qualification of products for critical applications. However, there are significant hurdles to turning raw x-ray and/or neutron scattering data into quantitative microstructure information that can be used to develop and/or validate PSPP models. In particular, measurements at relevant data rates often preclude the ability to probe the sample in multiple directions. This makes it difficult or impossible to determine inherently three-dimensional information that is necessary to develop and validate advanced process models. These limitations include the quantitative determination of stress, texture and in some cases phase evolution. We will present data collected during *in situ* manufacturing and heat treating as an exemplar of some of the difficulties.

12:30 PM - 2:00 PM Lunch Break

Breakout Session: 1

2:00 PM - 2:30 PM

Developing a Pathway to Microstructure-Aware Predictive Capability for the Shock / Dynamic Response of Materials

George T. (Rusty) Gray III, Los Alamos National Laboratory, Los Alamos, NM 87545; rusty@lanl.gov

It is sixty years since Cyril Stanley Smith's seminal paper describing the effects of shock loading on the structure / property behavior of metals. While numerous experimental observations have fostered the correlation of post-shock microstructural parameters, such as dislocations, point defects, deformation twins, shock-induced phase products, etc., with particular shock parameters, quantitative predictive capability of the defect generation and damage evolution in materials subjected to dynamic loading has yet to be realized. Broadly based defect generation/storage phenomenology presenting a unified view of the material structure/property aspects of shock-wave deformation for a wide range of crystal structures has proven very difficult. However, changes in design and manufacturing paradigms applied to events dominated by dynamic-loading processes have placed increased emphasis on developing physically-based predictive materials models of shock / dynamic loading effects on materials as well as amazing innovations in *in situ* shock diagnostics. In this talk, a survey of the evolution in the state-of-our-understanding of defect generation and damage evolution is discussed and thoughts on the evolving capabilities to move shock /

dynamic behavior of materials research from observation to design and control, and the role of 3-D imaging techniques, is presented. Examples of how utilizing "real-time", post-mortem, and *in situ* experimental approaches together are needed to facilitate quantification 4D processes during shock-wave loading including dislocation / defect generation, shock-induced phase transitions, and damage evolution and spallation.

2:30 PM - 3:00 PM

Landscape of new light source diagnostics for frontier dynamic compression experiments

Arianna E Gleason-Holbrook, SLAC/Stanford University; ariannag@stanford.edu

Understanding the processes which dictate physical properties in condensed matter, such as strength, elasticity, plasticity, and the kinetics of phase transformation/crystallization, requires studies at the relevant length-scales (e.g., interatomic spacing and grain size) and time-scales (e.g., phonon period). Experiments performed at 3rd and 4th generation lightsources, combined with dynamic compression, with ever-improving spatial- and temporal-fidelity are pushing the frontier of condensed matter, materials science and plasma physics. The Matter in Extreme Conditions end-station at the Linac Coherent Light Source, SLAC combines a laser-driven dynamic compression pump and X-ray free electron laser (XFEL) probe to explore transformation pathways and mechanisms. Looking beyond X-ray absorption radiography to recent advancements in coherent X-ray diffractive imaging (CXDI) platforms, we will discuss several examples using phase contrast imaging (PCI). Ideas for near term XFEL-based singleshot CXDI (e.g., ptychography, Bragg-CDI, holography), including multidimensional platforms for 2D or 3D reconstructions, in concert with gated detector advancements, will be discussed. However, as the technology of accelerators and dynamic drivers move us forward to higher rep rates (e.g., MHz level) we will face new challenges surrounding real-time data analysis, real-time data storage for post-processing, and samples delivery systems.

3:00 PM - 3:30 PM

Discussions

Breakout Session: 2

2:00 PM - 2:30 PM

Unsupervised Learning of Dislocation Motion

Darren C. Pagan[1], Thien Q. Phan[2], Jordan S. Weaver[2], Austin R. Benson[3], Armand J. Beaudoin[1]
1 Cornell High Energy Synchrotron Source (CHESS)
2 Engineering Laboratory, National Institute of Standards and Technology (NIST)
3 Department of Computer Science, Cornell University

Every photon scattered from a sample contains information about its current microstructural state. Traditionally, connecting material microstructure to measured signal has required a physics-based scattering model and a choice to discard some portions of the data. Instead we propose the application of the unsupervised learning technique, locally linear embedding (LLE), to analyze *in situ* diffraction data and find lower-dimensional embeddings that characterize microstructural transients, by-passing the need for a scattering model chosen a priori. We apply the approach to diffraction data gathered during uniaxial deformation of additively manufactured Inconel 625. We then connect the evolution of the lower-dimensional representation of microstructure to the evolution of the defect densities that dictate strength and plastic flow behavior using a well-established material model. The implications of the findings for future constitutive model development and wider applicability to the study of material evolution during *in situ* processing and dynamic loading will be discussed.

2:30 PM - 3:00 PM

Real-time 3D nanoscale imaging enabled by deep learning and automatic differentiation

Mathew Cherukara, Argonne National Laboratory

Coherent X-ray diffraction imaging (CDI) is a powerful technique for operando characterization. Visualizing defects, dynamics, and structural evolution using CDI, however, remains a grand challenge since state-of-the-art iterative reconstruction algorithms for CDI data are time-consuming and computationally expensive, which precludes real-time feedback. Furthermore, the reconstruction algorithms require human inputs to guide their convergence, which is a very subjective process. I will describe our work in the use of deep convolutional networks (CDI NN) in accelerating the analysis of, and potentially increasing the robustness of image recovery from 3D X-ray diffraction data. Once trained, CDI NN is hundreds of times faster than traditional phase retrieval algorithms used for image reconstruction from coherent diffraction data, opening up the prospect of real-time 3D imaging at the nanoscale. Our networks are designed to be 'physics-aware' in multiple aspects; in that the physics of the transform is explicitly enforced in the training of the network, and the training data is drawn from a distribution that is representative of the physics of the material. We further refine the NN's prediction through automatic differentiation of the forward model that enables maximum accuracy at lowest computational cost. While we have used the phase retrieval problem in 3D as an example, our integrated machine learning and automatic differentiation approach is widely across inverse problems.

3:00 PM - 3:30 PM

Discussions

Breakout Session: 3

2:00 PM - 2:30 PM

Best-guess experiment needs to measure irreversible structural dynamics

Garth Williams, Brookhaven National Laboratory

2:30 PM - 3:00 PM

An Overview: Adaptive Co-design of Resilient Radiation Detector Materials

Anjana Talapatra, Blas Uberuaga, Chris Stanek, Ghanshyam Pilania, Los Alamos National Laboratory

Scintillators are detector materials with a wide variety of applications, ranging from medical imaging to radiation detection for global security. These materials convert a fraction of the energy deposited by incident gamma rays or X-rays into visible or ultraviolet photons. An ideal scintillator would exhibit high light output, fast response time, and emission at suitable wavelengths. However, no single scintillator is ideal for all uses; there is a need to design custom scintillators optimized for each application. Currently, the discovery and design of new detector materials relies on a laborious, time-intensive, trial-and-error approach; yielding little physical insight and leaving a vast space of potentially revolutionary materials unexplored. To accelerate the discovery of optimal scintillator materials with targeted properties and performance, efforts are ongoing to develop a closed loop machine learning (ML) driven adaptive design framework based on experiments and Density Functional Theory (DFT) calculations. This talk will present an overview of this framework detailing the close coupling between high throughput experiments, first principles computations and machine learning to efficiently screen a large chemical space of potentially promising scintillator chemistries with a view to identifying promising chemistries for materials with better scintillation properties for theoretical and experimental investigation. The developed framework is general and is expected to yield applications beyond scintillator discovery.

3:00 PM - 3:30 PM

Discussions

3:30 PM - 3:50 PM Coffee/Snacks Break

3:50 PM - 4:20 PM

Dynamic Convolutional Sparse Coding for Quantifying Elastoplastic Deformation in Polycrystalline Materials from High Energy X-ray Diffraction Time Series

Daniel Banco[1], Kelly Nygren[2], Darren Pagan[2], Armand Beaudoin[2], Eric Miller[1], Matthew Miller[2,3]
1 Department of Electrical and Computer Engineering, Tufts University
2 Cornell High Energy Synchrotron Source, Cornell University
3 Sibley School of Mechanical and Aerospace Engineering, Cornell University

High energy monochromatic X-ray diffraction data collected *in situ* during loading experiments permits probing of the crystalline microstructure of a sample during thermo-mechanical loading. An elastoplastic deformation is associated with the development of heterogeneity in both crystal orientation and lattice spacing each manifesting as azimuthal broadening and radial broadening of diffraction peaks respectively. Quantifying the spreading effect is challenging, especially in cases where the sample has a granularity between that of a single crystal and fine grain or powder material. The approach developed in this talk begins by modeling the intensity signal in the vicinity of a Debye-Scherrer ring as a nonnegative superposition of Gaussian basis functions. A convolutional sparse coding (CSC) approach, requiring the solution of a large scale but structured inverse problem, is used to determine a parsimonious collection of basis functions from a large "dictionary" of shifted and scaled Gaussians. The two-dimensional distribution of the azimuthal and radial variance parameters associated with the selected basis functions along with their recovered amplitudes are used to construct a meaningful statistic, the Amplitude Weighted Mean Variance (AWMV), to quantify radial and azimuthal spread.

Of particular interest in this talk are loading experiments where the impact of continuous deformation on a material sample is encoded in a series of diffraction data fames collected at regular intervals. For problems such as these, temporal variations in spot morphology as captured by the AWMV provide insight into the kinetics of crystallographic slip. Recovering the AWMV time series from raw diffraction data could be addressed by solving an independent CSC problem at each point in time. Such an approach results in a noisy AWMV time series as it fails to exploit the physical reality that the material is changing smoothly in time. To alleviate this problem, we develop a temporal regularization scheme to encourage similarity in the choice of basis functions selected by the CSC process (and by extension the AWMV) as a function of time. Specifically, the radial and azimuthal distribution of variances is viewed as an empirical two-dimensional probability density function (PDF). Temporal smoothness is enforced by adding to the sparse coding optimization functional a term penalizing differences in the Wasserstein distance between the PDFs at adjacent points in time. We discuss numerical methods for solving the resulting very large-scale inverse problem in which the individual CSC problems are now coupled. Results are shown for X-ray diffraction time series data captured using the highspeed mixed mode pixel array detector (MM-PAD)1; the time resolution permits observation of bursts

of dislocation movement in a tensile Ti-7Al sample which we quantify using the AWMV.

Broadly considered, modern machine learning and data science methods provide a wide range of options for addressing dynamic imaging problems such as the one of interest here. From recurrent neural networks or temporal convolutional networks to dynamic Gaussian processes and beyond, there is no shortage of models and associated processing schemes that could be brought to bear on the problems which concern this community. The real challenge lies in developing an understanding the potential and the pitfalls of all of these methods and subsequently constructing new, effective techniques based on this knowledge. The balance of this talk will focus on how this might be accomplished.

4:20 PM - 4:50 PM

In situ materials characterization using ultra-high-speed imaging with (partially) coherent hard synchrotron radiation

Alexander Rack and Margie P. Olbinado, European Synchrotron Radiation Facility (ESRF), 38000 Grenoble, France; alexander.rack@esrf.fr

The potential of hard X-ray imaging to tackle scientific questions especially related to materials sciences can be substantially increased when the dimension time is accessible. Nowadays, unprecedented temporal resolution with hard X-ray imaging can be reached at synchrotron light sources thanks to high-speed CMOS cameras combined with indirect detection schemes. Storage rings like European Synchrotron Radiation Facility (ESRF) can be operated in so-called timing-modes with reduced bunch number but increased electron bunch charge density per singlet [1,2]. The polychromatic photon flux density at insertion-device beamlines during timing-modes is sufficient to capture hard X-ray images exploiting the light from a single bunch (the corresponding X-ray flash length is a few 100 ps FWHM). Hence, hard X-ray imaging with absorption contrast as well as phase contrast depicting processes in real time on the picosecond scale is nowadays accessible. Common bunch-rates are in the MHz regime (1.4 MHz and 5.6 MHz in case of ESRF). Additionally, direct transmission with diffraction imaging can be combined, i.e. revealing stress and strain in single-crystalline materials such as wafers [3]. In this presentation, we will describe our strategies to push the limits of time-resolved hard X-ray imaging for materials characterization at ESRF. We will show visualizations of various transient processes such as crack propagation in Si wafers, explosion during electric arc ignition in an industrial fuse, laser-induced micro-cavitations and jetting in water, laser-shock-induced compression in polymeric foam [4, 5, 6].

1. M. P. Olbinado et al., “MHz frame rate hard X-ray phase-contrast imaging using synchrotron radiation,” Optics Expr. 25 (2017) 13857.
2. A. Rack et al, “Exploiting coherence for real-time studies by single-bunch imaging,” J. Synchrotron Rad. 21(4) (2014) 815.
3. A. Rack et al, “Real-time direct and diffraction X-ray imaging of irregular silicon wafer breakage,” IUCrJ 3(2) (2016) 108.

4. M. E. Rutherford et al., "Probing the early stages of shock-induced chondritic meteorite formation at the mesoscale," Scientific Reports, 7 (2017) 45206.
5. M. P. Olbinado et al., "Ultra high-speed X-ray imaging of laser-driven shock compression using synchrotron light," J. Phys. D: Appl. Phys. 51(5) (2018) 055601.
6. D. Yanuka et al., "Multi frame synchrotron radiography of pulsed power driven single wire explosions," J. Appl. Phys. 124(15) (2018) 153301.

4:50 PM - 5:30 PM

Combined discussions / Out-briefs from breakout sessions

WEDNESDAY (08/28/2019)

7:30-8:30 AM Breakfast/Registration

8:30 AM - 9:00 AM

X-ray imaging of crystal defects and nano-scale strain fields

Felix Hofmann, Department of Engineering Science, University of Oxford, Oxford, UK

Lattice defects control the mechanical and physical properties of crystalline materials. In metals, dislocations provide a low energy pathway for plastic deformation. Manipulating their propagation by alloying, introducing second phases or injecting pre-existing defects is at the heat of alloy development for high performance energy generation, transportation and aero-space applications. A very important question concerns the behavior of defects as a function of time-scale. Much work has focused on the observation of defects at quasi-static deformation rates, including TEM and XRD imaging of defects. At high deformation rates such detailed observations are scarce. The reason is that high resolution experiments tend to be very slow. Yet there is a multitude of applications where observations of the high rate characterization of defect behavior is urgently needed. For example, to design materials with optimized high rate properties, detailed insight into the competition between different deformation mechanisms, such as dislocation slip, twinning and transformations is needed. For materials exposed to intense irradiation environments detailed knowledge of the early stages of irradiation-induced defect formation, on sub nano-second time-scales during progression of collision cascades, is still missing. Yet this is key to designing materials with enhanced radiation resistance that are needed for next generation fission and fusion power.

A very important role in controlling defect interactions is played by the strain fields associated with crystal defects. Bragg Coherent X-ray Diffraction imaging (BCDI) is a powerful technique that uniquely makes it possible to probe these strain fields with 3D nano-scale resolution, even for quite complicated defect structures. For example, we have used BCDI to study irradiation-induced defects, as well as extended dislocation structures. To function correctly, BCDI requires crystallographically-isolated samples less than a micron in size. This challenge can be addressed using focused ion beam machining for sample manufacture.

BCDI works very well for the characterization of static defects. However, it is far too slow to probe dynamic behavior at anything less than minute timescales. Some progress has been made using pump-probe BCDI to probe reversible phenomena, such as acoustic phonons. The big challenge is that most defect interactions are not reversible. This means that the whole interaction history must be captured in one go in a single shot experiment. One approach would be to move to a mode of operation where a detailed image of the sample is acquired before loading and then snapshots of several projections are captured for stereo-imaging during deformation. This would allow a dramatic speedup, but will depend on the availability of sufficiently fast detectors and X-ray flux. A much greater conceptual challenge is to design new experimental schemes/approaches that allow the full 3D data from a crystal to be captured within a single shot, without the need for sample movement or multiple exposures. This would really revolutionize the field and could open the door to movies of irreversible processes.

9:00 AM - 9:30 AM

Modernizing the experiment-driven workflow to meet the needs of next generation DOE BES light source facilities

Harinarayan Krishnan, CAMERA, Lawrence Berkeley National Laboratory

Experiment-driven analysis at DOE BES light source facilities often have complex, stringent, and time sensitive requirements on resources, both human and computational, as part of delivering solutions for the scientific research mission. While current post-processing approaches have been adequate to drive experimental science research forward, next generation upgrades such as ALS-U and APS-U in addition to NSLS II and LCLS II will produce data at significantly higher rates (>10x) and at higher volumes (PBs/year) outpacing capabilities light source facilities can sustainably support.

A core mission of The Center for Advanced Mathematics for Energy Research Applications (CAMERA) is to develop and deliver novel algorithms with sound mathematical underpinnings essential for extracting scientific insight from raw data. The combination of technological advances at facilities and increased complexity of algorithmic workflows is estimated to cause the traditional post processing approaches and localized data solutions to be inadequate or fail outright for certain techniques such as Ptychography and XPCS. Additionally, the amount of resources required to address both data storage and computational needs require solutions that are more appropriately run and maintained by supercomputing facilities rather than user facilities.

Thus, a new need emerges for solutions that enable processing data at real-time, running analysis on distributed heterogeneous architectures, and providing feedback and insight to drive future experiments. This presentation will highlight three major efforts: autonomous steering, visual orchestration, and execution of highly parallel remote workflows. Additionally, this talk will also highlight efforts in addressing data lifecycle issues, providing programmable analysis, and refactoring existing algorithms to provide exploratory feedback on data processed at rates expected from detectors within the next decade. Each of these ongoing efforts are developed in close collaboration with partners at the light sources with the eventual goal of producing a standard common software ecosystem aimed at executing distributed end-to-end pipelines optimized for real-time processing and feedback.

9:30 AM - 10:00 AM

X-ray Imager developments in Hamburg

Heinz Graafsma[1,2], 1) CFEL; DESY Hamburg, Germany; 2) University of Mid Sweden, Sundsvall.

The Photon-Science Detector group at DESY is responsible for the development and deployment of new detectors for the photon sources in Hamburg: PETRA III; FLASH and the European XFEL. Due the different nature of the sources and the large span of photon energies different systems were developed. The main challenge was posed by the European X-ray Free-Electron Laser (Eu.XFEL), with its extreme peak intensity and 4.5 MHz repetition rate. From the beginning it was clear that only custom designed systems would be able to meet those challenges. The Adaptive Gain Integrating Detector (AGIPD) system is one of three projects for the Eu.XFEL. In this system each pixel individually and fully automatically adapts its gain to the incoming signal strength during the pulse, and with that provides at the same time low-noise performance for weak signals, allowing distinguishing between single photons, and high dynamic range for strong signals. In addition to the large dynamic range the AGIPD system also provides high speed imaging up to 6.5 MHz. The first system was deliver and installed at the Eu.XFEL, and successfully used for the very first user experiments in fall 2017. A short overview of its performance will be given.

Another challenge is presented by the low-energy FELs like FLASH. In order to be able to reliably detect photons down to 250 eV a system based on back-illuminated CMOS imagers is developed. This system, PERCIVAL, has a different adaptive gain structure providing single photon sensitivity as well as a large dynamic range. The results obtained with the first 2-million pixel monolithic sensors will be presented.

In the next decade the PETRA storage ring will be upgraded to a diffraction limited source, and the European XFEL will be extended with a CW-mode operation. Although the final parameters of the sources are not yet fixed, it is clear that the two sources, from a detector point of view are becoming more similar. We therefore, have started a development program for a high-speed imager. The design goals, and first of ideas of the implementation will be presented and discussed.

10:00 AM - 10:30 AM Coffee Break

10:30 AM - 11:00 AM

A continuum mesoscale perspective of the dynamic response of metals and explosives

DJ Luscher, Los Alamos National Laboratory

The dynamic thermomechanical responses of polycrystalline materials under shock loading are often dominated by the interactions of defects and interfaces. Polymer-bonded explosives can be initiated under weak shock impacts that would be insufficient to drive a reaction if the material response were homogeneous. Within metals, a prescribed deformation associated with a shock wave may be accommodated by crystallographic slip, void nucleation and growth, and fracture; the competition amongst these processes is often influenced by the behavior of grain boundaries. Direct numerical simulation at the mesoscale offers insight into these physical processes that can be invaluable to the development of macroscale constitutive theories. However, this approach requires that the mesoscale models adequately represent the nonlinear thermomechanical response of individual crystals and their interfaces. Here, we highlight a mesoscale modeling approach and then discuss progress towards improving the underlying theory and models for each constituent based on experimental observation.

11:00 AM - 11:30 AM

Imaging Failure and Fracture of Ceramics During Ballistic Impact

Brian E. Schuster, Andrew L. Tonge, Phillip A. Jannotti, Thomas W. Scharf and Nicholas J. Lorenzo, Army Research Laboratory, Aberdeen Proving Ground, MD

Boron carbide is considered in many armor applications because it has a high hardness (>30 GPa) and low density (2.5 g/cc). In practice, wider use of this material has been limited because it is well-known to show a loss of shear strength at pressures exceeding ~20 GPa. Reports in the literature have suggested that this loss of shear strength results from a crystalline to amorphous phase transition at high pressures. Here, the large-scale ballistic response was investigated using the High voltage *in situ* Diagnostic Radiography Apparatus (HIDRA) at ARL. The penetrator-target interactions and activated damage modes were observed using radiography, high speed imaging and velocimetry. The small-scale impact and shock response were investigated using phase contrast imaging (PCI) and X-ray diffraction under shock loading at the Dynamic Compression Sector (DCS, 35-ID-E) at the Advanced Photon Source. At the lowest peak stresses investigated, experiments at both length scales show the penetrator undergoes dwell and the target response is consistent with cone crack formation at the impact site. At higher striking velocities there is a distinct transition to massive fragmentation leading to the onset of penetration. Imaging and diffraction suggest that the loss of shear strength at high pressures can be attributed to brittle fracture above the Hugoniot Elastic Limit (HEL) and not from an amorphous phase transition. We will introduce applications of these experimental techniques to investigate the response of novel monolithic and composite brittle material systems, and for computational model calibration and validation.

11:30 AM - 12:00 PM

Dynamic 4D Reconstruction

Charles A. Bouman, School of ECE/BME, Purdue University

There is an increasing need to reconstruct objects in four or more dimensions corresponding to space, time and other independent parameters. Traditional approaches to space-time reconstruction require that a full set of projections be taken at each time step; however, this is not practical or even possible in many applications. Fortunately, algorithms such as time-interlaced model-based iterative reconstruction (TIMBIR) have demonstrated that it is possible to dramatically reduce the number of required samples while still maintaining high quality space-time reconstructions.

In this talk, we present both the state-of-the-art as well as the likely future directions for reconstruction in 4 and higher dimensions. The key to innovation is the solution of the space-time inverse problem with both an accurate model of an informative sensor, along with an advanced machine learning (ML) model of the object being reconstructed. Over the past decade, Plug-and-Play (PnP) methods have been shown to be an effective way to integrate advanced ML prior models with physical sensor models. More recently, multi-agent consensus equilibrium (MACE) has been proposed as an extension to PnP which allows for the integration of multimodal sensor models along with multi-modal priors. We present examples of how the PnP/MACE framework can be used to solve 4D reconstruction problems in applications such as the imaging of additively manufactured parts, cone-beam imaging of moving objects, and most recently imaging of dynamic grain structure in high-energy diffraction microscopy applications.

12:00 PM - 1:30 PM Lunch Break

Breakout Session: 1

1:30 PM - 2:00 PM

Ultrafast x-ray imaging and complementary techniques at 32-ID beamline of the APS

Niranjan D. Parab, X-ray Science Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne IL 60439; Email: nparab@anl.gov

High-speed synchrotron X-ray imaging can provide vital sub-surface information for opaque materials undergoing dynamic processes such as fracture and laser processing. 32-ID-B of the Advanced Photon Source has pioneered the use of x-ray white beam from an undulator source to do ultrafast inline phase-contrast imaging with exposure time down to 100 ps and repetition rate up to 6.5 MHz. We subsequently added the capability to do simultaneous diffraction, and the recent installation of a specialized undulator (short period, single line @ 24 keV) allowed us to add Small Angle Scattering to the mix of simultaneous techniques, all at an exquisite time resolution. Further, we have integrated several complementary techniques including high-speed thermal imaging and x-ray digital image correlation to record additional information about the processes. In this talk, along with the technical details of the beam line, I will also give an overview of the diverse programs running at the beamline, such as fluid dynamics, materials science, shock physics, and metal additive manufacturing. In the end, I will provide an overview of the future upgrades planned at the beam line and in the APS storage ring and how these upgrades will improve the imaging quality at the beam line.

2:00 PM - 2:30 PM

A new High Throughput-High Energy Diffraction Microscope at the Advanced Photon Source

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1) Carnegie Mellon University, 2) Purdue University, 3) University of Utah, 4) Colorado School of Mines, 5) Advanced Photon Source, Argonne National Laboratory

A second High Energy Diffraction Microscopy (HEDM) instrument is being developed at the 6-ID-D hutch at the Advanced Photon Source (APS) at Argonne National Laboratory. The development is funded by the National Science Foundation's Major Research Instrumentation program supporting a consortium including Carnegie Mellon University, Purdue University, University of Utah, and Colorado School of Mines; the APS is providing all front end beamline components and the hutch to house the instrument. Engineering and technical support and collaboration with Sector 1 staff is also supported by APS. The HT-HEDM instrument will split time with an existing instrument in the 1-ID-D hutch; the hutch has been extended so as to house both instruments with at most minor interactions. We expect to have beam in the hutch during the Fall 2019 run cycle and instrument commissioning should be completed in early 2020. Users will be able to obtain time on the instrument through the APS General User Program.

The "high throughput", or HT-HEDM, instrument will perform near-feld and far-field HEDM and high energy computed tomography (additional methods can be developed). Box beams, line and point focused beams will be available with the latter two being achieved with saw-tooth refractive lens. The 6-ID beamline is fed by a superconducting undulator similar to that at 1-ID where the current HEDM facility is located. Further, the existing horizontal bounce monochromator uses similar bent crystal optics, so comparable fluxes of high energy x-rays are expected. The HT-HEDM instrument will be restricted to "simple" sample environments so that major repositioning of apparatus will be avoided and consequent time devoted to realignment procedures will be minimized. NSF funding includes a furnace for high temperature studies; other sample environments can be developed by the consortium members or other users. A major justification for this project is that it will off-load significant usage demand at the existing 1-ID-E hutch so that measurements that use complex loading or other environments requiring significant rearrangements of hutch instrumentation will have increased time available and therefore reduced waiting times for beam allocation.

This talk will discuss design criteria for this updated instrument with an emphasis on implementing new data collection protocols to accelerate measurements, new GPU-based reconstruction software, and data pipelining. While the HEDM methods are far from being single pulse based, they may be relevant in a number of ways, for example, screening samples for high rate deformation measurements and providing samples with known microstructures for modeling such processes.

2:30 PM - 3:00 PM
Discussions

Breakout Session: 2

1:30 PM - 2:00 PM

COHED: Coherence for High-Energy Diffraction

Stephan O. Hruszkewycz[1], Siddharth Maddali[1], J.- S. Park[2], P. Kenesei[2], S. Shastri[2], H. Sharma[2], J. Almer[2], R. Harder[2], W. Cha[2], M. J. Highland[1], Y. S. G. Nashed[3], S. Kandel[4], P. Li5, M. Allain[5], V. Chamard[5], M. Wilkin[6], A. D. Rollett[6]
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Coherent diffraction imaging (CDI) with X-ray energies greater than 50 keV opens up new opportunities for nano-scale resolution of crystal strain and defects in macroscopic volumes. In this talk I describe computational and experimental advances in this direction, which include signal processing innovations, treatments of partial beam coherence and new generalized forward modeling methods that use automatic differentiation. I will also present proof-of-concept imaging results of nanoparticles with synchrotron X-rays at 52 keV energy, substantially higher than the energies employed in present-day coherent X-ray scattering measurements. These methods are meant to make timely use of the upgraded coherence capabilities of next-generation X-ray sources over the next few years. It is anticipated that this high-resolution strain field imaging capability will be eventually extended to other, hitherto difficult-to-access environments, such as crystals in dense catalytic media or deeply embedded grains in a polycrystalline bulk. The combined computational and experimental capabilities being developed could benefit a vast cross-section of materials research and solid-state physics, like structural and functional materials design, and validation of materials physics models, potentially including pre-characterization for pulsed imaging purposes.

2:00 PM - 2:30 PM

Dynamic 3-d X-ray diffraction microscopy: challenges and opportunities Joel V. Bernier and Saransh Singh, Computational Engineering Division, Lawrence Livermore National Laboratory, Livermore, CA 94550

The evolution of X-ray light sources has recently made "single bunch" materials probes a reality, opening up the possibility to make increasingly detailed observations of material state under dynamic compression. Concurrently, advances in detector technology provide a basis for making 3-D measurements. We will examine some of the fundamental challenges to obtaining spatial maps of intergranular orientation and strain/stress, and discuss several strategies for addressing the projection problem that typically limits resolution to 2-D projections.

2:30 PM - 3:00 PM

Discussions

Breakout Session: 3

1:30 PM - 2:00 PM

Proton Radiography at LANSCE and its uses in Mesoscale phenomena

Dr. Anna Llobet, P-23 Neutron Science and Technology, Los Alamos National Laboratory

In this presentation we will introduce proton radiography capabilities available at LANSCE. We will discuss the different types of experiments that can be performed as well as quantitative measurements of very fast phenomena. Examples of static, quasi-static and dynamic experiment will be presented as well as examples of mesoscale phenomena.

2:00 PM - 2:30 PM

Copper Reconsidered: Characterizing Materials' Interaction with Electromagnetic Waves

Diana Gamzina, Paul Welander, Emilio Nanni, Mike Kozina, Apurva Mehta, Arianna Gleason
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Recent advances in understanding material effects on accelerator systems have led to significant improvement in accelerator performance, but detailed knowledge of the temporal material changes due to its interaction with electromagnetic wave continues to be an unknown and hence material properties limiting accelerator performance cannot be easily identified and mitigated. While surface imaging prior to and post operation clearly show surface degradation, the practical findings provide limited insight into materials' behavior during operation of the accelerator. We evaluate the problem from mechanics of materials perspective laying a foundation for understanding transient material response to electromagnetic interaction. This analysis not only impacts development of advanced accelerators and radio frequency sources, it also informs development of materials resistant to damage caused by electromagnetic radiation and of material synthesis techniques that utilize electromagnetic fields for achieving far-from-equilibrium material states.

Furthermore, development of an RF-pump / x-ray probe (RFX) instrument, first of its kind, at the synchrotron facility at SLAC is underway to image *in situ* temporally evolving thermal strain induced by high power electromagnetic radiation at ~100 GHz frequencies. This instrument will help in validating material models describing its interaction with electromagnetic radiation. The instrument utilizes grazing incidence diffraction to measure change in a material's lattice constant in single-crystal copper samples, both during a single pulse and over the duration of many pulses. We have designed, built, and demonstrated the RFX instrument in the intended operating environment at the synchrotron facility at SLAC and we have collected the first material transformation measurements inside of the RFX instrument chamber. Experimentally validated expansion of our fundamental understanding of materials' interaction with high power electromagnetic wave will guide our invention of new materials with tailored micro- to macro-scale properties and enable low cost and high-performance accelerators required for the future discoveries.

2:30 PM - 3:00 PM

Discussions

3:00 PM - 3:30 PM Coffee/Snacks Break

Lightning Talks

3:30 PM - 3:40 PM

High-dimensional longitudinal classification with the multinomial fused lasso

Samrachana Adhikari, Department of Population Health, New York University School of Medicine, New York, New York;
Fabrizio Lecci, Department of Statistics, Carnegie Mellon University (CMU)
James T. Becker, Department of Neurology, University of Pittsburgh
Brian W. Junker, Department of Statistics, CMU
Lewis H. Kuller, Department of Epidemiology, University of Pittsburgh
Oscar L. Lopez, Department of Neurology, University of Pittsburgh
Ryan J. Tibshirani, Department of Statistics, CMU

We study regularized estimation in high-dimensional longitudinal classification problems, using the lasso and fused lasso regularizers. The constructed coefficient estimates are piecewise constant across the time dimension in the longitudinal problem, with adaptively selected change points (break points). We present an efficient algorithm for computing such estimates, based on proximal gradient descent. We apply our proposed technique to a longitudinal data set on Alzheimer's disease from the Cardiovascular Health Study Cognition Study. Using data analysis and a simulation study, we motivate and demonstrate several practical considerations such as the selection of tuning parameters and the assessment of model stability.

3:40 PM - 3:50 PM

The Role of Grain Boundary Structure in Determining Damage and Failure Materials

Saryu J. Fensin, Materials Science and Technology Division, Bikini Atoll Road, MS G755, Los Alamos National Laboratory; saryuj@lanl.gov

Understanding and predicting the response of materials under dynamic loading is a challenging problem due to complexities involved with the loading state and its interaction with various features in the microstructure. In general, it is heterogeneities like grain boundaries that can control the dynamic response of material. Hence, we can divide the problem into 3 pieces: 1) single crystal, 2) bi-crystals and 3) polycrystals that together help provide mechanistic insights that take us a step closer to developing a predictive capability for damage and failure in metals. Understanding how grain boundaries (GB) affect the deformation and spall behavior is critical to engineering materials with tailored fracture resistance under dynamic loading conditions. This understanding is hampered by a lack of a systematic data set, especially for BCC metals. To fill in this gap, Non-equilibrium molecular dynamics (MD) simulations are performed on a set of hundreds of Ta bi-crystals along various tilt axes to investigate the role of GB structure and properties (GB misorientation angle, energy, excess volume, etc.) on the deformation mechanism, the resultant spall strength. The spall strength is found to correlate directly with the capability of the GB to plasti-

cally deform by emitting dislocations and twinning. As the misorientation angle increases, a transition of dislocation-meditated to twinning-dominated plasticity is observed. Moreover, the local structure of the GB significantly affects the deformation behavior of Ta bi-crystals, resulting in significantly different spall strengths at the same misorientation angle.

3:50 PM - 4:00 PM

Indexing crystal grains with Laue diffraction at 34-ID-C end station of the Advanced Photon Source

Anastasios Pateras[1] (aptrs@lanl.gov), Jonathan Gigax[2], Wonsuk Cha[3], Ross Harder[3], Richard L. Sandberg[4] Saryu Fensin[1], and Reeju Pokharel[1]
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Bragg coherent X-ray diffraction imaging (BCDI) allows measurements of lattice displacement in a single nanoparticle or a grain. BCDI is compatible with *in operando* measurements under different external stimuli, such as compression or tension, femtosecond laser light pulses, electric and magnetic fields allowing the visualization of strain inside nanoparticles and ultimately the investigation of materials properties at the nanoscale. A chronic problem faced in BCDI experiments, is that it relies on satisfying the Bragg condition of a single crystalline grain within a large population of micron scale crystals or grains of arbitrary and unknown crystallographic orientations. Laue diffraction with the use of a large bandwidth (pink) X-ray beam allows finding the crystallographic orientations of crystals by simultaneously satisfying the Bragg condition for multiple reflections. Laue maps allow indexing grains by matching the measured data with the contents of a large database of Laue patterns from known material structures. Until recently, it was not possible to index crystal grains at 34-ID-C but only measure lattice displacements with BCDI. Here we present the commissioning of a new movable monochromator that allows easily switching between a monochromatic and a pink X-ray beam, with the one used for Laue diffraction and the other for BCDI strain imaging of single grains. This unique capability will be crucial for investigating properties of crystalline materials where the knowledge of the crystallographic orientation with respect to the axis of external stimuli is imperative. We discuss the potential for future research in diverse areas of materials science and condensed matter physics.

4:00 PM - 4:10 PM

Practical Considerations from Shock Experiments at DCS

Benjamin Morrow, MST-8, Los Alamos National Laboratory

The Dynamic Compression Sector (DCS) at the Advanced Photon Source (APS) is a powerful tool for plate impact shock compression testing of materials. The main advantage of this facility lies in the ability to record multiple frames of X-ray data during a single shock event in a single sample. This rapid rate comes with various tradeoffs, adding complexity to data analysis. These roughly break into hardware, software, and science issues. A selection of these considerations will be discussed, with potential solutions and paths forward.

4:10 PM - 4:20 PM

Adaptive machine learning for accelerator and beams

Alexander Scheinker, AOT-RFE, Los Alamos National Laboratory

Neural Networks (NN) can learn the input-output relationship of complex many parameter systems, but their accuracy will suffer as the system they have been trained to control or optimize changes with time. On the other hand, adaptive feedback methods are model-independent and will automatically respond to un-modeled time variation, but they are only local in nature and can get stuck in local minima if initialized too far away from the global optimum in a large parameter space. In this talk we describe the combination of a neural network (NN) with an adaptive feedback algorithm for global optimization of analytically unknown, time-varying systems. We present the results of an in-hardware demonstration at the Linac Coherent Light Source (LCLS) Free Electron Laser (FEL), where we used an adaptive machine learning approach to automatically adjust the longitudinal phase space (time vs energy) of an electron beam.

4:20 PM - 4:30 PM

High Resolution X-Ray Imaging and Diffraction to Study Materials Under Extreme Conditions at the Mesoscale

Richard Sandberg, Brigham Young University

The revolution in accelerator-based X-ray sources at synchrotrons and X-ray free electron lasers is drastically changing the way we understand materials, especially in extreme conditions. With the intense, ultrafast, and coherent X-ray pulses provided by these new sources, we are now able to probe inside materials under extreme conditions at unprecedented temporal and spatial resolutions. In this talk, I will review work on understanding materials strength, damage, and failure mechanisms under shock loading conditions using X-ray diffraction and coherent diffraction imaging at modern light sources.

4:30 PM - 5:00 PM

Discussions

THURSDAY (08/29/2019)

7:30-8:30 AM Breakfast/Registration

8:30 AM - 9:00 AM

Stuck in flatland: What to do when you can't do 3D

Todd Hufnagel (hufnagel@jhu.edu), Johns Hopkins University

Although 3D characterization techniques such as X-ray tomography and high-energy diffraction microscopy provide exceedingly rich data about the structure of materials, their use is limited to static or slowly-evolving systems. In many problems of interest, however, the structure of the system evolves too rapidly to permit collection of 3D data, and the question becomes how to maximize the information obtained in the limited time available for data collection. In this talk, we present two approaches to structural characterization of dynamic systems using X-rays. In the first, we describe X-ray phase-contrast imaging (XPCI) studies of the structure of geological materials subjected to dynamic deformation. Although the XPCI images are too complex for direct interpretation, by using a robust physics-based algorithm we can extract quantitative information about the 3D structure including the porosity and mean pore size. We illustrate the application of this model to dynamic wedge impact of sandstone, and discuss extensions to other materials systems. Our second approach to characterization is a proposal for a novel facility consisting of two high-brightness X-ray beams oriented orthogonally to each other. These two beams could be used simultaneously for imaging, with the with the potential for recovering 3D structural information from the orthogonal projections. Alternatively, the two beams could be used for multi-modal data collection, for example doing imaging with one beam and diffraction with the other. We will discuss the capabilities and expected performance of such a facility, and describe several potential areas of application.

9:00 AM - 9:30 AM

Detector technologies for high-energy X-rays and high rates

Gabriella Carini, Brookhaven National Laboratory

9:30 AM - 10:00 AM

Use of Broadband X-rays to Aide/Perform Bragg Coherent Diffraction Imaging

Ross Harder, X-ray Science Division, Argonne National Laboratory

In recent years Bragg coherent diffraction imaging (BCDI) has become a powerful tool for *in situ* studies and investigations of *operando* materials. This is especially the case for coherent imaging in the Bragg geometry. Here the crystalline sample reflects the beam to high angle, enabling imaging of distortions in the crystalline lattice at nanometer spatial resolution. Due to the crystalline structure of the sample, one must first align the sample and detector in the X-ray beam to generate and capture the Bragg peak. Here I will present some recent work at the Advanced Photon Source (APS) to enable *in situ* broadband Laue diffraction on the same diffractometer used for BCDI measurements. This development will enable one to obtain the orientation of a crystalline component of the sample, switch to monochromatic beam and measure Bragg coherent diffraction patterns, then switch back to broadband mode and track the orientation of the crystal while *in situ* processes, such as stress loads, are applied. Another recent development at the APS is meant to enable 3D coherent diffraction imaging utilizing parallel measurements of reciprocal space slices. This is accomplished using broadband illumination and post sample analyzers. The proof of concept results will be presented with the proposition that single pulse, three dimensional BCDI could be performed at free electron lasers.

10:00 AM - 10:30 AM Coffee Break

10:30 AM - 11:00 AM
Out-briefs from breakout sessions

11:00 AM - 11:40 AM
Discussions

11:30 AM - 12:00 PM
Closing Remarks
Cindy Bolme, Los Alamos National Laboratory

12:00 PM - 3:00 PM
Report writing
Organizing committee / Participants

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