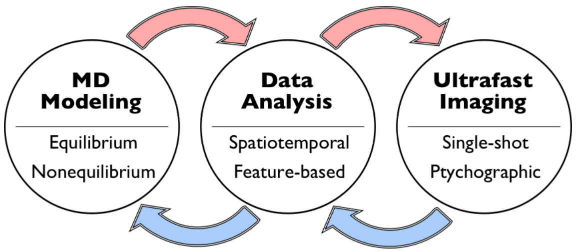
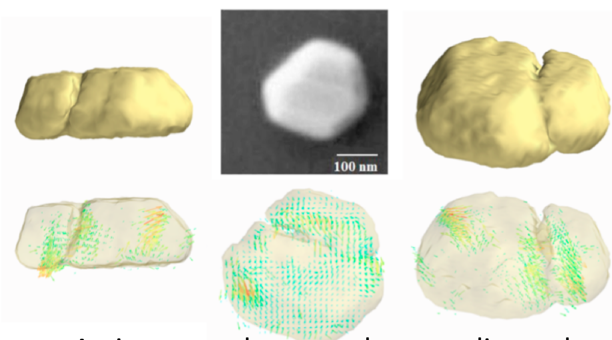
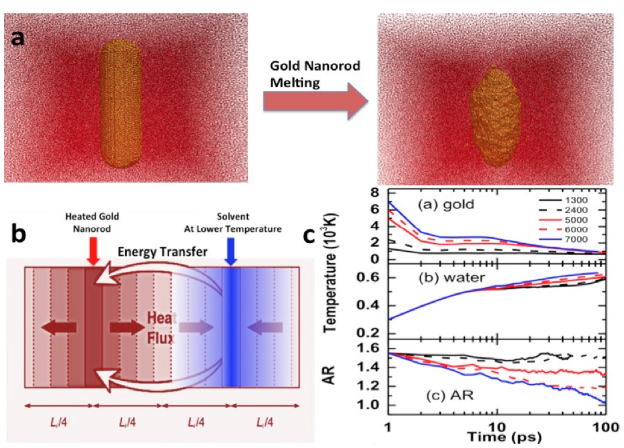
MAUI: Modeling, Analysis, and Ultrafast Imaging



Above: Simulation and experiment are integrated through a common language of data analysis.



Above: An integrated approach to predict and validate material response to external stimuli shows density and distortion vectors that lead to identification of cracks along slip planes.



Scientific Achievement

Integrated Imaging, Modeling, and Analysis of Ultrafast Energy Transport in Nanomaterials

Significance and Impact

Understanding lattice vibrations in individual nanoparticles can enable energy applications such as photocatalysis, photonics, thermoelectrics, semiconductor design, groundwater photo remediation, and heat transfer in battery interfaces.

High Level Research Details

– Modeling: MD will be used to model the phonon transport and lattice thermal conductivities for the proposed systems.

– Analysis: In order to combine the reverse (image reconstruction) with the forward (simulation) models, data transformations between model spaces will be investigated.

– Ultrafast imaging: We will conduct laser pump-probe imaging experiments to study the structure dynamics originating from electron-phonon interactions.

Left: (a) Million-atom MD simulation showing a laser-heated gold nanorod in water (b) Typical schematic of an NEMD simulation to compute heat transport (c) Temperature dissipation and aspect ratio in our preliminary MD calculations.

Additional information

- **Additional Information**

Integrating ultrafast time-resolved imaging with large-scale molecular dynamics modeling and in situ data analysis and visualization in order to design, conduct, and understand spatiotemporal measurements can provide crucial insights for energy research. The temporal behavior of in situ externally stimulated materials beyond equilibrium can lead to breakthroughs, for example, in heat dissipation of next-generation semiconductors, conversion of wasted heat into electricity in thermoelectric materials, and electrochemical processes across liquid-solid interfaces in water purification. All these diverse applications share a common behavior: they transport energy through phonons (sound waves that carry heat) in a time-evolving crystal lattice. We anticipate that our integrated approach to predict, image, and analyze phonon dynamics can be applied to other externally stimulated (for example, heated, pressurized, laser-pumped, acid-dissolved, or electromagnetically induced) systems measured by various imaging techniques including x-ray, electron, and optical microscopy.

- **Research Team (All from ANL)**

Tom Peterka (PI) is assistant computer scientist at MCS. **Ian McNulty** is a physicist and Senior Scientist at NST. **Nicola Ferrier** is a computer scientist at MCS. **Ross Harder** is a physicist at the APS. **Todd Munson** is a Computational Scientist in MCS. **Sven Leyffer** is a computational mathematician at MCS. **Subramanian Sankaranarayanan** is an assistant scientist at CNM. **Haidan Wen** is an assistant physicist at APS.

- **Sponsors**

Department of Energy Office of Science, Materials for Energy Strategic LDRD

- **References**

[1] Clark et al. Science 341, 5659 (2013) demonstrated a “pump-probe” experiment, whereby an infrared laser pumps (pulses) the material sample followed by x-ray diffraction probes at various times after the pump event.

[2] Tom Peterka, Dmitriy Morozov, Carolyn Phillips. High-Performance Computation of Distributed-Memory Parallel 3D Voronoi and Delaunay Tessellation. To appear in Proceedings of SC14, 2014.

- **Acknowledgements**

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