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Title: Structural Materials Under Extreme Conditions Workshop

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Structural Materials Under Extreme Conditions Workshop
July 29-31, 2009
Executive Summary

LANL is in the process of holding a series of focused workshops designed to engage the external scientific community and help define the facilities and capabilities to be incorporated into MaRIE. A three-day workshop focused on structural materials was held July 29-31, 2009 at LANL. The purpose of the workshop was to assess future needs in structural materials applications and supporting research, and to identify the developments and innovation necessary in the next ~10 years. Of particular interest was the development of in situ characterization techniques during processing, synthesis, and functioning of structural materials, along with supporting modeling to develop a predictive capability of materials performance.

The workshop was structured around a series of talks by both internal and external experts in structural materials development, production, application, and characterization. Speakers and attendees represented industry, academia and other National Laboratories. The talks and group discussions were asked to build upon current state-of-the-art work to define the experimental and modeling capabilities that will not only shape of the future of materials research at LANL and more broadly, but provide a new set of tools for the structural materials community at large. An external executive committee composed of Tresa Pollock (U. Michigan), Ian Robertson (U. Illinois), Darryl Butt (Boise State U), and Jim Williams (Ohio State U) played an important role in defining the overall structure of the workshop and the conclusions that emerged.

The workshop was organized into five sessions: (1) materials needs – specific applications, (2) materials modeling, (3), materials processing (4) materials characterization, and (5) specific properties/materials interactions. At the end of the talks we brought the speakers back to the front of the auditorium to facilitate a broader discussion based upon what was presented during the session and previous sessions. The following themes were common to all sessions:

- Modeling is integral to materials design and optimization – see the Integrated Computation Materials Engineering (ICME) report by the National Materials Advisory Board of the National Research Council of the National Academies.
- In situ probes that can characterize the structure or properties of a material under multiple extreme environments (e.g. high temperature, high radiation field, under fatigue) are needed.
    - Other environments of interest: pressure, corrosive, cyclic fatigue
- Advanced n-D microstructural characterization techniques and the tools to analyze the enormous data sets are needed. (n is 3D for spatial, plus time, grain orientation, strain, chemical signature, etc.

- Current experimental capabilities require approximately 2 weeks to setup and collect microstructural data with 1 μm resolution and grain orientation. Volume of sample analyzed is 200 x 500 by 1000 μm.
- Data sets are in the 3-10 Tb range and data analysis can take months to years. A graduate student may spend his entire thesis analyzing one data set.
- Today's time resolution for 3D characterization of the volume above and mapping only grain orientation is on the order of days to weeks. For many of the structural materials applications of interest we would like timescales on the order of msec to sec. There are some applications that also require time resolution down to ns or μs for science problems looking at nucleation events, e.g. twin nucleation or martensite nucleation.
- Require higher order dimensions, orientation, chemical analysis within 3D spatial structure, and dynamically time resolved.
- Possible method on roadmap to M4 would be the combination of 3D atom probe with electron tomography to give both structural and chemical resolution down to atomic scale. Drawback is that 3D atom probe is destructive and time resolution is poor.
- Multiple characterization techniques that can be utilized on the same sample. One suggestion was to combine multiple characterization tools and materials processing into a single connected instrument so that a material may be processed, exchanged in controlled environment to characterization wing, transferred back to processing, then transferred to further characterization of structure or properties.

- Many talks focused on need for improved detector technology for neutrons and X-rays: increased sensitivity, spherical shapes, semi-transparent, etc. Not much discussion or need for "brighter, more" intense beams. It sounded like the beam brightness and coherency were sufficient for many of the applications. The detectors however have a great need for advanced development. Most beam users today rely on commercial technology developed by the medical industry. Advanced deyector development is a potential opportunity for MaRIE to help overall scientific community and meet MaRIE goals. Good way to gain community acceptance of MaRIE.

- In the design and development of advanced materials, need models to design a material system with multiple optimized properties. From the industry perspective, cost needs to be an integral part of the modeling and materials design framework. Note that cost is not part of the traditional materials tetrahedron and may need to be included.

- Prediction of structural material lifetimes based on properties like fatigue, fracture, corrosion, etc. depend upon the "weakest structural link". Future facilities need to be able to fully characterize a microstructure at the micron scale looking for the defect "needle in a haystack". Then be able to observe the evolution of this defect in situ while being exposed to the stressor and environment.

- Many structural material applications rely upon casting as the processing route because it is relatively quick, cheap and efficient. Most codes today only predict the thermal history of a casting, then use either inference or empirical tools to predict microstructure in a general sense. In order to become more predictive with our casting modeling codes, we need a better understanding of the microstructural processes occurring during solidification, e.g. nucleation & growth phenomena, chemical partitioning, grain orientation, and phase changes after solidification. For most applications this would need to be done at micron scale and in the time scale of seconds.

- There is a need for a large-scale facility dedicated to environmental/corrosion science.

In addressing the above needs in a proposed facility, such as MaRIE, the following facility considerations are important:

- Facility where state-of-the-art characterization and modeling tools are available in addition to the "beamline tool". More enhancing experience for visiting users. Example: having SEM, FIB or spectroscopy available to further characterize sample tested in novel in situ tool.

- Need to develop the right kind of students and staff for a multi-disciplinary facility like M4. Students have to be trained to work as a team and understand multiple disciplines as opposed to be narrowly focused on their specific research area.
    - Consider a summer school model similar to Lujan

- Shared experimental tools at a user-facility.

- Shared data and models at a user facility. Possibly follow NIH model where NIH requires that models and data be available to all who are funded by NIH.

- Customer support in setting up experiments, and acquiring, storing, and processing the huge amount of information generated is vital for the user. In the words of Matt Miller: 'go from heroic to routine effort for analyzing the data collected'.

- General software and hardware should be maintained by the facility. Personnel needs to be allocated to this effect.

- Need for fast measuring times and techniques.

Finally, workshop participants offered some specific comments on how to define/position MaRIE and M4 in the context of broader capabilities.

- Need to focus the mission of MaRIE / M4 to only 2-3 areas and do them wholistically and very well.
    - Focus on specific material and understand from cradle-to-grave
    - Focus on application area
- Focus on a scientific problem area and develop personnel, tools and models to solve, e.g. nucleation and growth phenomena, corrosion science, or radiation tolerance. For a long-term vision like MaRIE, this would be the preferred approach.