NSF Workshop on Emerging Areas in Ceramics and Glass Science
September 12 -14, 2016

Executive Summary (10/3/16)

A workshop to identify emerging research areas in ceramic and glass science was held in Arlington, VA, September 12 through 14, 2016. Forty-one domestic and international researchers in glass and ceramic materials, representing academia, industry and national laboratories, assembled to share both expertise and vision in defining outstanding materials challenges. In preparation for the meeting, participants suggested topics for discussion through an e-mail survey. Based upon these suggestions, co-organizers Katherine Faber, Jennifer Lewis, Clive Randall, and Greg Rohrer organized the ideas into five sessions: Advanced Processing, Defect-Enabled Phenomena, Low-Dimensional Phenomena, Materials for Extreme Environments, and Glass and High Entropy Materials. Based on presentations and panel discussions in the five areas, eight challenges emerged that are summarized below. A full report of the workshop will be published in *The Journal of the American Ceramic Society*.

1. **Programmably Design and Assemble Ceramics with Prescribed Architecture**
   As additive manufacturing continues to gain attention in the materials community, the development, characterization, and modeling of preceramic polymers, colloidal systems and fluids as inks, based upon fundamental science, are still lacking. Added complexities arise from heterogeneous materials, i.e., multiple phases, transient fluxes, porous and hierarchical structures. Addressing these deficiencies should lead to strategies for simultaneous optimization of material composition, microstructure, and topology to arrive at a science of synthesis. The outcome is to create new materials and constructs with unprecedented properties and architectures by low energy sustainable routes.

   Defect-Enabled Phenomena
   Defects in ceramics exist over a multi-dimensional space, defined by time-scale, length-scale, concentration, and even defect dimensionality (point, line, planar and volume defects). The structural anomalies that define defects give rise to the possibility of exquisite control of material properties. In this context, two challenges emerge.
2. **The Defect Genome: Prediction, creation, manipulation and characterization of defects across time and length scales**
   Many of the desirable functional properties of ceramics are dependent on defect populations and their character. Envisioned here are new classes of ceramic materials wherein defects concentrations span from a few, precisely placed, isolated anomalies to those so numerous in concentration that the high entropy associated with their presence stabilizes unexpected phases. Advances in imaging and spectroscopy will allow direct defect analysis in realistic environments. Application of stressors, either during or after synthesis, will generate dynamic defect response that can be further manipulated for material design and property control. Along

with appropriate theoretical and computational techniques, the defect genome will complement the materials genome for comprehensive materials design.

3. **Functionalizing Defects for Unprecedented Properties**
   Using defects as components in the toolbox for materials design, one might anticipate the creation of defect complexes from which emergent phenomena arise. Examples include cascaded motion (motion of one defect triggers motion of many others), engineered reliability (defects trap one another), and neuromorphic properties (the existence of multiple, reconfigurable, interacting states). Full understanding of the relevant defect interactions, defect dynamics and defect-property relations will require the creation of new tools for *operando* characterization. Ultimately, materials which exhibit, via the presence of such functionalized defects, high response to applied stimuli are anticipated.

4. **Ceramic Flatlands: Defining structure-property relations in freestanding, supported and confined two-dimensional ceramics**
   Two-dimensional structures, whether freestanding layers, supported surface films, or confined complexions at grain boundaries or interfaces, are noted for their high anisotropy in mechanical, electrical and transport properties, and hence, provide unique functional and structural capabilities. The discovery of many 2D structures and their processing has outpaced our understanding of their properties. Establishing an understanding of structure-property-processing relations for 2D structures is expected to lead to easily tunable properties through small changes in chemistry, processing, or external fields. Such 2D structures may have impact on energy applications (batteries, super capacitors, catalytic materials), miniaturization of switching devices, low energy computing, and novel mechanical properties.

5. **Ceramics in the Extreme: Discovery and Design Strategies**
   Ceramic materials are the key enabler in meeting society's imperatives in energy, transportation, and aerospace. However, the menu of materials that can withstand extreme fields/loads/fluxes (thermal, chemical, mechanical, radiant, electromagnetic) is currently inadequate and critical properties are often unknown. Therefore, strategies based on chemical and physical principles and their effect on properties are essential. These must combine interactive modeling and experiments to guide the discovery and design, as well as their synthesis, to meet the basic functional requirements in severe environments. Compounding the challenge is the shortage of characterization approaches for very high temperatures, including thermodynamic properties to support modeling activities, as well as mechanical and thermal property characterization.

6. **Ceramics in the Extreme: Complex systems**
   Because of the complexity of extreme environments, materials are likely to involve multiple phases, doping or alloying, and tailored microstructures and architectures. A science-based approach that captures the complexity of these material interactions is essential. The includes modeling of the thermochemical and thermo-

mechanical interactions of the constituents in different configurations, requiring input from thermodynamic measurements, phase equilibria and kinetic models; processing approaches to develop the desired architectures; and experimental assessment of the multi-phase/microstructurally designed material systems to evaluate performance in extreme environments. This would involve *in-situ* and *in-operando* measurements that may require development of testing systems for extreme conditions.

7. **Rational design of functional glasses guided by predictive modeling**
   Despite the 5000+ year history of glass making, the computational design of multi-functional glasses and the atomistic understanding of their properties, are in their infancy. Modeling beyond well-ordered covalent polyhedral is challenging, in large part, due to inadequate interatomic potentials and limited time- and length-scales accessible by current computational power. *In operando* characterization and modeling of glasses and melts are needed to develop predictive computer models. Through advances in modeling and experimental verification, it is anticipated that fundamental knowledge of glass behavior, such as selective chemical reactivity of certain polyhedral arrangements, or mechanical strength and toughness can be garnered.

8. **Understanding glasses and melts under extreme conditions**
   There is little structural information, physical and thermodynamic data, and limited connection between modeling and experiment for glasses and their melts under extremes in temperature, pressure, or steep chemical, electrochemical and magnetic gradients. By using the responses of glasses and melts to such extreme conditions, it is anticipated that our knowledge of the glassy state can be extended, resulting in new glasses, including some non-traditional glass formers, with unanticipated properties. These studies, though being difficult, to some extent due to the lack of facilities, are expected to provide guiding principles to advance the discovery of new glasses.