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RPPR Final Report
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STEM Degrees: **STEM Participants:**

Major Goals: This project sought to support a workshop, called the Controversies Colloquium, which was aimed at providing a venue where a small-group of thought-leaders and subject matter experts could gather to discuss long-standing or new “controversies” in our field. The first workshop in what we hope it a continuing event on a biannual timeline focused on the subject of the Stability of Nanostructures, and occurred February 1-2, 2018 at the University of California, Irvine in Irvine, CA. To unravel the complex phenomena associated with nanostructured material stability, two key controversies were critically debated:

1) Is true stability ever achievable and how will we know when we get there?
- What are the gaps in our current understanding of boundary stabilization using solutes, second phases, and boundary type (e.g., twins)?
- Are stabilized grain boundaries true interfaces or new phases?
- How do triple junctions and the connectivity of grain boundaries in a real material affect stability?
- How does faceting of grain boundaries fit into the discussion of thermodynamics and stability?
- Can excess grain boundary free energy be negative?

2) Are thermally-stable boundaries also mechanically-stable?
- What are the critical differences and similarities between the mechanisms of grain boundary migration due to temperature and stress?
- Are boundaries more mobile in nanostructured materials or can these materials simply experience higher stresses?
- Can doping grain boundaries to lower their energy also drive mobility under stress to zero?
- Is there an analogy to mechanical work for temperature-driven grain growth that allows us to compare how hard we are driving boundaries in various scenarios?

The central concept of this workshop was in stark contrast to the status-quo workshop presentation format wherein speakers give a series of presentations and minimal time is usually left for critical discussion. Instead, the focus was on the discussion itself, with participation by all attendees in an interactive format.

Accomplishments: The organizers invited approximately 65 people to the event, with ~50 responding that they would plan on attending and a final count of 48 attendees (see Participants). The high level of participation shows that the community sees a strong need for such an event and is enthusiastic about the Controversies Colloquium. The attendees came from across the globe, with Germany, France, and Austria represented in addition to the United States, and from National Labs, Academia, and Industry. In the future, we will plan these workshops to be

close to the time of another major materials science conference to promote even more widespread attendance, as our invitees from Asia reported that it was difficult to plan a separate trip to the U.S., especially since this would require a visa.

The two day event was full of energy and vigorous discussion. Non-traditional small-group presentation and discussion formats were chosen to encourage and promote free-flowing scientific dialogue and critical debates. We found that the Chalk Talk format was especially good, as the audience remained very engaged and the idea of boiling a complicated topic down to a classroom lecture made us all be more critical of the basic concepts. Two examples of the unique formats are:

Flipped Classroom Discussion
The assigned speaker was responsible for writing a 2-3 page white paper on an open question, unexplained phenomenon, or area for rapid growth in the near future. A high-level discussion followed the presentation of this concept to the group.

Chalk Talk
The presenters gave talks on topics related to the stability of nanostructures, but used a whiteboard for all schematics and talking points. The basic idea was to force ourselves to condense our ideas into a form that could be easily expressed in a simple diagram, equation, etc., rather than a complicated schematic or graph.

A key outcome of the workshop was to identify key questions for the field, then make some progress toward finding the answers. Here, we break some of these questions or topics down into groups. A discussion of these topics is the core of the Perspectives paper that is being written.

(1) Impurities are everywhere and are very important
- Should efforts be focused on getting rid of them or exploiting them?
- What particular challenges exist with nanocrystalline processing techniques?

(2) Kinetics matter more than we think and must also be included in the conversation
- Kinetics and thermodynamics are coupled.
- What is the temperature-dependence of both?
- Can a set of experiments answer whether kinetics or thermodynamics dominates the stability of a certain material?
- What models are needed to isolate a dominant mechanism?

(3) What is the essential descriptor of our material that controls thermal stability?
- Are individual boundaries or grain boundary networks most important?
- How do we best describe individual boundaries? For example, should we use the concept of free volume or descriptors such as CSL number?
- Can the metallic glass community ask as a guide?
- What are the available continuum, mesoscale, or nanoscale descriptors?

(4) Role of mechanical driving forces
- Does pressure or normal stress influence migration?
- Does zero grain boundary energy affect mechanically-driven migration?
- How does dopant addition affect this migration?

(5) Figure of merit for thermal stability
- Are there more practical definitions of stability than zero grain boundary energy?
- What practical connections can we make to processing or service conditions?
- Is there a dimensionless parameter that represents kinetic limitations?
- Can we use the concept of “degeneracy of states” to describe metastability?

(6) Describing grain boundary transformations with equilibrium thermodynamics
- Should the field use the term complexion or grain boundary phase?
- What is the role of entropy on complexion/phase formation at a grain boundary?
- How can we describe the full grain boundary phase space, to understand all of the options like we do for bulk thermodynamics?

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In summary, a vibrant, engaging workshop was held for the inaugural Controversies Colloquium. The ARO support for this workshop was invaluable, as it helped us support the cost of the meeting rooms, the audio/visual expenses, working meals that enabled open discussion, and finally the writing of the Perspectives paper. From discussions with attendees in the months since the workshop, it appears that this workshop also served as a nucleation event for new ideas in the area of interface science and nanostructured materials. A number of colleagues have reported that they have pitched some of these ideas to the Army Research Office. If the Controversies Colloquium leads to great new research at ARO, then it will have been an even bigger success.

Training Opportunities: No direct funds for student or postdoc training were provided. However, the Controversies Colloquium was a unique exercise where, rather than have one “teacher” lecturing to the audience, a room full of notable scientists all acted as the students. This experience will help us all become better advisors for our own research groups in the future. In addition, a number of early career scientists and faculty attended the meeting. While this is not direct training for them per se, we hope that the workshop will have an impact on their career development.

Results Dissemination: Our intention is to publish a Perspectives paper on the outcomes of the workshop. The goal of the manuscript is to close the book on old issues and identify new problems of interest for the research community to tackle. The five organizers of the workshop (Rupert, Boyce, Gianola, Mathaudhu, and Trelewicz) are currently working on a draft manuscript, which is approximately 50% finished. Our plan is complete this paper and have it submitted by Nov. 30, which includes some time needed to circulate the draft to a few key participants in order to solicit feedback. The paper is being prepared for Materials Research Letters due to its open-access format and moderate impact factor (2017 IF = 6.16) which will enable broad dissemination to the community.

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

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