Accelerating Materials Discovery for Global Competitiveness Focus Topic
Room: 202 B - Session MG+EN+MS-WeA

Education for Interactive R&D & Industrial Implementation
Moderator: C. Eom, University of Wisconsin-Madison, B. Nelson-Cheeseman, University of St. Thomas

2:00pm **MG+EN+MS-WeA1 21st Century Skills and Educating the Next Generation Workforce for Expedited Innovation and Deployment**, ***C.C. Broadbridge***, Southern Connecticut State University **INVITED**

The goal of the Materials Genome Initiative [MGI] is to expedite materials discovery, innovation and deployment via the development of new approaches to materials research that exploit interdisciplinary collaboration and innovation. Successful implementation will require a workforce possessing 21st Century Skills including critical thinking, problem solving, communication, collaboration, technological fluency and creativity. To address the need for US competitiveness in a global economy, educational reform has been initiated at the K-12 level with the development of 21st Century Skills Standards [1], Common Core Standards [2] and the Next Generation Science Standards [3]. Similar reform is needed at the university and post-graduate [PG] professional development levels to assure the optimal development of a STEM educational pipeline. At the university level, reform has been initiated with the development of novel approaches to all university [non-major] requirements as well as courses and programs for majors (e.g., [4,5]). For the effective implementation of the MGI, it is important to realize the natural synergies that exist between these efforts and those within the materials science education and research communities. Arguably, individuals acquire and refine these necessary skills best via exposure to, and active participation in, authentic science research. NSF funded Materials Research Science and Engineering Centers [MRSECs] support interdisciplinary and multidisciplinary materials research and education of the highest quality [6]. All MRSECs include education and outreach components that effectively integrate the collaborative and innovative aspects of materials research. Components are developed and implemented at the K-PG levels and also include programs that educate the general public. For this presentation, educational reform at all levels will be reviewed with an emphasis on approaches with the greatest potential positive impact on the implementation of the MGI. In particular, an interdisciplinary team-based approach to materials research effectively leveraging programs within the Center for Research on Interface Structures and Phenomena (CRISP) MRSEC will be described that integrates materials science education and research while maximizing on the attainment of the 21st Century Skills necessary for successful implementation of the MGI.

1.http://www.p21.org/overview/skills-framework/351

2. http://www.corestandards.org/

3. http://www.nextgenscience.org/

4. http://www.aacu.org/resources/generaleducation/index.cfm

5. http://www.tms.org/pubs/journals/jom/0910/thornton-0910.html

6. http://www.mrsec.org/

2:40pm **MG+EN+MS-WeA3 High-Performance Ceramics – Challenges for Next Generations**, ***W. Rossner***, *S. Lampenscherf*, Siemens AG, Germany **INVITED**

Ceramics play an important role in system engineering for demanding industrial applications because they provide functionality of key components that are critical for overall system performance and operational benefit. The continuous development of high performance ceramics over the last decades was aiming mainly towards 'better' properties and 'deeper' understanding of material behaviour.

For today's applications in areas such as power engineering, medicine, automotive, aircraft and high-end electronics the time-to-market aspect is an important success factor. Product cycles become shorter while R&D cycles especially including materials development are not able to keep up with such pace. The complex relationship between ceramic performance and processing plays a special role for accelerating the R&D process. An additional time-consuming factor is the need for extensive qualification and testing of high-performance ceramics to guarantee functionality and reliability under desired operation conditions.

Based on the very much improved understanding of the dependencies of processing, performance and application as well as the availability of advanced computational methods and tools materials engineering can be a vital part to overcome today's limitations for accelerating materials development and product implementation.

In the talk we discuss these aspects in the context of current industrial examples for next generation high performance ceramics.

4:00pm **MG+EN+MS-WeA7 Educating for High-Impact Computation - Skills vs. Acceptance**, ***W.E. Windl***, The Ohio State University **INVITED**

As an integral part of the Materials Genome Initiative (MGI), the task of materials computation, in concert with experiment and theory, is to help accelerate the discovery and maturation of new materials by at least a factor of two. During the first rounds of MGI-related solicitations, two major groups of challenges that always existed became very evident. For one, the obvious question about the skill set available in the Materials Research community to actually perform the necessary computations. Secondly, and much less apparent on the surface, was the frequent lack of acceptance of computational work as a valid input, maybe foremost in the experimental community, which can lead to awkward situations, missed opportunities, and frustration in collaborative projects. Beginning with the 2012-2013 academic year, The Ohio State University has moved from a quarters-based academic calendar to a semesters-based calendar. As part of this change, the Department of Materials Science and Engineering has elected to revise degree program curricula in a significant manner. A key objective in our revision was to respond to the challenges in skill set and acceptance of computational work from Integrated Computational Materials Engineering and MGI described above. We have developed a curriculum that attempts to integrate congruently database use, visualization, simulation and computational approaches in materials science with other core educational content. At the undergraduate level, our goal was to produce graduates who are cognizant of the broad range of computational tools available to materials engineers and what they can do to solve engineering problems, and who are able to use a number of those tools proficiently to solve problems of practical importance themselves. The MSE core curriculum includes 9 credit hours (four courses), or 20% devoted to these topics. Students may take an additional 4 credit hours (two courses) in elective content on computational methods in materials science. In this presentation, details will be presented on the specific course offerings, course content, exercises, and software packages used. How the courses are postured in the curriculum will also be addressed. The experiences, challenges, and recommendations resulting from the first year of teaching will finally be discussed, where the author was involved in four different courses relying on different combinations of traditional teaching with reverse and peer teaching approaches as well as with significant fractions of active-learning work.

4:40pm **MG+EN+MS-WeA9 MGI in the Laboratory: Closing the Feedback Loop in Aerospace Materials Design and Development**, ***E. Sapper***, *P. Kinlen*, Boeing Research & Technology **INVITED**

The aerospace industry has continuously driven major developments in material science as technology has evolved from wood and fabric to lightweight metal alloys and advanced polymer composites. Future aerospace materials systems will require even more advanced technologies, such as those afforded by smart and responsive systems like electroactive polymers and composites. The unique properties of these materials provide the ability to construct intelligent systems which produce a defined, predictable response to an input.

Concurrent with state-of-the-art chemical technology, the increasing availability of high-performance computing power has facilitated the entry of various computational simulation and modelling methods into the research and development production cycle. Quantum mechanics, molecular dynamics, and multi-scale simulation approaches, developed and applied within a Materials Genome Initiative paradigm, are providing insight into aerospace material properties of interest, such as species-specific transport rates, electrochemical response, service lifetime prediction, material color and appearance, and quantitative structure-property relationships.

The ultimate goal of a coupled experimental-computational approach is the closed and tightened feedback loop between laboratory results and computational predictions. This leads to the incorporation of more theory into experimental practice as well as more heuristics into computational method development, expressed in the form of semi-empirical models and empirically-pinned property response surfaces. This presentation will review some of the challenges involved in applying advanced computational methods alongside state-of-the-art laboratory procedures. The development of novel, more environmentally friendly aerospace coatings that release site-specific corrosion inhibitors on-demand will be presented as a case-study in closed-loop computation-experimentation.

5:20pm **MG+EN+MS-WeA11 Condensed Matter Physics in an Age of Computation**, ***M. Marder***, University of Texas at Austin **INVITED**

Condensed matter physics and materials physics have grown so enormously that no one can hope to know everything done in the last five years let alone the last fifty. This does not relieve researchers of the charge of educating new generations of students. I will discuss the balance between acquisition of skills and acquisition of knowledge, and the way that computing power changes what is taught and how.

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