The Materials Genome Initiative: NIST, Data, and Open Science

Abstract: In this talk I will present an overview of the Materials Genome Initiative, covering the current and planned efforts across the Federal government. After an overview where I will provide insight into community-led activities, I will discuss our attempts at NIST to address some of the challenges to creating the materials innovation infrastructure that lies at the heart of the Materials Genome Initiative. In particular, NIST is now devoting considerable effort, in concert with its partners in industry, academia, and government, to develop the tools, standards, and techniques for (i) establishing model and data exchange infrastructure (ii) establishing best practices and new methods for ensuring data and model quality and (iii) developing the Big Data analytics to enable "data driven" materials science.

To properly address these problems involves a deeper examination of the nature of materials data than is typical. In particular, the essential linkage between models and measurements implies that many of the conceptual challenges with materials data can be most efficiently resolved using methods that address the role of materials models as the core concept of the scientific method. This insight, and associated examinations of the manner in which we collect and disseminate data are the keys to overcoming the impediments to a materials innovation infrastructure.

James Warren, Ph.D.

Dr. James A. Warren is the Director of the Materials Genome Program at NIST. His aspirations of an academic physicist’s career took a turn in 1992 when he received an NRC post-doctoral appointment at NIST. He came to the Metallurgy Division after receiving his Ph.D. in Theoretical Physics at the University of California, Santa Barbara, which was preceded by an A.B. (also in Physics) from Dartmouth College. In 1995, with three other junior NIST staff members, he co-founded the NIST Center for Theoretical and Computational Materials Science, which he has directed since 2001. From 2005-2013 he was the Leader of the Thermodynamics and Kinetics Group. His research has been broadly concerned with developing both models of materials phenomena, and the tools to enable the solution of these models. Specific foci over the years has included solidification, pattern formation, grain structures, creep, diffusion, wetting, and spreading in metals. In 2010-11, Dr. Warren was part of the ad hoc committee within the National Science and Technology Council (NSTC) that crafted the founding white paper Materials Genome Initiative (MGI), and has served as the Executive Secretary of the NSTC MGI Subcommittee since 2012.