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LARGE DATASET GENERATION, INTEGRATION AND SIMULATION IN MATERIALS SCIENCE (PREPRINT)

Jeff Simmons

Metals Branch

Metals, Ceramics, and NDE Division

J.-C. Zhao

The Ohio State University

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MATERIALS AND MANUFACTURING DIRECTORATE
WRIGHT-PATTERSON AIR FORCE BASE, OH 45433-7750
AIR FORCE MATERIEL COMMAND
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14. ABSTRACT As new and rapid materials characterization tools become widely available, large datasets are being generated at a faster and faster pace, which is both exciting and challenging. The exciting aspects are that large amounts of composition, structure, and spectral information about materials are being gathered routinely. This promises to accelerate the traditional scientific pursuits in Materials Science of establishing processing-structure and structure-property relationships and hypothesis testing. Even more exciting is the promise to provide quantitative validations of the physics-based forward models of these input-response relationships by providing statistically significant datasets for this validation. The main challenges presented by the emergence of these techniques are (1) rapid acquisition of larger and larger datasets, (2) using this information to provide predictive capabilities in materials systems, and (3) analysis of the increasing volumes of data.						
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Large Dataset Generation, Integration and Simulation in Materials Science

Jeff Simmons and J.-C. Zhao

As new and rapid materials characterization tools become widely available, large datasets are being generated at a faster and faster pace, which is both exciting and challenging. The exciting aspects are that large amounts of composition, structure, and spectral information about materials are being gathered routinely. This promises to accelerate the traditional scientific pursuits in Materials Science of establishing processing-structure and structure-property relationships and hypothesis testing. Even more exciting is the promise to provide quantitative validations of the physics-based forward models of these input-response relationships by providing statistically significant datasets for this validation. The main challenges presented by the emergence of these techniques are (1) rapid acquisition of larger and larger datasets, (2) using this information to provide predictive capabilities in materials systems, and (3) analysis of the increasing volumes of data. The selected articles highlighted here provide a snapshot of some current activities in this expanding field, but, in no way, attempt to cover the entire field-such an attempt would be well beyond the page limit of a JOM issue.

Four articles were chosen to highlight data generation. The article by Uchic, Groeber, and Rollett describes the current state of the art of automated serial sectioning. That by Barabash, Bei, Ice, Gao, and Barabash describes one of the exciting developments in X-ray characterization: that of characterization of internal strains in materials. The article by Kotula and Sorensen describes recent advances in hyperspectral X-ray materials characterization and some techniques used to fuse the signals from multiple wavelengths into a single coherent picture of material structure. J.-C. Zhao and D. Cahill describe recent development of femtosecond-laser based measurements of thermal conductivity, expansion coefficients and elastic modulus in micron-scale spatial resolution and their applications in rapid collection of composition-phase-property data.

Beyond characterization, Materials Engineering and Materials Science are concerned with prediction and explanation of properties, from a structural standpoint. Two articles were chosen to highlight important considerations when making this connection. The article by Lewis, Qidwai, Geltmacher, and Jackson highlight the actual details of turning a 3-D characterization into property predictions. We take it for granted what a microstructure is, but the actual definition of a microstructure must be a statistical one, whose true description is currently an active area of research. The article by McDowell, Ghosh, and Kalidindi describes the current state of the art of representing random media for the purposes of modeling properties in Materials Science and Engineering.

The increasing data rate of modern microscopy is generating a new focus for research: that of converting measurements to context. The output of a microscope observation is typically an image that the eye can interpret, if sufficient care is taken. Microstructure images actually consist of thousands or millions of individual measurements that the eye interprets. The actual value stored in each pixel was the magnitude of a measurement. For this reason, image data is often referred to as a

memory-based representation. Converting this to a Materials context-based representation required by the physics-based models used to compute properties constitutes an emerging problem in large dataset generation: that of analysis.

The article by Rowenhorst presents a comprehensive description of the issues involved in converting 3-D serial section data to a Materials context. Since this is a painstaking process, research is being devoted towards developing algorithms that require less human interaction to analyze the datasets. The field of image segmentation is an exploding field, mostly fueled by the proliferation of medical imagery and the introduction of the digital camera: it is not possible to cover this field with any fidelity. Instead, we have chosen to highlight several techniques currently in development for performing segmentations in Materials images. The articles by Bouman and Comer, Pollak, Wang and Waggoner, and by Shiflet describe four promising techniques: (1) statistical segmentation, including Bayesian methods, (2) inverse diffusion, (3) graph-cut methods, and (4) level set methods, respectively.

The articles covered in this issue represent only a sampling of the exciting developments in this rapidly expanding field. It is with regrets that we could not cover all of the interesting developments in the field, including 3D Atom Probe, MultiModal data collection and Fusion, 3-D + t time series tomography, the many physics based “forward models” that can be validated for the first time with the rich datasets being collected, among many others. Watch this space for further developments.

Jeff Simmons is with the Air Force Research Laboratory and is a member and former chairman of the Advanced Characterization, Testing and Simulation Committee of the Structural Materials Division of TMS.

J.-C. Zhao, professor, is with the Department of Materials Science and Engineering, The Ohio State University and is the advisor to *JOM* from the Advanced Characterization, Testing and Simulation Committee of the Structural Materials Division of TMS.