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Future Directions in 3D Materials Science: Outlook from the First International Conference on 3D Materials Science

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The First International Conference on Three-Dimensional Materials Science was held in July 2012 in Seven Springs, Pennsylvania. The final session of the meeting consisted of a panel and audience discussion of the future directions of 3D materials science. Here we summarize these directions in four categories: improving data collection capabilities; increasing efficiency of collection, analysis, and modeling of data; error quantification; and data management.

INTRODUCTION

At the First International Conference on 3D Materials Science (3DMS-I), held July 2012 in Seven Springs, Pennsylvania, researchers in the fields of three-dimensional (3D) data collection, processing, analysis, and modeling gathered to share their research, exchange ideas, and discover the state of the art in this rapidly growing field. The format of the conference allowed for in-depth discussions throughout the week, and the numerous oral and poster presentations set the tone for the last session of the conference, which concluded with a panel discussion on the future directions of 3D materials science.

The aim of this discussion was to establish goals and actionable tasks for the 3D materials science community. As the field emerges, expertise is being developed in five critical areas of 3D materials science: data collection, data and image processing, microstructure quantification and analysis, modeling and simulation, and data management. As these five interrelated areas develop and expand, it is critical to maintain proper communication among them. The discussion was therefore focused on advances and directions in these areas and on the tasks required to maximize the integration of all aspects of 3D materials science.

The panel, which comprised six leaders in the field (J. Christodoulou, Office of Naval Research; H. Fraser, Ohio State University; P. Midgely, University of Cambridge; M. Miller, Cornell University, G. Olson, Northwestern University; and G. Rohrer, Carnegie Mellon University), led the discussion, with input from the roughly 150 attendees in the audience. Several recommendations were brought forth by both the panel and the audience, which fell into four general categories. These are improving data collection capabilities; increasing efficiency of collection, analysis, and modeling of data; error quantification; and data management.

DATA COLLECTION

One of the most important factors contributing to the rapid emergence of 3D Materials Science has been the automation of 3D data collection. Although serial sectioning, x-ray tomography, atom probe tomography, and other data collection techniques have been employed for some years,[1–8] new collection methods are being introduced that are either partially or fully automated.[9,10] Automated data collection techniques, particularly those that can incorporate crystallographic measurements, remove the initial barrier to 3D materials analysis—the perception that unsupportable investments of time and resources are required for data collection. (Although data collection certainly requires significant investment of time and resources, many have noted that far more time and resources are expended on the processing and analysis of the data.)

The need for better detectors was proposed during discussions. This refers both to spatial resolution and speed, as well as refers to confidence in detector accuracy. Many 3D researchers rely on commercial products for data collection and are therefore limited in speed and resolution by the parameters of commercially available cameras, tomography units, etc. As the field of 3D expands to more laboratories and classrooms around the world, consumer demand for better detectors may drive great advances in a number of technologies. A good example of this phenomenon is the collection speed of electron backscatter diffraction (EBSD) patterns used in measuring crystallographic orientation. Initial measurements took on the order of two seconds per pattern, but as illustrated in Fig. 1, current commercially available cameras can collect more than 900 patterns per second. As the power of desktop computers has increased substantially, it is feasible to index these patterns and create orientation maps in real time.

Although the example of EBSD pattern collection speeds is just one type of measurement critical to 3D materials science, it illustrates the potential path that a number of technologies may take, whether they are commercial products or "home-grown" facilities. As a community, 3D materials scientists must focus on improving not just the speed but also the precision and accuracy of the detectors we use to measure microstructures by creating the demand for these devices and driving innovation in data collection.

Besides increasing the speed and accuracy of our varied detectors, another important path forward in 3D materials science is the use of complimentary techniques on a single sample. For some measurement techniques, the effect of sampling methodologies is not completely understood. Coupling two or more techniques allows assessment of any systematic error that may be introduced by specific techniques (for example, sample damage caused by a focused ion beam), which in turn may serve as a pivotal aspect of technique optimization. The complementary use of destructive and nondestructive techniques, such as serial sectioning and x-ray tomography, is one approach to this type of artifact and error assessment, as is the coupling of backscattered or forescattered electron images with high-resolution chemical composition maps.

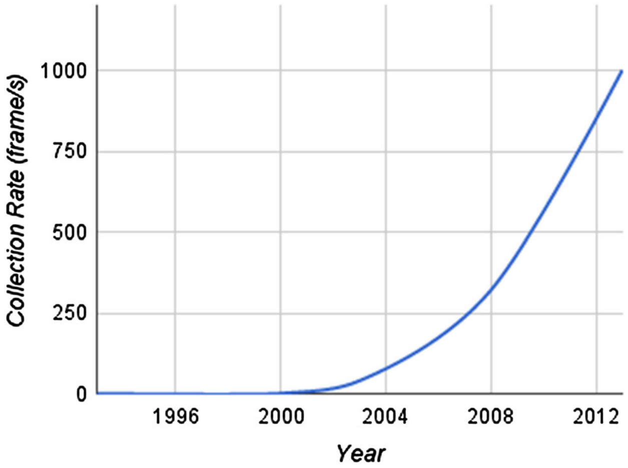

Fig. 1. Collection rates of electron backscatter diffraction (EBSD) patterns in the past two decades. From Ref. [11] and self-reported manufacturer values

EFFICIENCY AND INTEGRATION OF DATA COLLECTION, MODELING AND ANALYSIS

Despite significant advances in data collection and automation, the collection of a 3D dataset remains a time-consuming step, and in some cases, it is not readily available to all users. Three approaches to improving the accessibility and availability of 3D data to the community were suggested.

First, data collection techniques must become more efficient. Many groups (i.e., Refs. 9 and 10) have begun automating the collection of data through serial sectioning, and this remains a critically important path for the future of 3D materials science. Although faster and more efficient detectors play a critical role in improving the speed of data collection, true automation—that which allows for continuous, unsupervised data collection—is vital to the 3D materials science community. Efforts to automate these processes are nontrivial and require a significant time investment on the front end. This investment of time, however, will pay off in immense time savings as automated systems come online and unsupervised data collection becomes possible.

In addition to automating the processes of 3D experimental measurements, a second approach to increasing the efficiency of integration of 3D data into models and simulations is the generation of synthetic microstructures. The generation of statistically accurate, physics-based computed microstructures allows for simulations to be carried out on several different systems without the need for 3D data collection for each system. Although the generation of synthetic microstructures has a long history, it is only through integration of experimentally measured 3D microstructural metrics, and incorporation of materials physics into microstructure simulation tools, that truly accurate synthetic microstructures can be generated. Efforts to match synthetic microstructure parameters to measured statistics have resulted in new capabilities, and the expansion of synthetic microstructure generation is a key area for the future direction of 3D materials science.

Finally, the processing of 3D data, which is often the most time-consuming step, was identified as an area where automation could greatly improve the accessibility of datasets. Image processing of both serial sectioning data and tomographic data is typically tailored to specific datasets and is often based solely on grayscale image values rather than on materials physics. Incorporating prior knowledge of the materials system, such as grain crystallography or known morphologies, of the materials system into the image processing steps was identified as a potential pathway to the automation of image segmentation and processing techniques for 3D data processing.

ERROR QUANTIFICATION AND MODEL VALIDATION

Although not specific to 3D materials science, the concepts of uncertainty and error quantification, and verification and validation of models, are particularly important to 3D data. The nature of 3D data collection makes uncertainty quantification somewhat challenging. Those parameters that can be reported, however, should be included in 3D analyses. Sampling size, machine uncertainty, signal variation and noise, and known artifacts are often factors that can be quantified for an individual dataset. It was stated that as a community, 3D materials scientists should strive to report these values whenever possible.

Validation of materials models is another often-discussed endeavor that is not unique to the 3D community, but it is nonetheless vitally important. Both the experimental validation of performance models (e.g., mechanical tests to validate plasticity models) and the verification of tools for synthetic microstructure generation by experimentally collected data are critical to the future integration of 3D materials data into computational models. Experimentalists and modelers have long strived to collaborate for this purpose, and the conference attendees agreed that the 3D materials science community should continue to work toward integrating these approaches.

DATA MANAGEMENT

Data management, which entails the long-term preservation, storage, and sharing of datasets, is critical because of both the expense and the effort required to obtain rigorous 3D experimental datasets, as well as of the utility of such data. 3D experimental datasets are typically large and complex, requiring advanced data analytics. Although 3D data are typically gathered with a specific question in mind, the same datasets may offer even greater possibilities for broader analysis and discoveries by other researchers and data scientists.

Data management has different implications for different sectors of the scientific community. For government-funded research in particular, there is an increasing push to make data more broadly available. A February 2013 memo from the White House Office of Science Technology and Policy (OSTP) put this need in clear language, expressing a commitment that “federally funded scientific research is made available to and useful for the public, industry and the scientific community… [including] peer-reviewed publications and digital data.”[11,12] For incentivizing data sharing, those gathered at the 3DMS-I Conference suggested that the amount and quality of data that a scientist makes available to the general public should become a basic metric for career achievement much as the “h-factor” is today. Data management in the private sector may have less to do with cross-organizational sharing and more to do with developing internal systems to derive maximum value from datasets. Mutually beneficial sharing of private data is also encouraged primarily at a precompetitive level.

Although the community’s requirements for long-term data management and sharing are still evolving, some resources exist that can fulfill many data management needs. One early vehicle in this area is the 3D Materials Atlas (www.tms.org/3DMaterialsAtlas), which was developed as an open-access database for 3D Materials Science data. A milestone in the push for increased sharing of 3DMS research is a special feature on 3D Materials Science planned for the open-access journal *Integrating Materials and Manufacturing Innovation* (*IMMI*). The articles themselves will be publically available, and much of the data will also be made available through the *IMMI* site (www.immijournal.com/series/3DMS).

An ongoing challenge for data management is the cost of long-term data storage. 3D datasets are often massive (on the order of terabytes), and it is not always feasible to store all relevant data. Although this can often limit the scope of what can be done with such data subsequently, for data management to be feasible, it will likely remain necessary to be selective about what datasets are stored even as computational storage prices continue to fall. Likewise, a major hurdle for the community is to develop standards of metadata and data annotation to make it easier for scientists to make use of one another’s data.

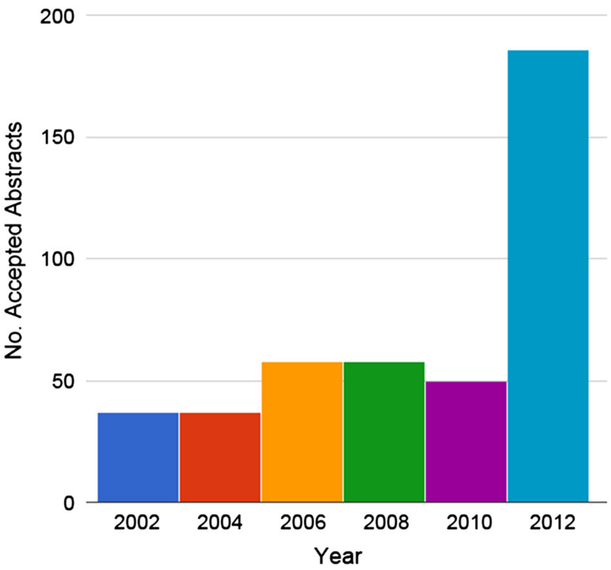

Fig. 2. Number of abstracts submitted for 3D materials science symposia at TMS Annual meetings, MS&T meetings, and 3DMS-I (2012)

LOOKING TO THE FUTURE (3DMS-II)

The 2nd International Congress on 3D Materials Science 2014 will be held June 29–July 2, 2014 in Annecy, France. Like 3DMS-I, this conference will continue to explore the topics of three-dimensional characterization, visualization, quantitative analysis, modeling, and investigation of structure–property relationships of materials. Figure 2 shows a snapshot of the participation in the 3D materials science symposia at TMS Annual Meetings as well as at recent Materials Science & Technology (MS&T) meetings, with the 3DMS-I conference in 2012 representing more than 180 abstracts. A larger number of participants is anticipated at 3DMS-II, and the event will culminate with a panel discussion focused on progress made up to that point and future directions of the field. As progress continues in the field of 3D materials science, overcoming the critical challenges surrounding 3D data collection, integration of data collection with modeling and analysis, error quantification and model validation, and data management will lead to significant advances in the way we look at and work with materials.

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