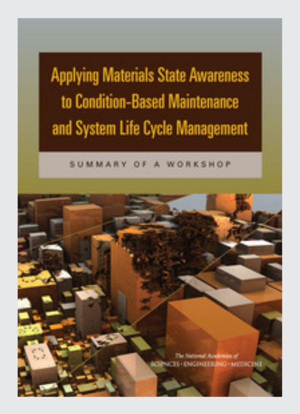

Applying Materials State Awareness to Condition-Based Maintenance and System Life Cycle Management: Summary of a Workshop

DETAILS

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Applying Materials State Awareness to Condition-Based Maintenance and System Life Cycle Management

SUMMARY OF A WORKSHOP

Robert J. Katt, *Rapporteur*

Defense Materials Manufacturing and Infrastructure Standing Committee

National Materials and Manufacturing Board

Division on Engineering and Physical Sciences

The National Academies of
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Cover: By knowing the initial state of materials and the environment they are in, and on a larger scale the whole system, it is possible to predict the expected progression of the conditions. It is possible to "slice through" to the future and predict when to do maintenance. Unfortunately, the detailed initial state is not often known for a material. However, progress is being made. *Artist:* Erik Svedberg. Image created by computing the progression of decay from an initial state.

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PLANNING COMMITTEE ON APPLYING MATERIALS STATE AWARENESS TO CONDITION-BASED MAINTENANCE AND SYSTEM LIFE CYCLE MANAGEMENT: A WORKSHOP

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Acknowledgment of Reviewers

This report has been reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise, in accordance with procedures approved by the Report Review Committee. The purpose of this independent review is to provide candid and critical comments that will assist the institution in making its published report as sound as possible and to ensure that the report meets institutional standards for objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process. We wish to thank the following individuals for their review of this report:

E. Ward Plummer, Louisiana State University,
Paul Kern, The Cohen Group,
Robert H. Latiff, R. Latiff Associates, and
Susan B. Sinnott, University of Florida.

Although the reviewers listed above have provided many constructive comments and suggestions, they were not asked to endorse the views presented at the workshop, nor did they see the final draft of the workshop summary before its release. The review of this workshop summary was overseen by Lyle Schwartz, University of Maryland, who was responsible for making certain that an independent examination of this workshop summary was carried out in accordance with institutional procedures and that all review comments were carefully considered. Responsibility for the final content of this summary rests entirely with the author and the institution.

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APPENDIXES

1

Overview

The Standing Committee on Defense Materials Manufacturing and Infrastructure (DMMI) convened a workshop on August 6-7, 2014, to discuss issues related to applying materials state awareness to condition-based maintenance and system life cycle management. The DMMI Standing Committee is organized under the auspices of the National Materials and Manufacturing Board of the National Research Council (NRC)[1] and with the sponsorship of Reliance 21, a U.S. Department of Defense (DOD) group of professionals that was established in the DOD science and technology (S&T) community to increase awareness of DOD S&T activities and to increase coordination among DOD services, components, and agencies.

The workshop was conducted as a convening activity. In accordance with NRC procedures for a convening activity, all views expressed at the meeting are solely those of the individual participants who made them. No consensus findings, conclusions, or recommendations were developed at the workshop or as an outcome of the workshop, and no statements reported here are attributable to the DMMI Standing Committee, the NRC, or any other corporate entity. This report is a summary of workshop events prepared by the workshop rapporteur, and any statements or views summarized in the report reflect the rapporteur's understand-

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[1] Effective July 1, 2015, the institution is called the National Academies of Sciences, Engineering, and Medicine. References in this report to the National Research Council (NRC) are used in a historical context to refer to activities before July 1.

ing of the statements and views expressed by knowledgeable individual participants at the workshop, not a consensus view.

To organize the Workshop on Applying Materials State Awareness, the DMMI Standing Committee first selected a workshop planning group to identify workshop topics and agenda items, speakers to be invited to give presentations, and invited guests. The workshop planning group consulted with Reliance 21 and members of the defense materials and manufacturing communities to develop and organize the workshop. The workshop was held at the Keck Center of the National Academies of Sciences, Engineering, and Medicine, 500 Fifth Street NW, Washington, D.C., and was open to the public. Approximately 40 participants, including speakers, members of the DMMI Standing Committee, representatives of Reliance 21, other invited guests, and members of the public participated in the 2-day workshop.

The workshop was structured around three focal topics: (1) advances in metrology and experimental methods, (2) advances in physics-based models for assessment, and (3) advances in databases and diagnostic technologies. Appendix C lists the presentations in the workshop agenda under each of these topics. In addition to short questions and discussion sessions after individual presentations, the agenda included longer discussion sessions at the end of the first day and at the end of the workshop. Along with the three focal topics and the agenda shown in Appendix C, the announcement and invitation for the workshop offered the following list of areas that the planning group suggested as relevant for presenters and discussants:

- Three-dimensional characterization at multiscales—what is the next step in tomography?
- New methods for the inversion of nondestructive evaluation measurements to provide information on material state and damage state
- Imaging, from electron wave functions through atoms and nanostructures to mesoscale granular structures and macro engineering scale structures
- Metrology: property measurement techniques for advanced materials
- Materials qualification
- Modeling to predict material state evolution
- Condition-based maintenance
- New science in nondestructive evaluation of complex microstructures

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Themes

This workshop was in some respects a follow-up to a 2007 National Research Council Workshop on Materials State Awareness (MSA). Whereas the first workshop dealt with themes such as how to define MSA and what its future prospects might be (see the introductory presentation, by James Malas, of highlights from the 2007 workshop), this second workshop focused on current and emerging MSA applications across a number of aspects of system life cycle management. Condition-based maintenance (CBM) recurred as a major topic throughout the workshop, and in many ways CBM provided a defining context for the perspectives on MSA offered by both presenters and audience participants. But other aspects of system life cycle management were also addressed, including system life prediction (SLP), system life extension, structural health monitoring (SHM), qualifying a new material for an application or qualifying a known material for a new application (qualification), and life cycle cost management. For purposes of this summary, "MSA applications" includes all of these aspects of system life cycle management.

The workshop's 14 presentations and 2 crosscutting discussion sessions covered a wealth of technical detail. To help readers trace connections among all of these details, the rapporteur has identified four themes that ran through multiple presentations and came up repeatedly during discussions. These themes are offered solely to aid comprehension and do not represent findings or conclusions of the workshop participants as a group.

THEME 1—WHAT IS MATERIALS STATE AWARENESS? WHAT SHOULD IT BE?

In his presentation of highlights from the 2007 MSA workshop, Dr. Malas said the participants in that workshop debated how to define and delineate MSA but did not arrive at a comprehensive definition. He expressed approval of the characterization included in the invitation-agenda document for this workshop:

> Materials state awareness seeks to quantify the current state of a material and/or damage [to a material or structure] with statistical metrics of accuracy located in individual systems, structures, or components and is the heart of condition-based management strategies. In principle, such quantitative evaluation should be based on knowledge of the initial state, damage or failure process, operational environment, and nondestructive evaluation (NDE) assessment of state. However, most frequently the initial state is not known and the assessment must be done from an unknown reference state.

Whereas the 2007 workshop focused on MSA for bulk materials such as metal alloys, this workshop expanded the scope of MSA to include composites, interfaces and complex assemblies, and hierarchically structured materials. Robert E. Schafrik encouraged the participants to think beyond MSA of monolithic structures to consider how it could be applied to degradation mechanisms at interfaces such as those between coatings and substrates or at material joins.

Another participant said that the degradation information from MSA needs to be related to functional characteristics of the system and its subsystems to provide a practical CBM solution. Mr. Eric Lindgren expressed a similar view, saying that ensuring the integrity of a system is the rationale behind trying to understand material state or the state of the system.

Jan D. Achenbach distinguished between the MSA methodologies for quantitative NDE (QNDE) and SHM. The former, he explained, consists of a toolbox of sensor applications and techniques used for *periodic inspections* of a structure, particularly safety-critical structures such as aircraft, bridges, or nuclear reactor facilities. In SHM, by contrast, the sensors are permanently installed in the structure, and near-real-time prediction of material properties of interest is possible if there are sufficient sensors and if the data from them can be transferred readily to a data processing facility. Other characteristics differentiating QNDE and SHM are listed in Table 3.1 in the summary of Dr. Achenbach's presentation.

Dale L. Ball focused his presentation on applications of integrated computational materials engineering (ICME) and integrated computational structural engineering at the airframe level, particularly in the design phase of an aircraft structures development program. He stressed that what the materials science community does with MSA has direct and important impacts on directions in the structures community. He sees physics-based modeling as a key technology in the set of evolving MSA technologies and capabilities that not only will be applied throughout the operational lives of engineered systems but also will enable higher-fidelity definition of the initial state (post-manufacture) of a materials system.

With respect to what MSA *should be*, the workshop discussion at the end of Day 1 led Michael F. McGrath to frame the question, "If we had perfect MSA, what would we do differently [in applications such as materials specification for design or CBM for legacy systems]?" Following up on this question, the facilitators of the closing discussion on Day 2 asked the participants, "What are the implications for perfected MSA?" The suggestions they received are summarized in Box 3.9. They also asked for participants' views on how CBM and SHM might change as MSA improves over time, and the responses are summarized in Box 3.10.

THEME 2—MSA REQUIRES THE INTERPLAY OF MODELING AND CHARACTERIZATION-DETECTION CAPABILITIES

The presentations by Dr. Philip Withers, Dr. Jan D. Achenbach, Dr. Joannie W. Chin, Dr. Kevin J. Hemker, Dr. D.J. Luscher, and Dr. Susan B. Sinnott each noted the necessity of studying material structure and damage state on multiple spatial scales, particularly for composite materials and components. Each presentation shows how this multiscale problem requires the interplay between modeling methods and techniques to detect and characterize microstructure properties in the material of interest. For instance, Dr. Withers emphasized, using several detailed examples, that the various mechanisms and effects of degradation or damage in a heterogeneous composite structure have to be identified and followed across a range of spatial and temporal scales, using multiple tools, including multiple sensor modalities and their associated imaging-modeling systems.

Dr. Achenbach stressed the need for probabilistic approaches to modeling SLPs from NDE and SHM sensor data. Measurement models are needed, he said, that incorporate probabilistic considerations in arriving at an overall interpretation of sensor readings. His presentation elaborated on how this general point can be applied to probabilistic predictions of fatigue crack growth.

Dr. Chin explained how her team at the National Institute of Standards and Technology incorporated a Total Effective Dosage Model into a reliability-based cumulative damage model for SLP. Exposure data from both outdoor testing and laboratory-based exposure chamber experiments are used as inputs to this model.

Speaking as an experimentalist, Dr. Hemker discussed ways that multiscale modeling for MSA needs experimental input to improve the models themselves. He gave examples related to operative failure mechanisms, three-dimensional structures with salient resolution, and benchmarking of model results at relevant length scales. He sees the kinds of detailed quantitative data coming from an increasing number of laboratories, such as Dr. Withers's, as providing "a tremendous opportunity" to couple microstructure with physics-based models.

Dr. Luscher described how models for properties and behaviors on at least three different scales—the microscale (e.g., single crystals and grain boundaries), mesoscale (e.g., polycrystalline microstructures), and macroscale (the length scale of engineered components and systems)—have to be coupled to successfully simulate how actual materials and components will behave in extreme environments. Abdel E. Bayoumi described how the Smart Predictive System his team has been developing incorporates data fusion of inputs from a range of condition indicators into measurement-based models. The final phase of development will involve iterated correlation and comparison between results from the measurement-based models and predictions from physics-based models that incorporate algorithms based on theories of materials behavior.

Dr. Sinnott's presentation focused on the smallest spatial scales in this hierarchy, where computational methods are used to model the electronic structure and atomic-scale properties and behavior of materials. Among her examples was a collaboration with two experimentalists to simulate the behavior of the intermetallic phases at the interface of platinum contacts with thin-film piezoelectric components of microelectromechanical systems. A second example was modeling the defect formation energies in a nickel-based superalloy, where confirmation of the computational results with experimental data was critical. The question period after her presentation included several enlightening discussions with workshop participants on the interaction of atomic-scale models with the models used to capture properties and behaviors at larger scales and on the interplay between these multilevel models and experimental systems.

THEME 3—FUTURE VISIONS FOR MSA, CBM, SLP, AND OTHER ASPECTS OF SYSTEM LIFE CYCLE MANAGEMENT

The plural "visions" in this theme refers to the plurality of long-term views expressed by various workshop participants. These views overlap but also diverge in some respects.

- Dr. Malas viewed MSA as becoming a critical input to a number of Air Force and Department of Defense programs for system life management, but he also said that much work remains to be done and that MSA implementation will have to be tailored to the application. He asked the participants, "Do we need a national initiative in Integrated NDE for Life Management of Advanced Materials?"
- Dr. Achenbach foresaw computational mechanics and multiscale modeling, supplemented with experimental information (see Theme 2), being

used in the future to provide a computational link from microstructure to material properties at the macrostructural level. These models, he suggested, together with signals from diagnostic embedded sensors, will provide ways to monitor the evolution of damage and enable what he called *intelligent system health monitoring*. Near the close of his presentation, he discussed the elements of his vision for a "structural health monitoring grand plan."

- Dr. Bayoumi contrasted CBM with corrective maintenance, which is reactive and event driven, and with preventive maintenance approaches that are time-based (hours of operation) or usage-based (duration and duty-cycle conditions of use). CBM is an approach to proactive maintenance based on one or more condition indicators, and he sees it as part of a paradigm shift from reactive maintenance to a holistic, systems-engineering approach that combines historical and logistics (current use) data on components and subsystems with onboard smart sensing and integration of data from electronics and avionics systems to optimize system operations. Furthermore, this systems engineering approach can be carried forward from maintenance of existing operational systems to optimizing the design and manufacture of new components and systems.
- Dashiell Kolbe described the holistic view of CBM (or Integrated Vehicle Health Management) that his company, an original equipment manufacturer of aircraft, uses. The aim is to provide aircraft customers with a "total solution" incorporating the entire chain, from health monitoring data inputs to decision support and user action.

THEME 4—CHALLENGES AND OPPORTUNITIES FOR MSA AND ITS APPLICATIONS IN SYSTEM LIFE CYCLE MANAGEMENT

Mr. Lindgren contrasted the relative maturity of modeling for bulk metals in propulsion-system materials with the status of modeling for composite materials, where he does not yet see a unifying theory of failure progression from an initiating event emerging, despite a great deal of past and ongoing work. He illustrated the difficulties for MSA of complex fabrications with the example of corrosion, noting that there is still no way to predict the time course of corrosion in an assembled complex aircraft system. Similarly, Haydn N.G. Wadley cautioned that, as high-strength material systems become more heterogeneous, the challenge to metrology for adequate MSA increases.

- Dr. Withers ended his presentation on correlative tomography by listing both the promising possibilities for this MSA methodology and several technical challenges that still need to be addressed.

- Dr. Achenbach expects that SHM will have to justify its existence by showing a favorable cost-benefit profile built on factors such as reduced maintenance with increased safety, advantages in affordability and maintainability, a near-zero rate of false alarms, and reduced design margins that do not compromise performance and safety goals.
- Service life prediction (SLP) is difficult, according to Dr. Chin, because remaining service life is not a fundamental material property; it is measured with respect to a minimum acceptable value for one or more critical performance properties. The SLP challenge is to relate the performance properties of interest to the fundamental material properties that govern them.
- Dr. Sinnott described how multicomponent microscale systems can be modeled with “next generation” energy potentials, but she also noted technical/tactical limitations to more widespread use of these atomic-scale computational approaches. She concluded her presentation with a list of four “big-picture” challenges for computational methods at this small end of the scale and suggested directions for addressing the challenges.
- Dr. Kolbe described the real-world challenges for an aircraft manufacturer in applying system health management technology to practical CBM and system life extension decisions. But he also stressed that many components and subsystems on modern commercial and military aircraft would be high-value areas for applying CBM and system health management approaches.
- Dr. Ball described the vision for ICME as developing both computational tools and experimental tools, then integrating these tools with information technologies, manufacturing-process simulations, and computer-based component design systems to develop and deliver optimized materials and manufacturing processes and to provide improved product performance at reduced time and cost.
- Prasun K. Majumdar addressed the challenges of SLP for composites again, going into even greater detail. He said that research on predicting the life of composites has been a moving target because the problems are more complex than for homogenous materials. His presentation brought out the complex interrelationships between the scale hierarchy for composite materials and the evolving material state as it affects service life.
- James A. Warren highlighted opportunities for MSA technologies stemming from the Materials Genome Initiative (MGI) and its goal of facilitating access to materials data. But he also raised “foundational issues” that he believes must be addressed if the full promise of the MGI is to be realized.
- Stephen Freiman picked up on the theme of uncertainty in MSA modeling, which Dr. Achenbach, Dr. Luscher, and Dr. Hemker addressed earlier in

the workshop. He illustrated how more sophisticated statistical approaches to the fundamental issues in quantifying uncertainty in specimen measurement data and in models for mechanical reliability can provide more realistic quantification of the uncertainties in service life estimates.

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Presentations and Discussions

The order in which workshop presentations are summarized differs somewhat from the agenda order of presentations, to bring together those presentations that were more closely related to each of the four themes extracted by the rapporteur as important messages from this workshop. Please see Appendix C for the order in which speakers presented at the workshop. The full names and affiliations of workshop participants are noted at the first mention of a particular participant. For a list of all presenters and other workshop participants who provided information on the daily sign-up sheets, see Appendix B. Appendix D lists all of the acronyms used in the summary.

Discussions that immediately followed a presentation and were focused on it are summarized with the presentation. The special discussion sessions held at the end of the first day and at the end of the workshop are summarized together after all of the presentations, as they focused on crosscutting topics and issues.

CONTEXT FOR THIS WORKSHOP: THE 2007 WORKSHOP ON MATERIALS STATE AWARENESS

The DOD/NRC Materials State Awareness Collaboration

James Malas, Associate Director, Manufacturing and Systems Support, Universal Technology Corporation

Dr. Malas opened his review of highlights from the 2007 National Research Council (NRC) Workshop on Materials State Awareness by noting that the U.S. Department of Defense (DOD) materials community and the NRC's National Materials Advisory Board (recently renamed the National Materials and Manufacturing Board) have been collaborating for many decades on both studies and workshops consistent with enhancing the mission of DOD's Project Reliance. The 2007 workshop, which explored the prospects for materials state awareness (MSA) as a "promising contributor to managing the life of defense assets,"[1] was part of this long-running collaboration, he said, and this collaboration continues with the present workshop.

After describing how the first workshop was planned, Dr. Malas summarized key points made by the presenters during the introduction and five sessions of that workshop. His summary emphasized the following themes and points:

- [System] failures begin at the material level. . . . Advanced materials are increasingly complex, requiring new materials science understanding to assess [their] behavior. . . . Life management of aircraft, turbine engines, and space systems is expensive and time-consuming. . . . The future paradigm for maintaining USAF [U.S. Air Force] systems is condition-based maintenance (CBM), [whose] successful implementation hinges on MSA (from the introductory presentation by Kumar Jata, U.S. Air Force Research Laboratory [AFRL]).
- Then-current sensor technologies were incapable of detecting the key properties, damage states, and conditions necessary for nondestructive evaluation (NDE) to support MSA. Sensor-related costs and sensor reliability in severe environments were also roadblocks (from the Session 1 presentations on "Key Issues for MSA").
- Another major roadblock to MSA implementation was inadequate understanding of the primary material degradation modes for a component in

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[1] James Malas, Universal Technology Corporation, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 2.

the application environment (from Session 1 presentations on "Key Issues for MSA").

- Although the first workshop did not arrive at one comprehensive definition of MSA, the presentations and discussions implied that it includes knowledge of the initial state (of a material/component), the damage or failure process, and the operational environment, as well as the NDE assessment of current state. Beyond the use of NDE for damage detection, MSA should also include nondestructive characterization of material structure and properties (from Session 2 presentations on "What is MSA?").
- Selecting an effective MSA implementation strategy requires a systems approach with careful consideration of design for inspectability, design for detectability, and material condition assessment (from Dr. Malas's summation of details from eight presentations in Session 3 on "What Should We Sense and How?").
- Variability in components, structures, and interfaces, as well as variability in operational history and environments of use, makes diagnosis of material state extremely challenging (from Dr. Malas's summation of Session 4 on "MSA Application Issues").
- For MSA to support CBM, the primary advance has to be in new approaches and capabilities in NDE for MSA (from Dr. Malas's summation of Session 5 on "What is the Future of MSA?").

Dr. Malas concluded with some observations of his own on the importance of MSA and this second MSA workshop. He views MSA as a critical input to a number of DOD and U.S. Air Force programs on system life management such as the Aircraft Structural Integrity Program, the Propulsion System Integrity Program, integrated computational materials engineering (ICME), Digital Twin and Digital Thread, and High Velocity Maintenance, as well as other major initiatives. However, MSA implementation will have to be tailored to the application, Dr. Malas said, and there is still a lot of work to be done. The terminology can be difficult, he noted; for example, he distinguishes between MSA, which aims to characterize the material state, and structural health monitoring (SHM), which uses embedded sensors to detect specific features such as a vibration. Dr. Malas approved of the definition of MSA included in the workshop agenda. He foresees this work requiring a long-term initiative, and he asked the participants, "Do we need a national initiative in Integrated NDE for Life Management of Advanced Materials?"

Questions and Discussion

Robert E. Schafrik (retired, GE Aircraft Engines) commented that a gap in the 2007 workshop was its lack of attention to degradation mechanisms at interfaces, including those between coatings and substrates and at material joins. He suggested that participants in this workshop think beyond the MSA of monolithic structures.

Kevin Curtis (General Dynamics), who explained that his company works with DOD and the other services on implementation of remote monitoring and Condition Based Maintenance Plus Prognotics (CBM+) applications, said that simply going to a customer with data on material state degradation is not seen as offering a solution. He suggested that degradation information from MSA needs to be related to functional characteristics of systems and functional subsystems (e.g., fuselage, landing gear, or engines of an aircraft) that ensure the integrity of the asset and its capacity to continue to function, to provide a "practical solution" for the user. Doing that, he continued, is necessary for CBM+ as defined by the Office of the Secretary of Defense.

Michael F. McGrath (McGrath Analytic, LLC, *Workshop Chair*) said that, based on Dr. Malas's presentation, the 2007 workshop, which predated the current interest in ICME and related computational approaches, seems to have emphasized NDE and sensing technology. He asked if there had been much discussion of physics-based modeling and whether that would change the perspective on directions for MSA. Dr. Malas replied that the 2007 workshop did discuss physics-based modeling, but participants did not want MSA to be defined by that, although it certainly informed the MSA strategies they discussed. The emphasis on actually sensing and evaluating material state, in his view, reflected how little was known [through the models] and what could be learned by examining actual materials in use.

Dr. Malas agreed with the points that Dr. Schafrik and Mr. Curtis made about expanding MSA to more complex materials fabrications and applying MSA to functional characteristics of importance to the system users. Nonetheless, an important concern of the 2007 workshop, he continued, was to raise and address questions of knowing what was important to characterize [in the state of a material] before one could get into a practical application of MSA.

With respect to physics-based models, Mr. Eric Lindgren (AFRL) said that important questions are what can be modeled and what can be accurately predicted and used. The historical focus on propulsion materials, particularly metals, reflects the practical knowledge acquired during the past 30-40 years of how these materials degrade and of their fracture mechanics, which, he noted, enables predictions to be made. He contrasted this application of modeling with the situation of organic composite materials, where, despite a lot of past and ongoing work on prediction, he does not see a unifying theory of failure progression in a composite as the result of some initiating event. He went on to describe the complexity of factors whose influence needs to be unraveled, with techniques such as multiscale, multivariable analyses and sensitivity analyses, to determine what affects the integrity of a system. Ensuring the integrity of a system, he said, is the rationale behind trying to understand material state or the state of the system; the question is what can be predicted and what can only be known in a reactive mode. He illustrated the difficulty for complex material fabrications with the example of corrosion, saying that there is still no way to predict the time-based evolution of corrosion in an assembled, complex aircraft system with its protective coatings and inhibitors and taking into account the maintenance practices for that system.

Jan D. Achenbach (Northwestern University) said that modeling of the results from [NDE] sensing is both difficult and important. Measurement models are needed, he said, that include probabilistic considerations in arriving at an overall interpretation of the sensor readings. "The sensing process is not deterministic; there is a probability of detection, and the sensors do not always operate the same way."

Haydn N.G. Wadley (University of Virginia) offered the following argument in favor of the need for increased MSA capabilities: As material scientists create stronger and stronger materials, the size of strength-degrading flaws in the material decreases. Their detection becomes an increasing challenge to the measurement science described by Dr. Achenbach. And as high-strength materials systems become more heterogeneous—for example, with complex coating systems on a composite material substrate—the challenge to metrology for sufficient MSA increases. Some complex materials have been developed that, although they offered substantial functional benefits, were never applied because their safety with respect to potential degradation and failure could not be demonstrated with the NDE capabilities then available. Dr. Wadley cited silicon nitride ball bearings as an example. In his view, the lag in measurement science will be an increasing impediment to the introduction of higher-performance materials into DOD systems.

Kevin J. Hemker (Johns Hopkins University) recalled a workshop he and Dr. Wadley led for the Defense Advanced Research Projects Agency (DARPA) entitled "Future Engines." When he asked the participants (U.S. jet engine manufacturers) whether it would be of value to have DARPA develop a new generation of microsensors for them to use, the immediate response was "no" because false positives posed a real problem for them. In his view, the problem to which the manufacturers were responding is not one of having too many sensors but of needing higher-fidelity sensors that provide highly reliable signals. This comment led to further discussion of whether high sensor loading was more appropriate for the design-development stages, as opposed to SHM during operational use. One participant suggested that many newer engines and other aircraft subsystems already have embedded sensors, but the issue is fusion of the real-time sensor data with sufficiently reliable historical failure data to make useful decisions about materials degradation and useful subsystem life. Other participants commented on additional types of data needed to provide benchmarks against which quantitative NDE (QNDE) data could be compared. Summarizing her view of many of the comments about model limitations, sensor capabilities, and interpretation of sensor data, a participant suggested that together these issues represent a data fusion problem. She suggested that, given adequate fusion of data from many of these approaches, an “85 percent solution” from each contributing approach would provide useful knowledge about the material state of a component.

E. Ward Plummer (Louisiana State University) noted that, based on aircraft crashes reported in the news, environmental events (such as lightning or other extreme weather events) are often the critical events in a system failure. He asked whether sensor-based monitoring for those kinds of nonstandard external events is done as part of MSA, as the types of material state monitoring that had been discussed so far seemed focused on “standard operating conditions.” Dr. Malas responded that MSA includes monitoring for environmental effects such as corrosion and weathering, but the application focus has been on sensing for system life management in operational environments, rather than on detecting single-event conditions that lead to immediate system failure.

Dr. McGrath added that, for DOD systems, battle damage represents another category of critical external events that cause system failure, like the “mother nature” events that Dr. Plummer had mentioned. Referring to one of Dr. Malas’s final observations about this workshop, he agreed that the workshop represents an exciting opportunity to pull together the key aspects of MSA and many other considerations to fully develop an integrated capability for system life management. Dr. McGrath also suggested that, in addition to reviewing the advances in MSA as narrowly defined, there is now growing interest in larger application problems.

THE STATE OF THE ART IN APPLIED MSA

Three of the presentations on Day 1 dealt primarily with state-of-the-art applications of an approach to MSA. Although these presentations by Dr. Withers, Dr. Achenbach, and Dr. Chin also touched on other workshop themes, they provide a good starting point for what is currently feasible in MSA applications.

Correlative Three-Dimensional Imaging Across Time and Length Scales

Philip J. Withers, Professor of Materials Science,
University of Manchester, United Kingdom

Materials design, Dr. Withers began, has required bringing together four areas that traditionally have been studied in separate laboratories: microstructure (typically in a microscopy suite), materials chemistry in a chemistry lab, performance and degradation in a materials testing lab, and processing in a processing workshop. Work in these four domains has been poorly connected, he said, and a key objective of his work has been to bring all four together in a more closely coordinated approach. To design better high-performance materials, he advocates identifying the critical time and length scales and spatially correlating an array of structural information, obtained with multiple imaging tools, ranging across these scales. For example, optical microscopy shows material features at scales from 10^{-1} meters down to a micrometer (10^{-6} meters); x-ray computed tomography (CT) provides information about features at scales from a meter down to 100 nanometers (10^{-8} meters); scanning electron microscopy (SEM) displays features at scales from a millimeter (10^{-3} meters) to a nanometer (10^{-9} meters); and scanning transmission electron microscopy (STEM) provides information about material features whose scales range from hundreds of nanometers (10^{-7} meters) down to individual atoms (angstroms, 10^{-10} meters).

To illustrate his point, Dr. Withers described how impact damage to a composite wing must be studied at various scales, using several tools, to understand how barely visible impact damage has affected the material structure and the temporal trajectory of the consequent degradation in material properties under service conditions. CT and imaging quantification tools allow one to "digitally unpick" the laminated layers one by one and to make virtual cross sections across the layers, so that the damage to individual fibers, laminate structure, and interlaminar interfaces can be examined. Because the damage analysis is performed nondestructively, the damaged structure can be subjected to subsequent stressing conditions, and one can follow how the damage site responds to those stresses. More generally, the various mechanisms and effects of degradation, or damage, in a heterogeneous composite structure need to be identified and followed across the time and length scales, using a combination of tools (Figure 3.1).

Dr. Withers described, with illustrations, how his team and collaborators have used x-ray imaging at multiple length scales, from large-scale x-ray images of 1-2 m components and structures down to micron-scale and nanoscale resolution images of structural features (micron and 50 nm x-ray imaging). To examine chemical structure, they are using three-dimensional (3D) x-ray detectors that identify elemental composition from the wavelengths of the diffracted x rays (Egan et al., 2013). They also combine 50 nm x-ray CT imaging with 3D SEM and electron backscatter diffraction analysis (EBSD) to examine crystalline structure at the micron and nanometer scales. STEM is used for ultrahigh resolution imaging and chemistry.

Next, Dr. Withers showed how his team follows material structure changes and degradation across time scales, using an example of tracing the growth of pitting corrosion in a stainless steel wire immersed in a brine (sodium chloride) solution. They used time-lapse macroscale x-ray CT to identify regions of interest for microscale x-ray CT; for example, they identified the slower and faster growing pits. Subsequently, microscale CT revealed the detailed morphology within a single corrosion pit, including the network of intergranular corrosion extending beneath

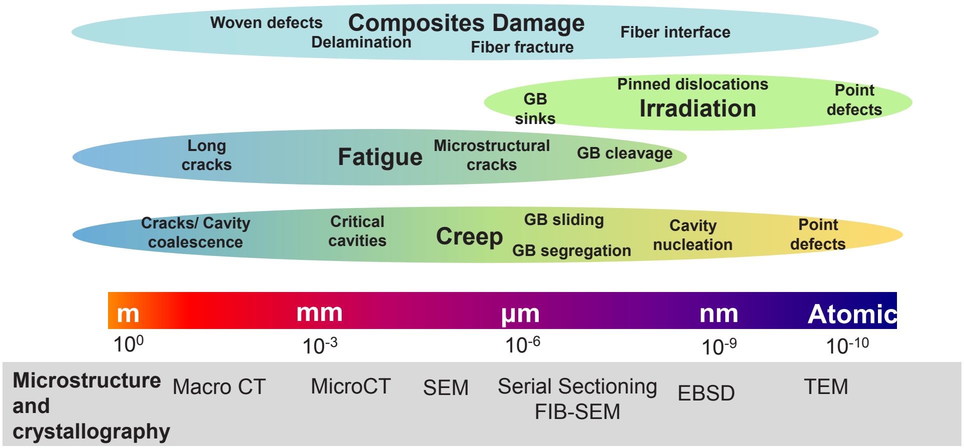

FIGURE 3.1 Degradation mechanisms in a heterogeneous composite material occur at different length scales, from a meter down to 10^{-10} meters. Similarly, degradation of metals by irradiation damage, fatigue, or creep has a variety of characteristic length scales. NOTE: EBSD = electron backscatter diffraction analysis; FIB-SEM = focused ion beam scanning electron microscopy; GB = grain boundary; TEM = transmission electron microscopy. SOURCE: Philip J. Withers, University of Manchester, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 7.

the much smaller opening at the surface of the wire. By carefully registering the sample in the SEM with the 3D subsurface images of the pit location, they were able to excavate the region of interest using a focused ion beam to obtain higher resolution (10 nm) serial section tomography within the dual beam focused ion beam scanning electron microscopy (FIB-SEM) for the same pit, which enabled them to characterize the shape, extent, and direction of intergranular corrosion cracks beneath the particular pit of interest. EBSD was used to analyze the crystallography local to the intergranular corrosion cracks, and the degree of structural disorder associated with different boundary conditions appeared related to the degree of corrosion at that front. STEM imagery of selected grain boundaries was then used to characterize the materials chemistry at the nanoscale (Burnett et al., 2014).[2]

Dr. Withers emphasized that, by correlating the electron microscopy analyses of grain boundaries and degradation phenomena with the x-ray CT imagery at multiple scales, one can assess how typical the microscopy results are and what types of larger-scale features (e.g., faster or slower growing pits) they characterize. In short, the lower-resolution (larger scale) information provides context for

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[2] BP, “ICAM focuses in on corrosion—New tools, new insights,” video, published October 22, 2013, https://www.youtube.com/watch?v=P5oUpiVvZVY.

interpreting the higher-resolution (finer scale) information. He explained that, whereas destructive sectioning of a sample to perform high-resolution analyses gives information about the material state just at the time of sectioning, the correlative tomography approach can be used to follow the progression of degradation and damage processes in the same sample of material over time. Examples that Dr. Withers presented in detail included progressive fatigue damage over a number of fatigue cycles in woven composites (Yu et al., 2014) and fatigue crack growth over time in a titanium–silicon carbide metal matrix composite (Withers et al., 2012).

In his summation, Dr. Withers noted the following as promising possibilities for correlative tomography:

- A huge variety of tools are available that can provide complementary insights.
- Together, these tools can bridge all of the key scales governing specific material behaviors.
- Time-dependent 3D data can be used to study
  —The fastest, smallest, or most potent defects/configurations,
  —The most representative microstructures, and
  —The least-damage defects and configurations.
- Selected areas of a sample for which low-resolution tools provide context can then be studied at high resolution.

He summarized the benefits of correlative tomography as (1) providing multiscale 3D information, (2) targeting and retaining the spatial context of critical regions of interest, and (3) bringing multiple signals (instrument modalities) to bear on the same region of interest. He added that the microscopy technology companies appear highly interested in participating in the development of the software algorithms needed to correlate imagery and other data across the different length scales and from the different instruments, to solve the registration challenge (spatial alignment and juxtaposition of data from multiple sources). Nevertheless, according to Dr. Withers, there are still technical challenges facing correlative tomography:

- No technique is currently available to excise regions identified by x-ray CT that are millimeters below the surface, for subsequent FIB-SEM serial sectioning.
- No software is currently available to manage the correlative workflow across instruments.
- No software is currently available that can co-register and co-visualize all of the data from different modalities and length scales.

Dr. Withers described some of the new instrument development and programming activities that his team at the University of Manchester and his industry collaborators are currently pursuing to meet these challenges. One of these involves use of plasma dual beam microscopy to perform serial sectioning at SEM resolution at depths greater than 100 µm and volumes up to many hundreds of microns on an edge (i.e., volumes 50 times greater than with a focused ion beam).

Questions and Discussion

In response to a question on whether the software programming is done in part by his University of Manchester team or entirely by the equipment manufacturers, Dr. Withers said that most of the software for deriving imagery from the signal used by a particular instrument is provided by the instrument vendors. His team has done some software development to analyze the 3D images. Image analysis and image reconstruction algorithms are shared with others through a U.K.-based network, the Collaborative Computational Project for Imaging.[3]

Mr. Lindgren asked if Dr. Withers had worked with or was familiar with the DREAM.3D software architecture.[4] Dr. Withers said he was familiar with it and maintains a good conversation with its developers. This software, he said, is particularly well suited to representing grain structure and grain orientation and provides results that can be input into a finite element analysis (FEA) model. He added that his team was collaborating with others to develop tools using diffraction contrast to measure grain structures and orientations such that the data would be suitable for input into DREAM.3D. Normally this would require synchrotron-based analytical methods. Mr. Lindgren and Dr. Withers discussed the capability in DREAM.3D to track workflow on the data sets being used within the architecture, and they agreed that the open-access, nonproprietary nature of the architecture is advantageous. Dr. Withers expressed interest in exploring a collaborative effort between his team and those who are working with DREAM.3D.

Dr. Hemker (Johns Hopkins University) asked about the use of lasers for sectioning below the surface of a region of interest and about work by Ji-Cheng Zhao and David Cahill to extract local information on mechanical properties. Dr. Withers replied that he was very interested in the laser work Dr. Hemker had mentioned and asked for contact information, to further discuss aspects with which he was unfamiliar. He described work in progress that compares some of the laser techniques, particularly those being developed by Pollock and colleagues (Echlin et al., 2014) at Santa Barbara and new plasma beam methods. At the present time, he added, the advantages and disadvantages of each of these methods were not clear.

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[3] The website for this network is http://www.ccpi.ac.uk, accessed October 2014.

[4] For information on the DREAM.3D architecture, see Groeber and Jackson (2014).

Quantitative Nondestructive Evaluation and Structural Health Monitoring for State Awareness of Materials and Structures

Jan D. Achenbach, Department of Mechanical Engineering, Northwestern University

Dr. Achenbach's presentation focused on QNDE and SHM in aircraft, reflecting his long tenure in working with the Federal Aviation Administration (FAA). QNDE, he explained, consists of a toolbox of sensor applications and techniques that are used for periodic inspections of a structure, particularly safety-critical structures, including aircraft, bridges, and nuclear reactor facilities. In SHM, the sensors are permanently installed in the structure. Prognostication (prediction of material state properties of interest) is possible in SHM, Dr. Achenbach continued, if there are sufficient sensors and the data are transferred directly to a data processing facility—which for aircraft requires wireless transfer of the sensor data. Table 3.1 is a contrast of characteristics of NDE versus SHM that he presented toward the end of his talk.

The category of NDE methods on which Dr. Achenbach focused in this presentation contains methods used for the evaluation of the fatigue of metal structures, but he noted that NDE for stress corrosion cracking and delamination are important areas of research as well. He defined the following four stages of metal structure fatigue:

- *Stage I:* pre-crack fatigue damage (extremely difficult to detect with current NDE methods in the field)
- *Stage II:* macrocrack formation (easier to detect with current NDE methods in the field)
- *Stage III:* macrocrack growth (can be predicted using an evolution law)
- *Stage IV:* optimization of inspection schedule

TABLE 3.1 Comparison of Nondestructive Evaluation with Structural Health Monitoring

Nondestructive Evaluation	Structural Health Monitoring
Noncontact probes	Built-in sensors
Human interpretation	Automation
Labor dependent (intensive)	Minimal labor
Local control	Remote or local control
Universal system	Structure-dependent

SOURCE: Jan D. Achenbach, Northwestern University, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 27.

What can be detected and quantified in stages I through III, plus probabilistic considerations, is important, Dr. Achenbach noted, for the inspection optimization in stage IV.

The need for probabilistic considerations in predictions of fatigue crack growth, he said, arises from the many sources of uncertainty in crack formation and growth, in inspection scheduling, and in crack detection and sizing as a result of inspection. To illustrate this overarching point, he described a probabilistic analysis of fatigue crack growth originating at the rivets in a lap joint between two sections of the aluminum fuselage skin of an aircraft (Cohen and Achenbach, 2013). A fatigue failure of this type, he explained, was responsible for the catastrophic loss of the upper fuselage skin from the first class cabin of Aloha Airlines Flight 243 on April 28, 1988.

To begin his exposition on probabilistic approaches to monitoring for fatigue-related cracks, Dr. Achenbach discussed mathematical models for evolution of fatigue-related damage. He began with Paris's law, a common heuristic model for fatigue crack growth (Box 3.1),[5] applied to the classic experimental data by Virkler and colleagues (1979) on crack growth during fatigue cycling in 68 samples of an aluminum alloy used in aircraft (2024-T3 aluminum). Paris's law expresses the change in the crack length, A, as a function of the fatigue cycles, N, and the range of the stress intensity factor (the difference between the stress intensity factor at minimum and maximum loading during one fatigue cycle); ΔK, A, and m in the accompanying equation for Paris's law (see Box 3.1) are constants for the material.

Dr. Achenbach noted that even a plot of Virkler's original data for the 68 samples shows that A and m need to be viewed as stochastic parameters, but for his example in this presentation he used values of A and m for one of the "average" samples from the Virkler set.

He acknowledged that more sophisticated approaches to modeling the evolution of structural damage such as fatigue cracking are emerging; for example, he foresees computational mechanics and multiscale modeling, supplemented with experimental information, being used in the future to provide a computational link from microstructure to material properties at the macrostructural level, such as strength, hardness, toughness, cracking, and perhaps even corrosion. These models, together with signals from diagnostic embedded sensors, will, he suggested, also provide a way to monitor the evolution of damage for "system-state awareness," which is sometimes called *intelligent* system health monitoring. Even so, in his view, simple damage-evolution equations like Paris's law, verified by this multiscale

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[5] Dr. Achenbach noted that some recent research suggests that Paris's law and its material-specific constants A and m may be derivable from the fundamental physics of material properties. If so, it could be viewed as a simplified approximation to a more rigorous physical model for fatigue crack growth, rather than as simply a heuristic model.

BOX 3.1
Paris's Law

$$\frac{da}{dN} = A\left(\Delta K\right)^{m}$$

modeling grounded in computational mechanics, will still be highly valuable for use in testing, inspecting (NDE), and monitoring (SHM) critical structures.

Next, Dr. Achenbach summarized the mathematical approaches he has used (Kulkarni and Achenbach, 2008) to represent the evolution of the probability distribution of fatigue cracks as a function of the number of fatigue-stress cycles; the probability that a crack of a certain size exists after a given number of fatigue-stress cycles; the probability of no detection of the crack during inspection, assuming an inspection or monitoring method with a known probability of detecting a crack of that size; and the probability that a crack exists that is near to causing structural failure, given one of these inspection/monitoring methods.

Dr. Achenbach then presented an information flow schematic (Figure 3.2) for inclusion of these probabilistic considerations with an SHM system and remediation response (i.e., the capability to repair or replace structural elements found to have a high failure probability within a preset time interval after the SHM signal is diagnosed). He added that Paris's law or some other simplified form of modeling damage evolution from the observed current state could be used to derive the input to the probabilistic prognosis, along the lines of the example he had developed. This flow diagram reflects the following elements of what Dr. Achenbach called a "structural health monitoring grand plan." (His assessment of the difficulty and time frame for achieving each element is shown in square brackets.)

- Permanently installed microsensors [current capability or achievable in near term]
- On demand or continuous condition monitoring in real time with known probability of detection [intermediate level of difficulty/time to achieve]
- Wireless transmission to central station (for mobile or distributed systems) [intermediate level of difficulty/time to achieve]
- Instantaneous interpretation of sensor data [intermediate level of difficulty/time to achieve]
- Detection of unacceptable material damage at critical high-stress locations [current capability or achievable in near term]

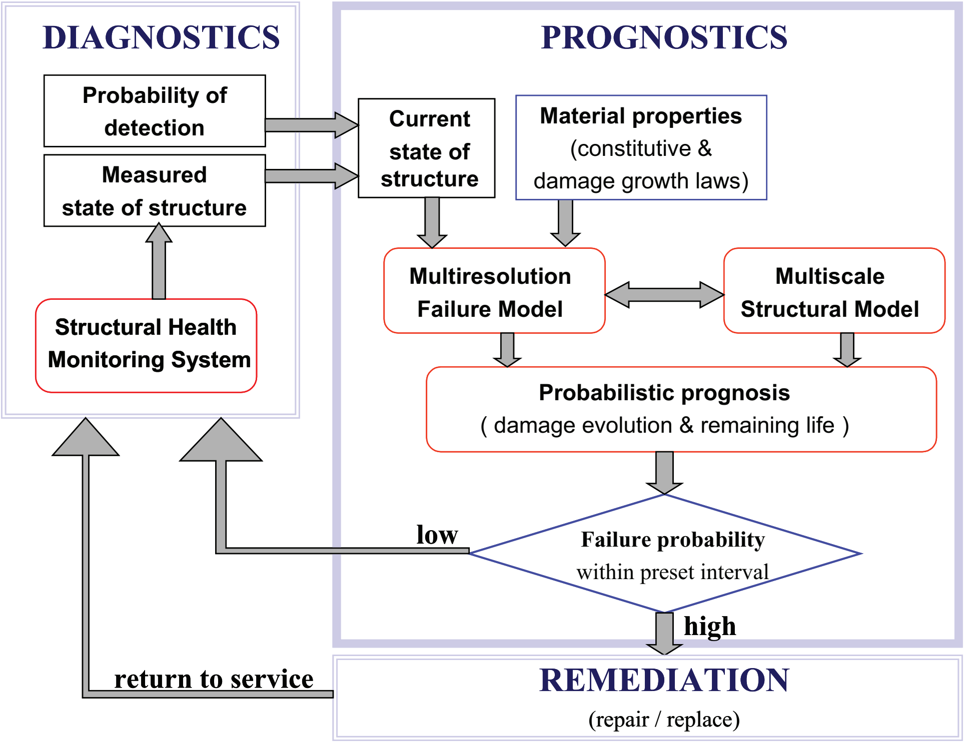

FIGURE 3.2 Schematic information flow for implementing SHM with explicit provision for probability of detection and probabilistic prognosis of damage evolution and remaining life. SOURCE: Jan D. Achenbach, Northwestern University, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 24.

- Monitoring of growth of material damage into critical size [current capability or achievable in near term]
- Growth prediction by a probabilistic procedure [hardest to achieve/long term]
- Adjustments for actual damage state at prescribed intervals [current capability or achievable in near term]
- Probabilistic forecast of damage state for near term and of remaining system lifetime [intermediate level of difficulty/time to achieve]

With respect to achieving his concept for the SHM system itself (as demarcated inside the Diagnostics section in Figure 3.2), Dr. Achenbach listed the following specific technical challenges:

- The *sensors* should be small (microsensors); autonomous (e.g., incorporating their own accelerometer, antenna, battery); cheap, robust, maintainable, and repairable; accurate, with known probability of detection; properly coupled to the structure; suitable for wireless transmission to a central station (for mobile/distributed systems); (probably) densely distributed in the monitored structure; capable of measuring both local and system-level responses; and designed to measure relevant damage parameters.
- *Monitoring* should be directed to detection of cracks and corrosion, multiple damage modes (stress corrosion cracking), and pre-crack fatigue damage; it should account for residual stresses.

He acknowledged that, taken together, these challenges are technically demanding and will take time to meet. Nonetheless, he continued, one can ask why SHM has been so slow in making the transition from research results to practical application. His answer focused on the competition from schedule-based inspections performed at maintenance facilities, which have a number of factors in their favor, including the safety record of aircraft they maintain, accepted prognosis methods, and a large inspection infrastructure already in place. He expects that SHM will have to justify its existence in terms of a favorable cost-benefit profile built on factors such as reduced maintenance, increased safety, affordability/maintainability, near-zero false-alarm rates, and reduced design margins. On the last point, Dr. Achenbach stressed that there could be huge benefits for SHM if it can justify reduced design margins for new generations of aircraft.

In his concluding summation, Dr. Achenbach said that either scheduled inspection or SHM is needed for safety-critical structures; he believes SHM will become the method of choice. A probabilistic approach is essential for all stages of fatigue damage under cyclic loading, he continued, with the probability of detection/nondetection defining the successful use of inspections (Stage IV in his paradigm). Referring to the research he had presented, he said that, for lap-joint structures under fatigue loading, the probability of cracks of unacceptable length has been determined.

The close of the presentation also included a quick overview on current SHM implementation and use of probabilistic approaches to system life management by Boeing and by Airbus. Mr. Lindgren commented that the PROF (Probability of Fracture) software and methodology used by Boeing is in fact an Air Force–developed product that the Air Force uses today for structural integrity and damage tolerance analysis. PROF is not new, he said; in fact, it has been around for many years. The Air Force manages its aircraft systems today using risk management approaches that require the probabilistic assessments of system integrity that Dr. Achenbach had pointed out in the PROF methodology. For Airbus, Dr. Achenbach summarized the four generations in Airbus's current SHM development and application roadmap.

In this stepwise implementation of SHM capabilities, Airbus now has online sensors embedded in in-service aircraft and expects to have fully integrated embedded sensor systems in its in-service aircraft by 2016-2018.

Dr. Achenbach completed his presentation with comments on the use of multifunctional materials. Such smart materials not only are load carrying, he said, but also have the capability to sense defects in materials and structures.

Predicting the Service Lives and Durability of Engineered Materials and Systems

Joannie W. Chin, Acting Director, Engineering Laboratory,
National Institute of Standards and Technology (NIST)

Dr. Chin began with some of the challenges to service life prediction (SLP), then described the programs in NIST's Engineering Laboratory relevant to SLP and MSA in applications for polymers, cement and concrete, and disaster resilience of structures. These programs, she noted, support NIST's mission to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve Americans' quality of life. She stressed that NIST's role is nonregulatory and that it does not actually develop standards documents. Rather, it advances the measurement science and technological foundations of standards, participates in a number of standards-development organizations, and provides reference materials and reference data that support standards.

SLP is difficult, Dr. Chin said, because service life, or remaining life, is not a fundamental material property. A former consensus standard, ASTM E632, defined service life as the "period of time during which critical performance properties exceed minimum acceptable values,"[6] and Figure 3.3 illustrates how service life would be measured with respect to a minimum acceptable value for one critical performance property. However, Dr. Chin said, the critical performance properties of interest are typically not fundamental material properties either. So the SLP challenge is to relate the performance property(ies) of interest to fundamental material properties that govern the performance property.

As other presentations had already stressed, tools are needed to measure properties at the smallest possible scale and over multiple scales, she continued, and one needs not only an understanding of the fundamental properties of the mate-

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[6] ASTM E632-82, *Standard Practice for Developing Accelerated Tests to Aid Prediction of the Service Life of Building Components and Materials,* was withdrawn in 2005 and has not yet been replaced. The standard is available from ASTM for a fee at http://www.astm.org/Standards/E632.htm, accessed September 2014.

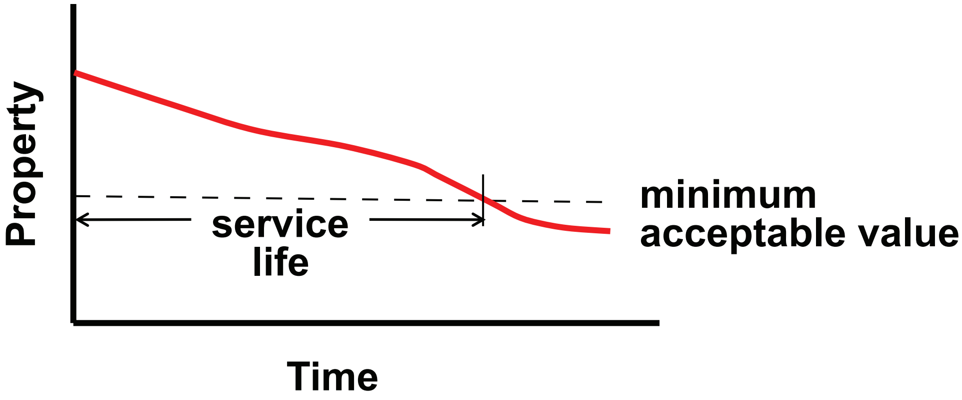

FIGURE 3.3 Predicting service life from a material property that degrades with time. SOURCE: Joannie W. Chin, National Institute of Standards and Technology, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 7.

rial and how they change but also a quantitative characterization of the end-use environment. To illustrate these points, she used the degradation and failure of a typical coating, observable as embrittlement and loss of adhesion on the scale of a centimeter, which can result from photoreactivity and surface chemistry effects that depend on size/distribution properties of the pigment at the microscale (~1 μm) and on pigment dispersion and orientation characteristics with scales around 100 μm, with degradation initiated as pitting at the nanoscale (10-100 nm).

Where NIST's role comes in, according to Dr. Chin, is that the methodologies, metrologies, and models are often lacking to relate the real-time environment to the laboratory data for accelerated exposure of the material to stresses that change the governing properties. For example, the Polymeric Materials Group in the NIST Engineering Laboratory has a primary focus on developing metrologies and methodologies for the characterization—including SLP—of high-performance polymers and composites. She highlighted three critical issues that affect the service life of these polymeric materials:

- Commercial polymeric systems are complex, multiphase, heterogeneous materials.
- Polymeric materials are susceptible to degradation via hydrolysis, photolysis, thermolysis, and combinations of these and other environmental stresses.
- Interfacial phenomena, prominent in polymers and composite materials, can complicate response to degradation stresses.

The traditional approach used by manufacturers of polymeric materials to test the degradation of critical performance properties, and thereby get a measure of service life, is through outdoor exposure in an environment with high ambient levels of sunlight, humidity, and temperature. There are probably hundreds of such sites around the world, Dr. Chin observed, often in exotic tropical settings. The limitations of outdoor exposure testing, she said, include that it takes a long time, is often laborious, and requires waiting for property degradation to occur. In addition, the data are typically highly scattered and difficult to replicate because conditions differ from one test site to another and even differ at the same test site over different exposure periods.

Laboratory-based methods for accelerated exposure, usually incorporating an ultraviolet (UV) light source, elevated temperature, and moisture, have their own problems, said Dr. Chin, and they generally have not given results that correspond with the slower outdoor exposure approach. A decade ago when NIST became interested in this problem, she recounted, the available accelerated-exposure chambers had so many problems that commercial manufacturers of polymers and composites generally felt they had to do outdoor exposure testing anyway. People who tested a number of materials by both methods found not only that there was no good (reproducible) correlation between the results but that materials even ranked in different order in predicted service life, depending on which methodology was used. In short, Dr. Chin said, outdoor weathering was the de facto standard for the industry, but there was no way to simulate that in the laboratory or to obtain reliable results from accelerated-exposure methods. Because outdoor testing results also varied from site to site and over time, standardizing on those results was a moving target.

In the early 1990s, Dr. Chin continued, the coatings industry came to NIST for help in developing a scientifically sound, reproducible methodology for getting quantifiable SLP results, not just rank-orderings of materials. The NIST team began from the insight that defining the question as outdoor exposure versus laboratory exposure made the problem intractable; they asked how the problem of relating field and laboratory exposures had been addressed in other fields where UV exposure is a key environmental factor, including biology, medicine, and agriculture. In those fields, she said, a model for total effective dosage was used, so NIST incorporated the Total Effective Dosage Model (shown in Box 3.2) into a reliability-based cumulative damage model for SLP. The model divides the total UV irradiance, E_0, into the energy absorbed and energy reflected; energy absorbed is divided between the dissipated energy and the energy that goes into damaging the material. The total effective dosage, $D_{total}(t)$, which represents the total amount of energy required to initiate damage to the material, is a fixed quantity for given material, all else being equal. Outdoor exposure testing data and laboratory exposure-chamber data were taken as equally valid input to the model. Temperature, relative humidity, and UV irradiance were monitored in the same way for both outdoor exposures and laboratory exposures and were incorporated into the model. This methodology

BOX 3.2
NIST Total Effective Dosage Model

$$D_{total}(t) = \int_{0}^{t} \int_{\lambda_{\min}}^{\lambda_{\max}} E_o(\lambda,t)\left(1 - e^{-A(\lambda)}\right)\phi(\lambda)\, d\lambda\, dt$$

$D_{total}(t)$ = total effective dosage
$E_o(\lambda,t)$ = spectral UV irradiance from light source
$1\text{-}e^{-A(\lambda)}$ = spectral absorption of specimen
$\phi(\lambda)$ = spectral quantum yield of specimen
$\lambda_{min}, \lambda_{max}$ = minimum and maximum photolytically effective wavelengths

SOURCE: Joannie W. Chin, National Institute of Standards and Technology, presentation to the Workshop on Materials State Awareness, August 6-7, 2014.

was adopted as the basis of an initial consortium on coatings, which ended about 5 years ago, and for two new consortia, one on sealants and the other on polymers used in photovoltaic materials.

To address the problem that the data from commercially available accelerated-exposure chambers were not reproducible or repeatable, Dr. Chin's team developed the NIST SPHERE (Simulated Photodegradation via High Energy Radiant Exposure), a 2 m spherical chamber that integrates UV exposures up to 84,000 W (equivalent to 22 "suns") with 95 percent exposure uniformity and precise control of the temperature and humidity around specimens (Chin et al., 2004). They also developed sample chambers to rigorously control temperature and relative humidity and an instrumentation suite for outdoor exposure testing. Dr. Chin described the parametric studies on model polymers that her team conducted to verify that the accelerated-exposure data obtained with the SPHERE chamber were well correlated with their outdoor exposure data. The SPHERE tests were completed in 3-4 months due to the substantial acceleration in total effective dosage enabled by the chamber; the outdoor exposure tests took about 3 years to complete, with each group of specimens exposed for about a year.

These studies, she said, demonstrated that the SPHERE chamber was a highly effective way to accelerate the effects of outdoor exposure without introducing any unnatural or new degradation mechanisms into the total effective dosage model. The team concluded that the overall methodology was an effective way to link outdoor-exposure and accelerated-exposure data sets (Gu et al., 2009).

For accelerated-exposure testing of sealants, Dr. Chin continued, the sample chambers of the SPHERE were modified to allow controlled tensile and compression forces to be applied to the sealant specimens while they are being subjected to the controlled UV irradiance, temperature, and relative humidity conditions. Testing of polymers used in photovoltaic systems using the SPHERE chamber and the reliability-based cumulative damage model began last year. A smaller (20-inch diameter) commercial version of the SPHERE chamber, called the Multiport Uniform Ultraviolet Solar Irradiance Chamber, is under development, she said; it will have a maximum UV intensity that is five times greater than the original SPHERE chamber.

Dr. Chin next described SLP programs of the Inorganic Materials Group, which focuses on developing experimental and computational methodologies, metrologies, and test standards to enable fundamental understanding of relationships between the chemistry, microstructure, performance, and service life of cementitious and other inorganic building materials. Here, a critical issue affecting service life is that many long-term degradation processes in concrete are controlled by transport of undesirable species such as chloride and sulfate. These processes involve chemical reactions that in some cases generate expansive reaction products, Dr. Chin said, and the expansive forces can cause cracking, which leads to loss of strength and increase in rates of transport of the undesirable species. The previous approach by industry to this issue was to increase the density of the concrete, but that led to early-age cracking, excess heat generation during curing, as well as other problems.

The NIST group has instead worked with a new paradigm for increasing service life by increasing viscosity—and hence the diffusion resistance—of the pore solution in the concrete. Dr. Chin showed the transport equation for modeling the transport rate for an ionic species and noted that this equation implies that doubling the value of the solvent viscosity of the pore solution should halve the transport rate, which should increase the service life. The NIST program to pursue this new approach, called Viscosity Enhancers Reducing Diffusion in Concrete Technology, or VERDiCT, is using nanoscale viscosity modifiers to reduce the diffusion rate into concrete of ionic species by a factor of two or more, she explained. Three 1-year studies were performed for three different methods of delivering the viscosity modifier into the concrete: (1) delivery directly in the mixing water, (2) immersion of the concrete structural element in a topical curing solution containing the viscosity modifier, and (3) delivery via pre-wetted fine lightweight aggregates (termed Fine Lightweight Aggregates as Internal Reservoirs, or FLAIR). Based on the inhibition of chloride transport from the surface into the interior of concrete test cylinders, the group estimated that the FLAIR method for delivering the viscosity modifiers increases service life by a factor of 2.7, while adding the viscosity modifiers directly to the mixing water increases service life by only a factor of 1.3, Dr. Chin reported. Similarly, using a standard (ASTM C1012) test for sulfate transport into concrete, the FLAIR delivery method significantly reduced sulfate ingress and deleterious expansion.

NIST has started another project on service life extension for concrete, this time with the Nuclear Regulatory Commission. An issue for concrete containment of aqueous solutions found in nuclear power plants is the alkali-silica reaction (ASR), in which the highly alkaline cement paste reacts with silica, found in many common aggregates, to form calcium silicate hydrate. This hydrate forms as a gel that increases in volume when water is present, causing expansive pressure inside the concrete that leads to spalling and strength loss. The project objective, Dr. Chin said, is to develop a technical basis for the Nuclear Regulatory Commission to issue regulatory guidance on evaluating ASR-affected concrete structures as part of relicensing procedures for nuclear power plants. She said the aim is to develop methodologies to determine the current structural capacity to resist static and dynamic loads and to estimate future structural capacity, based on nondestructive measures of the internal expansion and in-situ mechanical properties of ASR-affected concrete.

The last NIST program that Dr. Chin described is Resilience Strategies for the Built Environment. Its aim is to address issues of the capacity of aging infrastructure elements to continue to withstand natural or man-made disruptive events, including extreme weather events, for which it was designed. These issues, said Dr. Chin, "highlight the need for new technologies, materials, and retrofitting strategies to monitor structural health, detecting, and even repairing, damage; accurately predict remaining lifetime; and enable assessment of resilience of infrastructure elements to natural/man-made hazards." Components of the disaster resilience framework that NIST has been tasked with developing include assessment of degradation in infrastructure systems and components (risk-based condition assessment of aging infrastructure systems); methodologies to determine the remaining service life of infrastructure materials and to guide development and use of sustainable infrastructure materials; and methodologies to ensure the disaster resilience of structures under extreme conditions (specifically hurricanes, tornadoes, and other windstorms).

During the brief questions and discussion session, Dr. Achenbach noted a recent report that linear ultrasound techniques do not work for detecting ASR, and he suggested that nonlinear ultrasound may work better because the second harmonics in the signal can be followed. Dr. Chin agreed with these points and said that a number of researchers are working on ways to detect ASR, including using microwave technologies, although she is not directly involved in that area herself. Another participant asked what models researchers use to extrapolate to exposure times and volumes of material outside of those actually tested. Dr. Chin said she would provide further details offline, but that her teams work with a developer of stochastic models at Iowa State University, William Meeker.

THE INTERPLAY OF MATERIAL STRUCTURE MODELING AND EXPERIMENTATION

As noted in the "Workshop Themes" section of this summary, a point that recurred throughout the workshop, in different forms and contexts and expressed by a number of the presenters and discussants, was that MSA requires the interplay of modeling and characterization-detection capabilities. A corollary of this theme is that ongoing work to advance MSA in forms most valuable for the applications discussed at this workshop requires research in both model development and experimentation. This perspective on MSA research and development (R&D) was particularly evident in the presentations by Dr. Hemker, Dr. D.J. Luscher, Dr. Abdel E. Bayoumi, and Dr. Susan B. Sinnott, although all four presentations also contributed to other key themes of the workshop.

Supporting the Development of Physics-Based Models: An Experimentalist's Perspective

Kevin J. Hemker, Department Chair, Mechanical Engineering,
Johns Hopkins University

Dr. Hemker noted in his introduction that his perspective is that of an experimentalist whose recent work has largely focused on supporting development of physics-based models that fit within the themes of ICME or the Materials Genome Initiative (MGI), that is, "Materials by Design." In particular, Johns Hopkins has two major DOD-sponsored centers in these areas: a collaborative research alliance with the U.S. Army Research Laboratory called the Center for Materials in Extreme Dynamic Environments and an Air Force–supported Center of Excellence on ICME for nickel-based superalloys. He cautioned the audience that what he would be describing was still a work in progress: how experimentalists can feed into and support ICME or MGI activities by working closely with the modelers is "not a done deal." He also warned that he would be deliberately provocative at times, to stir discussion and debate.

Dr. Hemker then listed the following four "key takeaways" for his presentation:

1. The materials science and engineering community is at a tipping point in the development and use of ICME principles.
2. Multiscale modeling needs experimental input on
   a) Operative failure mechanisms,
   b) 3D microstructures with salient resolution, and
   c) Benchmarking at relevant length scales.

3. Representative volume elements (RVEs) in models must be both representative and descriptive; there is, therefore, considerable merit in splitting RVEs into microstructural volume elements (MVEs), property design volume elements (PVEs), and design volume elements (DVEs; Echlin et al., 2014).
4. Modeling and validation at the mesoscale are as important as modeling and validation at the macroscale and at the nanoscale.

With respect to the use of ICME principles being at a tipping point, Dr. Hemker said that processing-structure-property relations as part of materials science and engineering, physics-based modeling, and multiscale modeling are foundational tools for ICME that have all been around "for decades," but that he sees four recent developments bringing ICME to a tipping point: (1) Dramatic increases in computational horsepower (accessible computational capacity) enable modelers to use many more processing nodes and put more detail into better models. (2) An increasing number of laboratories, such as Dr. Withers's laboratory at the University of Manchester, can acquire incredibly detailed quantitative data in the form of 3D microstructures. This capability provides "tremendous opportunity" to couple the microstructures with physics-based models.[7] (3) Small-scale experiments, using new technologies such as FIB-SEM and ultrafast lasers (lasers guided on time scales of femtoseconds, or 10^{-15} seconds), can precisely excise very small bits of a material to be tested. (4) Integration of the experimental and modeling communities is enabling them to work together.

With respect to his second key takeaway, Dr. Hemker divided "what modelers want from experimentalists" into two categories: input for building better physics-based models and benchmarking of the predictions from the models. Under input for models he included identification of the governing failure mechanisms, 3D characterization of starting microstructure in a format that can be used as input to the models, and the constitutive properties of each of the phases in the microstructure. He gave two examples of the importance in failure-mode modeling of knowing which particular failure mechanism governs the circumstances being modeled: shock-induced amorphization of crystalline boron carbide (Chen et al., 2003a), which is used in body armor, and deformation modes in nanocrystalline metals (Chen et al., 2003b).

On experimentally informed characterization of starting microstructure, Dr. Hemker started with a reminder that "computer materials" or computer models are always more perfect than are "real materials." In response to a comment from Dr. Schafrik that models can be altered to more closely approximate the real

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[7] For an example of this coupling applied to the CBM of aircraft, see Dr. Bayoumi's summarized presentation.

microstructure, Dr. Hemker agreed with the comment but suggested that this is not always done; his reminder was meant to bring the focus onto how to provide experimental input to constructing a model from physics-based first principles *before* the step of heuristically modifying (“smoothing”) the model for a better “fit” to the empirical data. He elaborated on this point by comparing a minimal unit cell taken as the RVE for the cross-sectional microstructure of a continuous fiber–reinforced composite with a larger RVE that can more realistically characterize the variability in the relative positioning of the fibers within the continuous matrix material. Even for a highly regular microstructural pattern (Dr. Hemker used a simple black-and-white checkerboard pattern to demonstrate), sampling material volumes at different sizes when interrogating the material can lead to large differences in characterizing the variability of a microstructural property. He then showed how this point applies to a real material, studied by Tresa Pollock’s group at the University of California, Santa Barbara: a copper-tungsten composite used in hypersonics applications (Echlin et al., 2014). Because of the heterogeneity in the microstructure of the composite, the spread in the data for the volume fraction of copper in the composite varied over a wide range, depending on the size of the sampling volume (the edge length of the sampling box was varied from ~2 μm to ~65 μm).

Dr. Hemker used this example to show how Echlin and colleagues (2014) distinguished a hierarchy of volume elements of interest: the volume necessary to define a microstructural feature of interest (the MVE), the volume necessary to define a material property of interest (the PVE), and the volume necessary for the convergence of all relevant PVEs for component design (the DVE). As Figure 3.4 illustrates and Dr. Hemker emphasized, several different MVEs may be needed to get the right microstructural information to predict a material property of interest, such as yield strength or permeability, and an appropriate PVE for that property may be much larger than the largest MVE of a feature that determines that property. (This discussion and Figure 3.4 also pertain to his third key takeaway, that the RVEs used in a physics-based model must be representative and descriptive with respect to this entire hierarchy of MVEs, PVEs, and DVEs.)

Furthermore, he continued, different properties scale differently. Properties—such as melting temperature, thermal expansion, or elastic modulus—that depend on atomic bonding require only a very small volume element to capture the property. Other properties, such as thermal conductivity or permeability, require taking into account microstructure, at the scale of microns, whereas mechanical properties such as yield strength, fracture toughness, or fatigue life require a larger volume to capture flaws; Echlin and colleagues (2014) suggested that the latter require PVEs on the scale of millimeters.

Dr. Hemker next described the challenges of processing the EBSD scans of a polycrystalline nickel alloy (Rene-88DT), prepared as a voxelized data set by

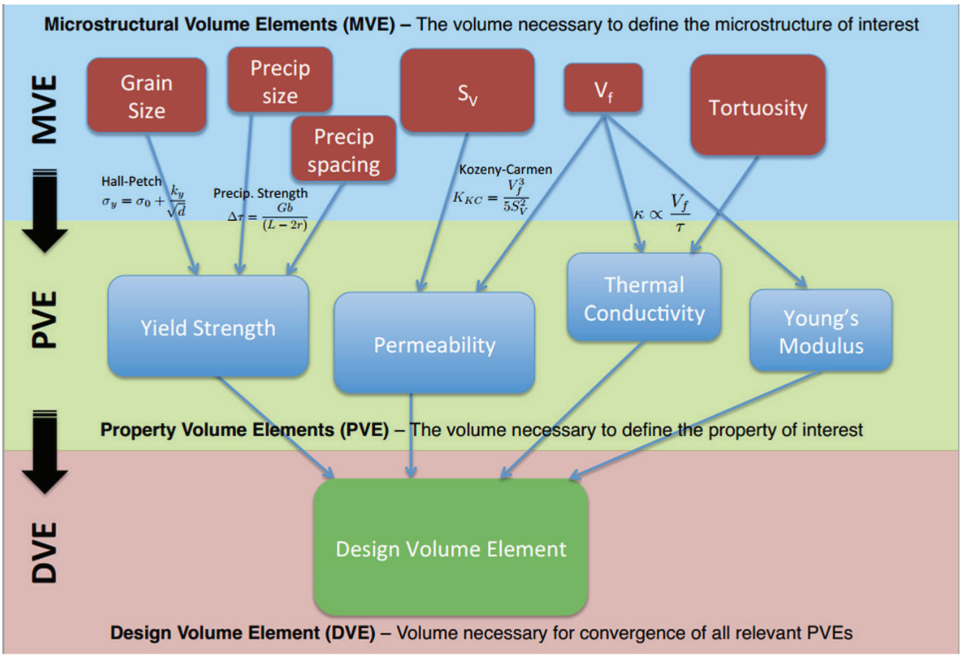

FIGURE 3.4 Hierarchy of material volume elements. Material volume elements can be divided into a hierarchy that is tiered based on their dependence. On the top tier, examples of selected MVEs are shown with their relative expected sizes (conveyed by box size). On the middle tier are PVEs, which depend on MVEs. Next to the arrows indicating the dependencies are the structure-property relations that model the expected relationship between the MVEs and the PVEs. DVEs are displayed on the lowest level. A DVE is defined for specific PVEs, for which it has been validated by means of property convergence. The DVE size is based on the geometric effects of the components that are being designed. SOURCE: Kevin J. Hemker, Johns Hopkins University, presentation to the Workshop on Materials State Awareness, August 6-7, 2014. Echlin et al. (2014), Figure 2 (including caption), Springer Open Access, Creative Commons Attribution License 2.0 (http://creativecommons.org/licenses/by/2.0).

Dr. Pollock's group, for use in an FEA model. Based on the features of the actual microstructure, which were too complex to capture fully in the FEA, Somnath Ghosh's laboratory at Johns Hopkins created a synthetic microstructure that had microstructural properties, such as mean grain size and grain size distribution, that were close to the properties in the real microstructure and preserved certain features such as twin boundaries, which are important in initiating cracks. The challenge, Dr. Hemker said, is getting the property-relevant details into the synthetic model at a resolution that the modelers can deal with, "and it's a dance [between the experimentalists and the modelers] that we are still learning how to do."

After a couple of additional examples of size-scale effects in measuring constitutive properties, Dr. Hemker turned to the second category of what modelers want from experimentalists: benchmarks for model predictions. He listed the following types of experimental measurements that can be used for benchmarking model results:

- Tensile characteristics
  —Tensile strength
  —Local plasticity maps
  —Texture formation
  —Geometric and necessary dislocation maps inside grains
- Fatigue characteristics (N = number of cycles to fatigue effect)
  —$N_{\text{local plasticity}}$ and the location and neighborhood of local plasticity
  —$N_{\text{crack initiation}}$ and the location and neighborhood of crack initiation
  —N_{fracture} and the location and neighborhood of fast fracture
- Fracture characteristics
  —Crack nucleation site and critical load
  —Crack propagation path
  —Role of material microstructure in promoting/inhibiting fast fracture

He then turned to how mechanical benchmarking properties can be measured at the mesoscale—the scale of what he called oligocrystals, or crystalline structures with hundreds of grains but not thousands or millions of grains, as found in macroscale measurements. This, he said, is the scale at which physics-based modelers can model a polycrystalline material; if the experimentalist can make a sample for which the modeler can model every grain in the sample, then the model-predicted properties of that sample can be compared with (or benchmarked against) the experimentally measured properties, he explained. “Where was the deformation? Where did the crack formation initiate?” And so on.

The mesoscale samples Dr. Hemker uses are “2.5D” specimens, which means they are just one grain in thickness (for a polycrystalline material) or are a cross section of a unidirectional fiber composite. Rather than the traditional benchmark measurement taken for a bulk property, where a single value of the property is expected, mesoscale benchmarking assumes there will be multiple benchmark values reflecting the different microstructures that exist in specimens at that scale. So the goal for benchmarking a model is for the model to be able to predict successfully the scatter of property values for the different microstructures in the modeled specimen.

He described how this approach has been used to benchmark simulated versus experimental surface strain maps of polycrystalline nickel alloy specimens of about 60 μm on a side, with the orientation of each surface grain measured by EBSD for input to the model as the starting microstructure (Turner et al., 2013). He also described a micro-bending technique for fatigue testing of metal specimens that was developed by a former postdoctoral fellow from his group (Straub et al., 2013). With this technique, he said, the grain in which plasticity first appears can be identified, and the subsequent spread of slip bands and cracks can be followed. These results can be compared with model predictions for the specimen when subjected to equivalent simulated micro-bending cycles. His third example was a technique for experimentally testing crack initiation in a fiber composite as modeled by David Mollenhauer of AFRL and colleagues (Swindeman et al., 2013). By placing controlled strain on a 2.5D specimen of a multiple-ply unidirectional composite, they could visually record crack initiation and progression in the specimen at the mesoscale. He hopes this information can be used to benchmark simulations of stress development in nonuniform cracking of the fiber composite.

Questions and Discussion

With respect to trade-offs on the size of RVEs and on computational volume elements generally, Dr. Luscher agreed that identifying the right size for an RVE is important for characterizing the mean field response of a material and that the size depends on the response of interest, as Dr. Hemker had noted. However, for many damage and failure mechanisms of interest, the mean field response is not as important as what's happening in the tails of the response distributions, Dr. Luscher said, so looking at *statistical* volume elements (SVEs), in contrast to *representative* volume elements, is useful. There is also a connection with probabilistic frameworks at multiple scales, he added, if one can look at multiple realizations (of a set of inputs to a probabilistic model) using volume elements with length scales relevant to the application of interest, to try to understand the statistics of different processes that can occur at that scale. Dr. Hemker concurred with the comment and noted that investigators at the Air Force Center of Excellence at Johns Hopkins University are working on that problem. "The statistical treatments are certainly an important step forward," he said.

A participant commented that a difficulty in choosing the right RVE for composites is that the failure effect can start a long way from the point of damage because of stress redistribution. Hot spots from damage at a given point can occur far from the area initially damaged, and crack propagation will depend on subsequent stresses and interactions among those hotspots.

Dr. Luscher and Profs. Hemker and Achenbach discussed the use of cohesive elements in a model and how the distribution of cohesive elements might affect the model's prediction of crack initiation and propagation. Dr. Hemker opined that cohesive elements provide an attractive method for modeling fracture but cautioned that prescribing fracture paths can influence the model predictions.

Dr. Wadley asked how Dr. Hemker's approach of mesoscale surface modeling of a 2.5D specimen translated to benchmarking the behavior of a bulk material, where there is no free surface. One approach to getting the response of an "interior" volume element, he suggested, is to rely on the modelers to translate what was observed experimentally on the surface specimens to interior elements without free surfaces. Another approach is to use experimental techniques that let one observe an interior 3D element that is the equivalent of what Dr. Hemker's methods can observe on the surface of a mesoscale element. He asked if digital strain mapping of an interior element, based on grain shapes, could be done using, for example, nanoscale x-ray techniques.

Dr. Hemker replied that there is a growing research community interested in using synchrotron data (i.e., using a synchrotron as the source of nanoscale-wavelength x rays directed at a material target), applying near-field techniques to map the polycrystalline microstructure and far-field techniques on the strained sample to examine dislocations and effects on individual grains. For deformation behavior, he believes it is thus theoretically possible to use these x-ray scatter techniques to observe the grain behavior of samples that are up to millimeters in thickness, instead of the hundreds-of-microns scale at which he works. His approach has been to provide the modelers with a benchmark that they can model as a free surface. A good first step for them is to see if they can successfully model a polycrystalline mesoscale specimen with free surfaces. He agreed, though, that the question of how that behavior relates to the behavior of the material in bulk is a very good one to raise. He thought the synchrotron techniques (near-field, far-field, and tomographic) might be the closest thing to the interior interrogation Dr. Wadley was describing. He suggested that the participants keep this potential experimental approach—high-resolution 3D interrogation of the bulk volume of a material—in mind when "big data" methods of analysis are discussed during the second day of the workshop.

As a final comment, Dr. Hemker said that work under the Materials in Extreme Dynamic Environments Collaborative Research Alliance is showing that extreme dynamic events such as projectile impacts can obliterate, or totally alter, the microstructure. The whole mechanism that occurs during the shock becomes very important to what happens to the material subsequently, he explained; this is an even more complicated problem waiting to be solved.

Physics-Based Mesoscale Modeling of Materials in Extreme Environments

D.J. Luscher, Fluid Dynamics and Solid Mechanics Group,
Theoretical Division, Los Alamos National Laboratory (LANL)

Dr. Luscher introduced his presentation as having two parts: first, a higher-level overview to define the terms used in the title of the presentation as his modeling group at LANL thinks about them; second, a discussion in more detail of what occurs in going from mesoscale to macroscale responses in a selected case of interest to his group.

Illustrative of the *extreme environments* of interest to LANL, he began, is the explosively driven dynamic expansion of a hollow spherical shell formed from a polycrystalline metal (Figure 3.5). Many length scales are spanned in moving from the mesoscale fine shear banding, reflecting highly localized plastic deformation, that is visible in micrographs of single fragments to the fragmentation pattern of the entire component (shown in the radiograph in the upper left of Figure 3.5). If one begins with consideration of the material state prior to this extreme event, he noted, the response also spans many time scales.

With respect to their modeling work, Dr. Luscher's group thinks of the micro-, meso-, and macro-length scales in terms of three distinct levels of material state representation as shown in Figure 3.6. Zooming in from the entire engineered system, the scale at which they can begin to resolve heterogeneous features of one "material"—for example, the polycrystalline microstructure of the containment shell material—is their mesoscale, he said. At this scale, the modelers can resolve the orientation distribution and morphology of individual grains. One example he described was a mesoscale simulation of the response of a polycrystalline material

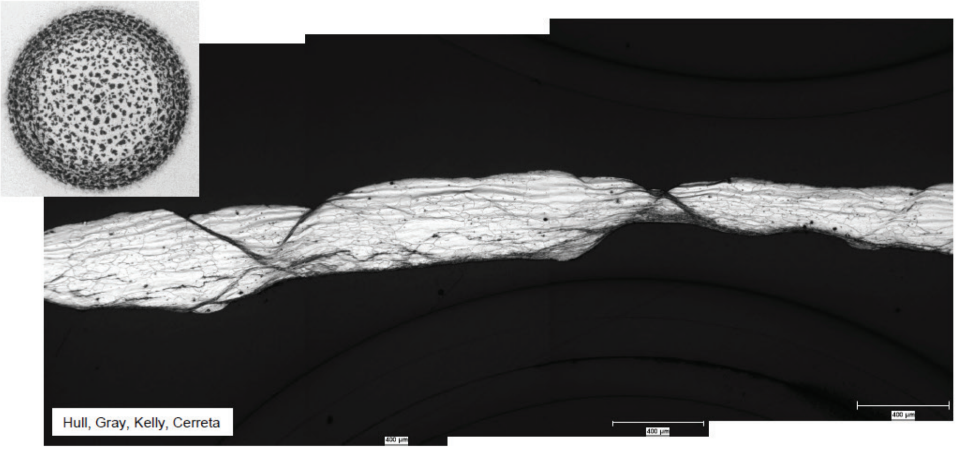

FIGURE 3.5 Macroscale response (radiograph in upper left corner) and mesoscale response (micrograph montage of shell fragment) of a polycrystalline metallic sphere to explosively driven expansion. Localized plastic deformation (shear banding visible in the micrograph) leads to fragment formation at the macroscale. Each scale bar along the bottom edge represents 400 µm. SOURCE: D.J. Luscher, Los Alamos National Laboratory, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 2. This image was generated through the ongoing research of Gray and colleagues (see Gray et al., 2012).

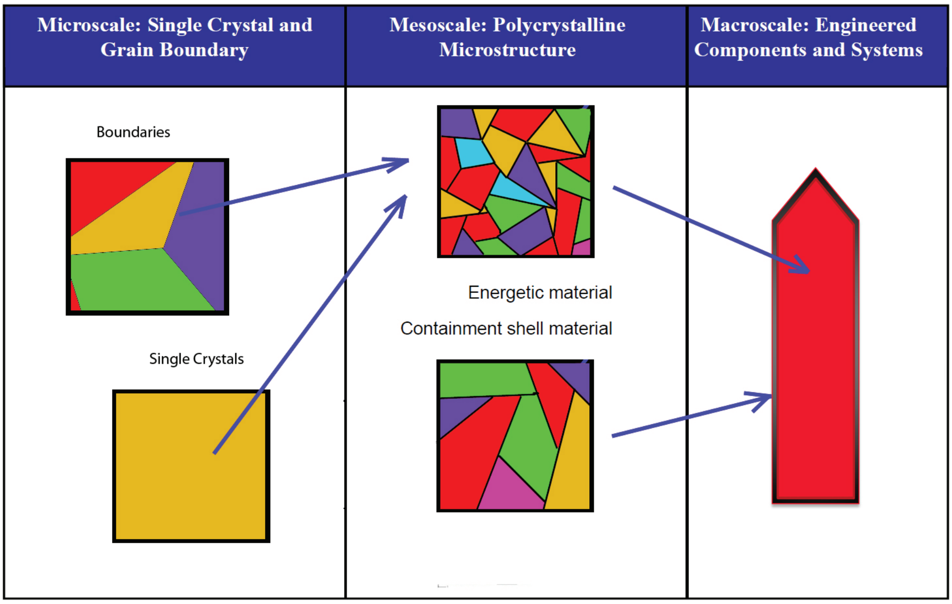

FIGURE 3.6 A modeler's perspective on micro-, meso-, and macro-length scales. SOURCE: Adapted from D.J. Luscher, Los Alamos National Laboratory, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 3.

to a shock wave, where the anisotropy due to differences in grain orientation and size leads to localized hot spots. Understanding the physics of hot spot formation, he explained, is useful for various applications, such as understanding the initiation process in explosive materials.

Within the model used to simulate a mesoscale behavior such as porosity, there may be models of properties and behaviors at the microscale, such as an atomistic-scale model. In particular, Dr. Luscher's group is developing "state-aware" single crystal and grain interface models that can be applied under the shock conditions of extreme events to obtain meaningful predictions for mesoscale SVEs. By "state aware," Dr. Luscher means a model that explicitly accounts for nonlocal interactions that are spatially coupled, such as a single-crystal model that includes field variables to represent evolution of dislocation velocities in a volume surrounding the crystal being modeled. He explained how his group has analyzed the representation of state awareness into three coupled sub-problems: deformation momentum balance, continuum dislocation transport, and dislocation-deformation compatibility.

In summing up the introductory part of his talk, Dr. Luscher said that the extreme environments of interest for his group's work span length scales from less than a micron to greater than a meter, temporal scales from nanoseconds

(10^{-9} seconds) to decades (greater than 10^{8} seconds), strain rates from 10^{-8} to 10^{8}, and temperatures from 200 K to 1500 K. Their modeling covers physical properties and behaviors from the microscale to the macroscale, as described above and illustrated in Figure 3.6, with the objective of handing off constitutive models to engineering analysts and weapons designers for application to entire components and systems at the macroscale. With respect to characteristics of the material state, they are interested in capturing classical thermodynamic state variables (elastic strain, temperature, stress, and entropy) augmented with a physics-based description of state that includes dislocation density and substructure, geometry and volume fraction of twins and transformed phases, porosity, and texture within the material (the distribution of nonuniform orientation).

The second part of the talk provided a more detailed look at modeling a specific phenomenon that has interested engineering analysts at LANL: the influence of material consolidation processes on the thermal expansion of explosives. In particular, Dr. Luscher said, the analysts want a continuum constitutive model of the thermal deformation of polymer-bonded explosives. With respect to descriptors defining the domain of this modeling, this application area encompasses quasi-static strain rates spanning minutes to years (the lifespan of weapons components) and temperature cycles from 200 K to 500 K. It requires models that can instantiate various homogenization theories and can span length scales from the mesoscale to the macroscale. Critical aspects of the material state to be modeled include texture, porosity, and the influence of the material's processing and deformation history on texture and porosity.

Polymer-bonded explosives, Dr. Luscher continued, have a high-volume fraction of explosive crystals in a relatively low fraction of polymer binder. One such explosive formulation, PBX-9502, contains polycrystalline aggregates of triaminotrinitrobenzene (TATB), which in its pure crystalline form has a triclinic unit cell and forms platelet-like crystals. The problem of interest, he explained, is that PBX-9502 shows an irreversible accumulation of strain from temperature cycling (e.g., temperature cycling between −54°C and 74°C). Although most of the strain increase from heating is reversed on the next cooling phase, some of the strain remains. This *ratchet growth* in strain with increasing temperature cycles is not exhibited by single crystals of TATB. So the goal for Dr. Luscher's group is to develop a constitutive model of this behavior that can be used in an engineering analysis of macroscale systems containing PBX-9502 as a material component.

The first part of the work has been to capture the reversible part of PBX-9502 thermoelasticity in mesoscale models of PBX-9502 homogenization because such models provide a bridge from single-crystal models to the mesoscale. The following high-level outline of his highly detailed discussion of the modeling work to date and what has been accomplished builds on three key points (the boldface questions below) through which Dr. Luscher framed his discussion.

1. **Why should engineers care about the texture of PBX-9502?**

   - A single crystal of TATB is highly anisotropic with respect to thermoelasticity in the three planes of the triclinic unit cell; thermal expansion normal to the *a*,*b* plane (the [001] normal) is an order of magnitude greater than thermal expansion in either the *a* or the *b* directions. In response to thermal change, individual crystals are pushing and pulling in interactions with each other, the highly irregular void structure interacts with the stress field, and the binder is not spread uniformly throughout the compounded material.
   - The many single crystals that make up one specimen of polycrystalline aggregate can vary in the distribution of crystal orientations in that specimen, but there tends to be a preference for orientation to the [001] normals. If there are relatively more [001] normals pointing in one direction, thermal expansion is expected to be higher in that direction than in others (thermoelastic anisotropy).
   - Specimens of aggregate are heterogeneous at the scale of microns; they differ in their degree and direction of this anisotropy.
   - Texture in the bonded aggregate indicates a lack of uniformity of the distribution of crystal orientations, hence thermoelastic anisotropy.
   - Texture is the key factor in the anisotropy of PBX-9502 thermomechanical properties at the macroscale.

2. **If texture is important, how can it be accounted for in constitutive models used for engineering analyses?**

   - Homogenization schemes provide a bridge from single-crystal behavior to macroscale properties. However, these schemes require that the orientation distributions of both individual crystals in aggregate specimens and aggregate specimens in the compounded bulk material are known or can be reasonably estimated.
   - Without measurements of the orientation distributions, a model for texture evolution during, for example, pressing operations is necessary to predict the thermoelastic behavior of the macroscale PBX-9502 component. The March theory holds that high-aspect-ratio crystals are rearranged according to the direction of the deformation vector of the consolidation process, and this response to deformation can be modeled—for example, Dr. Luscher showed the fit of experimental data for uniaxial die-pressed consolidation with the March theory model.
     - —For more complex consolidation processes, the deformation and material responses to it need to be modeled with greater complexity.

  - —If a purely volumetric consolidation process is used, so that there is no net effect of the deformation on platelet-normal vectors, then no texture is introduced by the consolidation process, he noted.
- Given an orientation distribution from the texture evolution model, a number of classical homogenization techniques (i.e., algorithms for deriving the macroscopic strain and stress from the single-crystal strain and stress) can be applied to scale up from the single-crystal properties of TATB to the properties of the bulk explosive component. However, Dr. Luscher noted, if uniform strain is assumed, the mesoscale representation will satisfy displacement compatibility constraints on a solution but will not necessarily satisfy stress equilibrium conditions. If uniform stress is assumed, then stress equilibrium is satisfied, but the mesoscale displacement field may not be single-valued and compatible. To resolve this conceptual problem, the modelers are pursuing a self-consistent homogenization technique to arrive at a result that meets both constraints.
- Dr. Luscher described work being done to compare their model simulations of the effects of porosity and texture on the bulk product's coefficients of thermal expansion, and the effect of consolidation on anisotropy, with experimental data for uniaxial compression consolidation. (In effect, these comparisons are like the experimental benchmarking discussed by Dr. Hemker.)

3. **How much influence does texture have on constitutive response, and can we connect that with some understanding of how the consolidation process during manufacture of PBX-9502 affects its thermoelastic behavior?**

- Dr. Luscher's group's macroscale constitutive model agrees with experiment. Dr. Luscher said that a macroscale constitutive model for engineering analysis has to take texture into account because of the high degree of anisotropy in single crystals and because the consolidation process itself can induce texture in the bulk explosive that conveys that anisotropy (depending on the consolidation process) up to the macroscale material.
- A finer point is that the more complex consolidation process for a real-world engineered explosive component has deformation that is spatially variable throughout the component. This means that macroscale material properties affected by the underlying anisotropy will differ "everywhere" throughout the component. Even at the macroscale, the material is not homogeneous.

- Texture has a significant effect on component properties. In the past, variability measured in the properties of explosive-material components taken from assembled systems has, according to Dr. Luscher, generally been attributed to stochastic differences; he now believes that spatial variability in texture is one factor in the variability measured in the properties.

In concluding, Dr. Luscher noted that the "real meat" of the group's work on the PBX-9502 problem will be to extend the theory instantiated in the model to cover the ratchet growth in thermal expansion. More broadly, he hoped the presentation had given the workshop participants a perspective on the breadth of what his group is interested in, the potential breadth of applications for this kind of modeling work, and how his group understands and uses some of the key terms and concepts employed in the mesoscale modeling of material state.

Questions and Discussion

Dr. Achenbach asked if the modeling group was looking into distributions of cracks. Dr. Luscher said that they have not yet done anything on crack distribution, but for this material (PBX-9502), that will be an important part of modeling the ratchet growth phenomenon. There are not cracks in the usual sense of cracks in the microstructure of a metal because the grains of aggregated crystals are bonded together by a polymeric glue. But material delamination allows relative slip between the anisotropic single crystals, and that leads to an irreversible deformation at the mesoscale and the ratcheting behavior at the macroscale. If all of the crystals stayed bonded together as in their original state after compounding, there would not be an irreversible component in the deformation in response to thermal cycling. Dr. Achenbach added that, if the group succeeded in modeling that behavior, it could make a major contribution to the modeling of fracking. Dr. Luscher responded that there are other people at LANL working on modeling fracking in terms of the stochastic nature of fracturing in geologic material, but that is not an area in which he works.

Dr. Rosario Gerhardt (Georgia Institute of Technology) commented that the concept of anisotropy is also applicable to electroresponsive materials. She has been doing measurements on many materials with a platelet structure (similar to the single crystals of TATB). When ceramic composites with boron nitride platelets are hot-pressed, the platelets align in a particular direction, either parallel or perpendicular to the direction of pressing. She suggested that hot-pressing might be an interesting experimental technique to use with PBX-9502—although she was not sure about the safety aspects of using hot-pressing with a polymer-based explosive.

Dr. Luscher agreed with the point about experiments involving explosives and noted that experiments on them at LANL get a high level of safety-related scrutiny. He added that a lot of approaches used to study other polymer-bonded materials do work with explosives, but getting approval to try them is difficult.

In response to a question about the difficulties of modeling the metallic casing fragmentation (see Figure 3.5), Dr. Luscher said that, in addition to the difficulty of capturing the detailed physics over the entire domain of the casing fragmentation, the necessary modeling at multiple scales, including fine-scale details within the microstructure, across that entire domain represents a very difficult computational problem. "Multiscale modeling has not yet been brought to bear successfully on this class of problem," he said. Further discussion included issues in modeling the fragmentation behavior and approaches that may help overcome the obstacles.

CBM+: A Smart Predictive Approach

Abdel E. Bayoumi, Director, CBM Research Center, and
Professor of Mechanical Engineering, University of South Carolina

Dr. Bayoumi said that talking about CBM means talking about cost, mission availability, and prediction. One driver for CBM is cost avoidance and keeping systems available: "if it isn't broken, don't fix it." But, he pointed out with examples of major system failures and crashes, "you cannot always wait until it fails" to fix it, which is where prediction comes in.

To illustrate the importance of cost as a driver for CBM, Dr. Bayoumi cited the following statistics on maintenance to indicate the potential for reducing unnecessary costs:

- Average cost of maintenance in food-related industries represents about 15 percent of the cost of goods produced.
- Maintenance costs represent up to 60 percent of the cost of iron and steel, pulp, paper, and other heavy industries.
- Recent surveys (not cited) show that 33 percent of maintenance cost is wasted as the result of unnecessary or improper maintenance. Assuming that U.S. industry spends $200 billion per year on maintenance, this wasted cost adds up to more than $60 billion each year.

To characterize how CBM differs from other schemes for preventive maintenance, Dr. Bayoumi first distinguished preventive maintenance from corrective maintenance, which is event driven by breakdowns and characterized by emergency repairs, and from improvement, which is driven by reliability objectives and characterized by modifications, redesigns, and retrofits. Maintenance to prevent failure events can be time based (i.e., at fixed intervals of calendar time or operational hours), usage based (e.g., dependent on a combination of load and time), or predictive (i.e., based on a condition indicator as in CBM). Examples of condition indicators that can be followed continuously as the basis for CBM are vibration monitoring, tribology, thermography, ultrasonics, and nondestructive testing.

Dr. Bayoumi sees CBM as part of the transition from reactive maintenance to proactive maintenance. This transition involves a paradigm shift in maintenance strategy to a holistic approach that combines historical and logistical data on components and subsystems, onboard smart sensing, integration of electronics and avionics data, and the limited data sets available from test stands, etc. CBM requires a systems engineering approach to optimizing system operation, Dr. Bayoumi continued, in which the system-level parameters to control might typically include minimizing down time and minimizing the combined cost of scheduled and unscheduled repairs. This systems engineering approach, he said, carries forward into the use of the holistic analysis results as input to optimizing the design and manufacturing of new parts and systems.

Achieving these CBM objectives requires developing accurate prediction models for diagnosis, prognosis, useful life, and operations, which come together in what Dr. Bayoumi called predictive analytics or a Smart Predictive System (SPS; see Figure 3.7 and Cao et al., 2013a). The first phase of SPS development at the CBM Research Center, started in 1998, has focused on *measurement-based models*

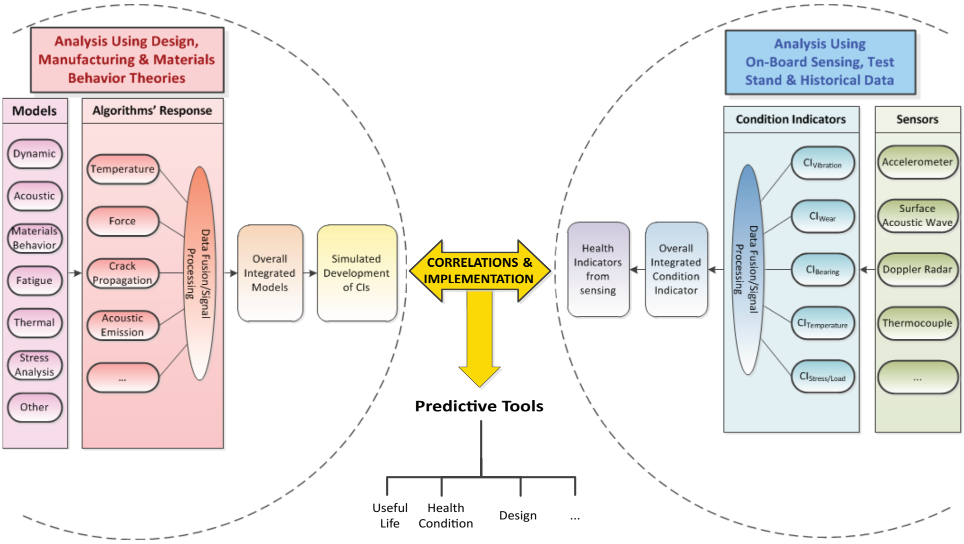

FIGURE 3.7 Three development phases to achieve a Smart Predictive System (predictive analytics). SOURCE: Abdel E. Bayoumi, University of South Carolina, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 7. Copyright 2014 CBM Research Center, University of South Carolina, all rights reserved.

that analyze data from onboard sensing, test-stand test and evaluation data, and historical/logistical data (right side of Figure 3.7). Data fusion of inputs from a number of condition indicators, tracked by appropriate sensor modalities, provides a system-level health indication and a set of tools for predicting useful life or other system attributes. The second phase of SPS development, which is the current focus of research at the CBM Research Center, is *physics-based modeling*, in which the models use algorithms that instantiate theories of materials behavior in design and manufacturing contexts (left side of Figure 3.7). The outputs from these algorithms are integrated into an overall model that can be run to simulate changes over time in the same condition indicators tracked by the measurement-based models.

The third phase in SPS development involves iterated correlation and comparison of the measurement-based model results with results from the physics-based models. This process, Dr. Bayoumi emphasized, involves the cross-validation and refinement of the models on each side, based on the results from the other side, as well as the integration of both modeling approaches to produce a practical set of tools for predicting useful life, system health, and inputs to design and manufacturing improvement (middle of Figure 3.7).

To differentiate CBM+ from CBM, Dr. Bayoumi said that CBM+ means "CBM plus prognostics." Another way to think about the information flows represented in an SPS is that feature-mapping functions relate sensor outputs to condition indicators (features) such as kurtosis temperature levels. Fault/diagnosis classifiers map these condition indicators onto diagnostic fault classes such as imbalance/misalignment, cracks, or spalling; probabilistic health/prognosis classifiers use this fault class information to make a prognosis about overall system health condition. Using these approaches, he said, the CBM and CBM+ work by his team is not just a materials problem, design problem, or manufacturing problem but is all of these.

He illustrated the CBM work being done on military rotorcraft with an example of the onboard and test-stand sensor systems used to monitor condition indicators for the main rotor and tail rotor drive train assemblies and swashplates in the Apache AH-64D helicopter (Cao et al., 2013b). The maintenance issue was a high rate of depot-level repairs related to leaking tail rotor gearboxes. The CBM approach they developed has reduced or eliminated unnecessary part replacements, reduced corrective maintenance, reduced inspections and test flights, reduced operating and servicing costs, and increased operational readiness of rotorcraft in the fleet. The demand for tail rotor gearbox replacements decreased 36.6 percent, for an average cost avoidance of nearly $3 million per year. To these tangible benefits of CBM, Dr. Bayoumi added intangible benefits: improved safety; improved feelings of safety, confidence, and morale for crews; and increased focus on mission objectives.

The areas of research focus at the CBM Research Center start with a cost-benefit analysis (to estimate the potential return on investment from transition to CBM) and include advanced signal processing (data fusion with an emphasis on the integration of data from existing sensors rather than on adding sensors); tribology (including studies of friction, temperature, lubricants, and wear); natural language processing (for automated collection of operational/logistical data from written logs); and component testing. These areas improve and expand on the inputs used in the modeling research for diagnosis, prognosis, and life prediction, the final phase of which will be SPSs as indicated in Figure 3.7. Dr. Bayoumi added that a planned new initiative will add inputs from rotorcraft avionics and electronics into the SPS.

In 2008, the CBM Research Center received an Indefinite Delivery/Indefinite Quantity (IDIQ) contract from DOD totaling $15 million over the 5 years of the contract. DOD awarded a second IDIQ contract in 2013 at the same level of funding. The center currently has about $6 million of infrastructure investments, Dr. Bayoumi said. They are expanding from the initial work on aviation platforms (military rotorcraft and the V22 Osprey) into aviation supply chains (sensing applications with instrumentation/control systems suppliers), systems integration and analytics (predictive analytics and the Connected Aircraft initiative under the Federal Aviation Administration's Next Generation Air Transportation System), and energy sector support (nuclear, wind turbine, gas turbine, and oil drilling applications). Dr. Bayoumi expanded on the initial effort that the CBM Research Center will undertake in data collection and data fusion for the aircraft usage/health management aspects of the Connected Aircraft initiative.

Dr. Bayoumi next elaborated on the system design and operational wear issues that were identified and diagnosed as part of the CBM research on the Apache AH-64 tail rotor gearbox problem. Testing showed that a leaking output seal was allowing the aviation gear lubricant to move out of the gearbox, leading to overheating of the output assembly ball bearings and, if uncorrected, eventual system failure during operation. His team also tested the addition of varying concentrations of graphite nanoparticles to the aviation gear lubricant to improve thermal conductivity, viscosity, and efficiency (Gouda et al., 2014). Dr. Bayoumi used this work to describe how a CBM approach can be combined with materials science and engineering (in this case, tribology) not only to improve the functionality and extend the operating life of existing systems but also to improve design standards and requirements through a structured process that starts with materials selection and behavior and continues with materials design, manufacturing, and "design for excellence" of structures and moving parts.

In his closing remarks, Dr. Bayoumi gave the following summary characterization of CBM and CBM+: They require a proactive, interdisciplinary program, so no one discipline can assume ownership. They require a systems engineering approach that includes every component of the system. They incorporate the science and engineering knowledge of materials, design, manufacturing, and sensing. They draw on the information technologies of data processing and analysis, data management, data fusion, data warehousing and mining, modeling and simulation, and predictive analytics. "CBM is no longer an art," he said in conclusion. "We have to see it now as a science."

In the limited time for discussion of this presentation, Dr. Schafrik suggested that the list of challenges for the Connected Aircraft initiative should include cybersecurity. He noted the sophistication of state-supported "hackers" and the security risk they represent. Dr. Bayoumi agreed and said that a retired U.S. Army general officer has recently joined the team at the CBM Research Center to add expertise and focus on security issues.

Advanced Approaches for Material Design and Discovery

Susan B. Sinnott, Department of Materials Science and Engineering,
University of Florida

Dr. Sinnott said her presentation would address the role of electronic structure and atomic-scale computational methodologies. In many respects, she added, her talk is a companion piece, coming from a computational perspective, to the presentation by Dr. Hemker on experimentalists and modelers working together.

As a computational materials scientist working at the nanometer scale, she said that the challenges at that scale are achieving both length and time scales that are meaningful to explaining experimental findings (Figure 3.8). Traditionally, electronic-structure and atomic-scale computational methods have been viewed as useful in determining mechanisms and providing valuable descriptions for problems of materials state and behavior. Her talk was intended to show how these methods can do more than that but have challenges to be addressed.

At the electronic-structure level, Dr. Sinnott said, high-fidelity methods are available, such as quantum chemical approaches and calculations based on density functional theory. Computational codes (software) for these methods are widely available and are usable "off the shelf" (with some caveats); within the computational community, there is widespread understanding of the strengths and limitations—such as where they can be used effectively and when not to trust the method's results, as in the case of highly correlated systems such as some metal oxides.

For her first example of electronic-structure modeling, she discussed her collaboration with two experimentalists on intermetallic phases at the interface of platinum contacts with lead zirconate titanate (PZT) thin films, which are piezoelectric and are used in devices such as microelectromechanical systems. These devices are used in numerous applications as transducers between an electrical signal and a sound wave, she said, including cellular telephones and smart phones. Solution deposition of the thin film is used because the process

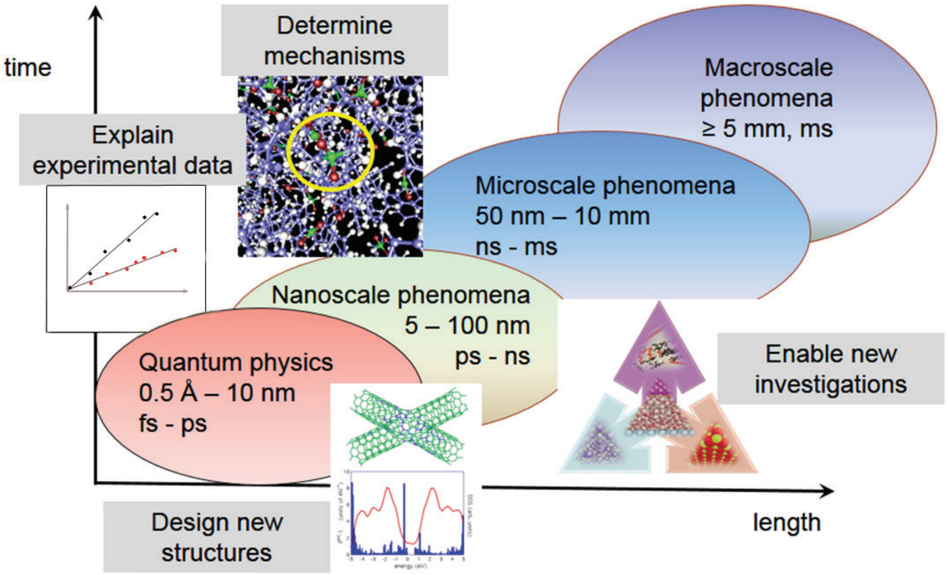

FIGURE 3.8 Length and time scales for phenomena relevant to the materials state at scales from quantum physics to the microscale and macroscale. Time ranges are shown in femtoseconds (fs, 10^{-15} s), picoseconds (ps, 10^{-12} s), nanoseconds (ns, 10^{-9} s), and milliseconds (ms, 10^{-3} s). SOURCE: Adapted from Susan B. Sinnott, University of Florida, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 2. *Determine mechanisms* image reprinted with permission from I. Jang and S.B. Sinnott, Molecular dynamics simulations of the chemical modification of polystyrene through C_xF_y+ beam deposition, *Journal of Physical Chemistry B* 108(49):18993-19001, copyright 2004 by the American Chemical Society. *Design new structures* image reprinted with permission from F. Cleri, P. Keblinski, I. Jang, and S.B. Sinnott, Localization and quantization in covalently bonded carbon nanotube junctions, *Physical Review B* 69:121412(R), 2004, copyright 2004 by the American Physical Society. *Enable new investigations* image from S.R. Phillpot and S.B. Sinnott, Simulating multifunctional structures, *Science* 325(5948):1634-1635, 2009, reprinted with permission from AAAS.

is inexpensive, simple, and versatile. Complete conversion of the film-contact interface to its perovskite working structure requires heating to around 600°C, but the heating also leads to formation of a platinum-lead alloy phase at the interface, which decreases the conductivity of the contact (Aksel and Jones, 2010). The question posed to Dr. Sinnott by her collaborators was whether the formation of the platinum-lead alloy was kinetically or thermodynamically driven. Her Density Functional Theory (DFT) calculations indicated that formation of the alloy phase was not thermodynamically preferred and was perhaps kinetically driven. She is currently investigating how the barriers to diffusion across the platinum-PZT interface are affected by composition changes. Although this is just one small part of a much larger investigation, she said, it illustrates the power of electronic-structure methods and how computational approaches and experimentation can work together to address material state problems.

Her second example involved work for the Air Force to design a new nickel-based superalloy as an alternative to the current nickel-based superalloys that incorporate rare-earth metals. These present aluminum-nickel superalloys are used in high-temperature applications such as gas turbine engines, she explained, and the scarcity and geographic locations of known sources for the rare earths raises source reliability and security concerns. The computational objective was to determine the energy involved in incorporating dopant atoms into the lattice structure of the superalloy. The defect formation energy of incorporating a currently used rare earth (cerium) as the dopant was compared with that of boron, chromium, and zirconium—three replacement candidates that are much more abundant. Defect formation energies were calculated for the dopant atom replacing either an aluminum or a nickel atom in the lattice. The computations indicate that cerium and zirconium have a lower defect formation energy when they replace an aluminum atom, whereas a nickel site is energetically favored for boron and chromium dopants. Her computational result for chromium, she noted, is confirmed both by a data-mining study performed as part of the MGI[8] and by experimental data from transmission electron microscopy measurements of the crystal lattice structure. She defended the value of materials informatics in opening up new potential lines of inquiry into materials alternatives rather than being a methodology that stifles creativity and innovation.

Turning to the use of atomic-scale computational methods in exploring materials state, Dr. Sinnott said that realistic energy potentials for many-body configurations that are meaningful in material behavior analysis have been available for more than 30 years. These energy potentials can be used to investigate dislocation generation, mechanical deformation, and nanomaterials, she explained, and they are especially good for examining material systems under extreme environments. "Blowing things up on a computer works well, and no one gets hurt." Furthermore, these atomic-scale energy potential computations can be used to study combinations of chemistry changes, microstructure, mechanics, and mechanisms, all occurring together. Dr. Sinnott said that if chemical changes are not an issue and material properties can be assumed as inputs to a model, then a micro-, meso-, or macro-level simulation may only need to be informed by experimental data or quantum-level electronic structure data. However, if models at any of those levels need to include the effects of changes in microstructure, chemistry, and composition, then the models need input from the atomic-scale level; the qualitative insights

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[8] The materials informatics work that Dr. Sinnott cited was performed by Dr. Krisha Rajan. For an account of his methods, see Rajan (2006).

from atomic-scale computations, she added, can contribute to developing physics-based models for higher-level phenomena.

In rejoinder to an earlier comment by Dr. Hemker that atomic-scale computations at best provide "a strong suggestion about what the atoms are doing," Dr. Sinnott said the computations are better than that description would suggest, but that the materials modeling and materials engineering communities are not yet sufficiently familiar and comfortable with the strengths and limitations of these computational approaches. As a readily accessible guide to the state of the art in many-body potentials, she recommended the May 2012 issue of *MRS Bulletin* (Volume 37, Issue 5), which was subtitled *Three Decades of Many-Body Potentials in Materials Research.*

These potentials have historically been developed for materials with specific types of bonds, she explained, including Tersoff and other bond-order potentials for covalently bonded silicon, carbon, hydrogen, oxygen, etc.; Embedded Atom Method (EAM) potentials for nanoscale indentation, deformation, and dislocation generation and propagation in metals, as well as variations for metals and metal oxides; and rigid ion or Buckingham potentials for ionically bound materials, including nuclear fuels. Until about a decade ago, a multicomponent material system—one that included different types of material bonding (e.g., covalent and metallic crystal for a coating on an alloy)—was modeled on an ad hoc, system-state-specific basis that meant the resulting model was not generalizable. But, Dr. Sinnott said, beginning about 10 years ago, the importance of multicomponent systems to many material state applications spurred the development of *next-generation potentials* such as COMB (Charge Optimized Many-Body) potentials (Phillpot and Sinnott, 2009; see Box 3.3),[9] ReaxFF (Reactive Force Field) potentials (van Duin et al., 2001),[10] and others. These potentials are able to handle multicomponent systems with multiple bonding types within a uniform expression, said Dr. Sinnott, although parameterizing the system appropriately can be difficult because of the range of physical interactions to be included. An important benefit is that once a component—say, zirconium oxide—is parameterized in the expression for its potential, that potential can be reused in other systems containing that component—for example, a zirconium oxide coating on an aluminum alloy.

Dr. Sinnott illustrated the type of multicomponent system that can be modeled with these next-generation potentials with an example of a metallic copper to amorphous silica interface. Because of the amorphous component, this system cannot be realistically modeled using electronic-structure methods. The energy

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[9] For a list of additional publications on COMB potentials, see http://phillpot.mse.ufl.edu/publications/charge-optimized-many-body-comb-potentials-2008-present/, accessed October 2014.

[10] For further information on ReaxFF potentials, see Dr. van Duin's webpage at http://www.engr.psu.edu/adri/, accessed October 2014.

BOX 3.3
General Equation for a COMB Potential

$$E_T = \sum_i \left[E_i^S\left(q_i\right) + \frac{1}{2}\sum_{j\neq i} V_{ij}\left(r_{ij},q_i,q_j\right) + B_i\left(q_i\right) + C_i\left(r_{ij},\theta_{jik}\right) + E^{polar}\left(q_i,r_{ij}\right) + E^{vdW}\left(r_{ij}\right) \right]$$

$E_i^S(q_i)$ is a term for the self-energy
$V_{ij}(r_{ij},q_i,q_j)$ is a term for short-range interactions
$B_i(q_i)$ is a correction term based on charge
$C_i(r_{ij},\theta_{jik})$ is a correction term for neighbor interactions
$E^{polar}(q,r_{ij})$ is a term for polarization and Coulombic interactions
$E^{vdW}(r_{ij})$ is a term for van der Waals interactions

SOURCE: Susan B. Sinnott, University of Florida, presentation to the Workshop on Materials State Awareness, August 6-7, 2014.

potential her team developed showed that copper-oxygen bonds at the interface play a crucial role in the adhesion between the copper and the silica and that oxidation of the copper is limited to the first two layers of copper atoms in the metallic lattice. The model predicted that the work of adhesion decreases as the number of oxygen-atom vacancies increases.

In another example, Dr. Sinnott showed how a model using COMB potentials predicts stacking fault energies in polycrystalline nickel subjected to a tensile strength test with a constant strain rate that are in good agreement with predictions by EAM potentials. She also presented results comparing COMB potentials with EAM potentials for predicting stacking fault energies for aluminum deformation and results for COMB potentials compared with experimental data on bulk properties and edge dislocations at the γ/γ' phase interface in a nickel-based superalloy of interest to the Air Force.

Despite these recent advances in atomic-scale computational approaches for multicomponent systems, there remain some technical limitations to their widespread use that Dr. Sinnott characterized as “fundamental barriers” for the following reasons:

- Parameterization of transferable, next-generation potentials is nontrivial and a continuing challenge. For example, each of the terms in the general equation for a COMB potential, shown in Box 3.3 above, has many associated sub-equations, and each set of sub-equations has multiple parameters. For some historical potentials, multiple parameterizations exist.[11] Funding agencies unfortunately consider the parameterization effort to be a routine procedure rather than fundamental development, even though it may require 6 person-months of work.

- Validation of predicted trends and quantification of error bars—important features of a useful model—are harder at the atomic-scale level than with electronic-structure computations. With so many embedded parameters and so many variants in the algorithms for the potentials (Dr. Sinnott quipped that there can be "thirty different flavors" of EAM potentials for a single metal), quantification of the uncertainty in the model results depends on the variant used for a potential and on the uncertainties in the parametric values.
- Perhaps the most important barrier, she suggested, is a "lack of comfort" within the broader community with how and when these potentials work well and when the transferability of parameterized properties breaks down. Every computational method, she noted, has strengths and limitations; there are problems to which a given method can be applied and other problems to which a given method should not be applied. Whereas the materials community is familiar with the strengths and limitations of electronic-structure calculations and continuum-level methods (e.g., FEA methods), nonexperts, she believes, are still uncomfortable with atomic-scale methods. Without that comfort level, many potential users are not going to use these methods for MSA because they don't know how far and in what circumstances to trust them.
- Although dissemination of the methodology and even of computed potentials is straightforward (see footnote above on the Internet availability of COMB and ReaxFF potentials), maintenance (the further application of algorithms to new problems, the proper use of parameterizations, dealing with software glitches, etc.) is challenging. Determining how to distribute the cost of moving the methodology into a broader community of practice is an issue.

The last portion of Dr. Sinnott's presentation described cyber infrastructures and databases and their role in addressing the technical challenges of broader community adoption and application of atomic-scale computational approaches

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[11] Dr. Sinnott emphasized that the barrier here is not access to the algorithms or the available parameterizations. The COMB potentials are freely available on the Sandia Laboratories website, and the ReaxFF potentials are also on an open website.

to MSA. She commented on the following representative (not comprehensive) selection of databases and infrastructures:

- Some databases enable the rapid design of materials, such as the Materials Project founded by Gerbrand Ceder of the Massachusetts Institute of Technology and Kristin Persson of Lawrence Berkeley National Laboratory,[12] AFLOWLIB.org at Duke University and other participating universities, and the Center for Advanced Vehicular Systems Engineering Virtual Organization for Cyber Design at Mississippi State University (Haupt et al., 2012). These sources enable experimentalists and manufacturing professionals to go online and see what data are available or can be generated from the cyber infrastructure.
- Some cyber infrastructures provide a "bookkeeping framework" for the different variants of software codes and provide access to computational tools. Examples include the nanoHUB at Purdue University (nanoHUB.org) and the Cyberinfrastructure for Atomistic Materials Science (CAMS) at the University of Florida.
- Repository projects that provide published atomic-scale potentials along with metadata on the source, the computational variant used, and the strengths and weaknesses of a particular potential include the NIST Interatomic Potentials Repository Project, led by Chandler Becker in the NIST Materials Measurement Laboratory,[13] and OpenKIM (the Knowledgebase of Interatomic Models, https://openkim.org/) at the University of Minnesota.
- Several technical societies are providing online tools for navigating all of the cyber infrastructure relevant to their field, such as the TMS Materials Cyberinfrastructure Portal (http://www.tms.org/cyberportal/showData.aspx?tooltype=all#grid).

Dr. Sinnott is the director of CAMS at the University of Florida. Her objective for this cyber infrastructure is to advance the atomic-scale modeling of materials by increasing the "comfort level" in the user communities with how and when to use the various computational methods and the potentials calculated using them. She described CAMS as providing a "forum for disseminating new atomic-scale methods, educating nonexperts, and acting as a bridge between atomic-scale and complementary modeling communities." In addition to disseminating software codes and other tools for atomic-scale methods, CAMS has run summer schools

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[12] The homepage of the Materials Project is http://www.materialsproject.org/, accessed October 2014.

[13] For further information, see the repository's website at http://www.ctcms.nist.gov/potentials/, accessed October 2014, and Becker et al. (2013).

for students who want to learn how to use these approaches. Many of the lectures (briefing slides and/or audio recordings) from the summer sessions are available on the CAMS website (CAMS.mse.ufl.edu).

To conclude her presentation, Dr. Sinnott presented the following "big-picture challenges" for the computational methods and modeling approaches she had discussed:

- What is the role of theory / computational modeling in the design, processing, and application of materials?
- How do we integrate the latest computational approaches with experimental data to improve predictability?
- To what extent are computational methodologies available that are applicable to the *physics of interest* in actual systems (actual materials, relevant length and time scales)?
- How do we ensure that the next generation of scientists and engineers can work in this new paradigm?

To meet these challenges, she suggested the following directions for needed improvements: (1) natural workflow from discovery codes to predictive software; (2) tight integration between processing, characterization, and computational approaches; (3) accurate error bars for the results of theoretical/computational methods; and (4) widespread dissemination of software with robust documentation.

Questions and Discussion

Dr. Hemker commented that Dr. Sinnott's presentation emphasized a significant point that the first day's presentations, including his own, had not highlighted: the importance of thermodynamics in ICME. He sees an important role for these computational approaches that address the thermodynamics of materials behavior and materials states changes directly. The property volume element as he had discussed it seems to him to be a reasonable way to think about when computational methods are appropriate. Given that the volume elements for DFT computations are very small (some thousands of atoms), he asked, what volumes are feasible with atomic-scale computational methods?

Dr. Sinnott replied that length scales of hundreds of nanometers (10^{-7} m) are now very accessible in atomic-scale modeling, although the feasible scale depends on whether one is using a "classical" potential such as a Lennard-Jones or EAM potential, for which the computation is very fast, or a multicomponent, "multiphysics" potential such as a COMB or ReaxFF potential. As a comparison, she suggested, if the computational time for that length scale using Lennard-Jones potentials is 1, then the time using EAM potentials might be 2, and the time required using COMB potentials with the charge correction turned off might be 50. If the charge term is turned on and can evolve in time, then the relative time for the COMB computation would be about 200. By contrast, even with a thousand fewer atoms, the relative time for a comparable DFT computation would be 10^6, she said.

She agreed with Dr. Hemker's follow-up comment that many mechanical properties of materials such as fatigue and fracture emerge at a much larger scale. In her opinion, atomic-scale methods will never compete with other modeling approaches for those properties because, for example, the atomic-scale methods do not capture the long-range stress fields. She also has doubts about the value of coupling atomic-scale modeling approaches to mesoscale or even microscale models and running them simultaneously because the problem of boundary values for the atomic-scale computation is not solved with current approaches to such coupling. Instead, she would like to see atomic-scale computations used to inform the higher-scale modeling methods with respect to chemistry, composition, and microstructure. That is feasible, she said, and the information from such computations can improve the accuracy of the higher-order models.

Dr. Wadley asked Dr. Sinnott to comment on the feasible time scales for these computational approaches; for example, for what period of time can a cubic nanometer of material be modeled by these methods? Dr. Sinnott replied that the time scale is indeed "the Achilles heel" of atomic-scale modeling of materials behavior. The time is on the order of picoseconds to nanoseconds, she said (see Figure 3.8), and the larger the system, the shorter the time that can feasibly be modeled. Some very smart people, she added, are working on many variants of "accelerated dynamics" approaches, which aim to bridge the time scale up to seconds. For her, a big issue with such approaches is that for systems with numerous local minima in the potential energy surface, such as the thin-film systems that are one of her research interests, the computation can get hung up in those local minima and go nowhere. These computational approaches do work well, she said, for systems with just a few, deep minima in the potential energy surface.

Because there are so many talented people working in this area, Dr. Sinnott believes the "time barrier" will be overcome and time scales relevant to practical materials problems will become feasible to model. In some cases, she added, there are computational shortcuts ("tricks") that can be used to incorporate thermodynamics, similar to the trick of using periodic boundary conditions to represent far larger numbers of neighboring atoms than are discretely specified in the model. Other computational "tricks" can be used to mimic the physics associated with longer time scales, she said, and she offered to discuss these approaches further with interested participants at another time. "Sometimes they work, and other times not so well," she said, "but they are available." This led her to emphasize a point about the purpose and role of modeling:

> The point is not to model the experimental system. Modeling the experimental system and showing agreement accomplishes nothing. What a model needs to capture is the physics that is needed to answer the questions you care about asking. As Dr. Hemker said, "It's a dance." What are the questions you want answered, and does the model answer those questions with the physics needed for them? If the model does that, then the system modeled need not be the same as the experimental system.

Dr. Plummer asked how the computational approaches discussed by Dr. Sinnott would handle the increasing importance of multifunctional materials. How can phenomena such as electron-phonon coupling and magnetic ordering be handled by these methods? Dr. Sinnott replied that any phenomenon whose physics requires explicit electrons will require first-principles types of computation. If there is ferromagnetism, lattice interactions, etc., then some form of quantum mechanical representation with explicit electron terms is necessary for the computation. In this case, system size becomes a limitation. This is where materials informatics can help, because it can be used to examine the experimental data and the first-principles data for systems of limited size and to identify potential trends to examine further. She sees the guidance toward innovations and "discovery" from such explorations as being helpful in suggesting new avenues of exploration.

In response to a question on "coarse graining" approaches to modeling metallic and metal oxide systems, versus polymers, Dr. Sinnott said that coarse graining is wonderful for molecular systems—covalently bonded materials where a chemical moiety such as CH_2 can reasonably be treated as a sphere. But within that assumed sphere there cannot be any chemistry or composition changes. She has, for instance, used a coarse-graining approach to model micelle formation in water. But when she was modeling the tribological deformation of polytetrafluoroethylene thin films, coarse graining could not be used because the model needed to allow for fluorine-carbon bond breaking. So again, she said, what you do in your model depends on the physics you care about. If conformation is the concern, then breaking covalent bonds is not an issue and coarse graining is a wonderful way to solve the "time scale" constraint. A question like "How does a protein fold [into its biologically active conformation]?" is a long–time scale problem, as is the question of the viscoelastic response of a polymer. For metals and ceramics, she continued, most of the problems of concern involve a metal atom moving or atoms of a metal and oxygen dissociating or otherwise changing their relationship. Those types of changes are not amenable to coarse graining, and she has not seen it applied to metallic or ceramic systems.

Dr. Hemker commented that earlier in the workshop, the effect of the environment on material state had been flagged as an important theme. That's a kinetics problem, he said; he asked how atomic-scale computational methods could be used to handle those kinds of kinetics-driven changes. Dr. Sinnott agreed with the importance of the question and illustrated her answer with a research problem on which she is currently working: the growth of a silver layer on a zinc oxide substrate. Her team is using DFT computations to calculate the barriers to silver atom movement on the zinc oxide surface. Those data on barriers and movements will become input to a kinetic Monte Carlo simulation of the system. That simulation will lose any mechanistic insights as to how the growth progresses (the time-dependent changes in state), she noted, but it can quite quickly predict the thermodynamic end state.

CHALLENGES AND OPPORTUNITIES FOR MSA APPLICATIONS

Each of the workshop presentations summarized in this section provided an individual perspective on one or more aspects of practical applications for MSA. In some cases, the focus was on the current status of an application area and ongoing R&D in that area. In other cases, the focus was on an emerging application area or a longer-term perspective on what might be feasible with the tools for MSA that the presenter described.

In addition to their contributions to the third workshop theme, "Challenges and Opportunities for MSA and its Applications in System Life Cycle Management," these presentations also provided valuable insights on what MSA is (now) and what it should be (or could be) in the future, next steps for MSA, and future visions—or at least the future visions of these particular subject matter experts.

Implications for Condition-Based Maintenance and Life Extension Decisions

Dashiell Kolbe, Staff Application Engineer,
Integrated Vehicle Health, General Electric Aviation

In his introduction Dr. Kolbe noted that in the aviation field, General Electric was formerly primarily an engine developer, supplier, and supporter. These roles are now being supplemented with work in avionics and aviation-related data analysis. Recent acquisitions and expansions have added capability in flight data analysis technology, airplane diagnostics and prognostics, and Tier 0 and Tier 1 support for aircraft development.

At a corporate level, GE has been doing system health management for a long time, he continued, and at multiple levels. For example, at any given time, GE has about 20,000 aircraft engines in operation, as well as 10,000 flight data recording systems, 9,000 diesel-electric locomotives (GE Rail), 20,000 industrial turbines (GE Energy), and 60,000 medical imaging systems (GE Healthcare). Dr. Kolbe works at the interface with GE's industrial customers, so he sees all of the technological capabilities GE has developed for system analytics (which includes both diagnostics and prognostics) as a large and diverse toolbox that can be offered in a customized solution set to meet a customer's needs.

His first example of system health management was the Integrated Vehicle Health Management (IVHM) capability developed for the U.S. Navy's F-18 fighter aircraft. During a mission flight, the aircraft records data from its health monitoring sensors in a mission computer, whose data storage capacity is hundreds of gigabytes, although that capacity is shared among a number of systems, including the IVHM system. Some data preprocessing/data fusion occurs on board. Because the data fusion algorithms were developed early in the F-18's history, problems have arisen in the intervening time. One such problem is that some data for health analytics that one might like to get from the monitoring sensor system are not available by the time the data are "on the ground."

The recorded data are not transmitted during flight; instead, when the aircraft has landed, the data cards with the stored data are pulled by a technician and plugged into a ground data receptacle to be read and transferred over a secure system. The data transfer rate is on the order of tens of megabytes per minute, so the data transfer time is measured in hours. (Dr. Kolbe said the data download rate of the new F-35 Strike Fighter is about the same as that of the F-18.) This leads to a second problem, said Dr. Kolbe; there may not be enough time to transfer all of the stored data from one mission before the aircraft is needed for its next sortie. Since all of the data cards must be in the aircraft before it can take off on the next mission, cards can be "marked as processed" by the technician pressing a single button on the data receptacle. This erases any untransferred data but allows the card to be returned to the aircraft. When data are missing, Dr. Kolbe explained, any Life Usage Indicators in the health management analysis system that rely on those data cannot be computed.

A final problem or bottleneck for effective health management is that there is no single repository for the flight data downloaded from a given aircraft. Military aircraft have different data repositories at different levels of maintenance, including operational levels and depot levels. Although there are handoffs of data between these repositories, Dr. Kolbe said, the handoff processes still introduce additional errors into the data sets.

The consequence of all of these data collection and integrity issues, he said, is that the analytics can signal for premature equipment exchanges or can signal safety-related flags that do not accurately reflect the operational experience of an aircraft. Or, a data handoff error can lead to a safety issue not being noted. In addition, even when an anomaly is detected and correctly reported, Dr. Kolbe said, those responsible for acting on the anomaly report often want to first download and review all of the relevant flight data themselves, to determine if the anomaly report is valid, because they do not trust the system. With time, the number of e-mails questioning details in anomaly reports does decrease, he added, as people build trust in the system.

Dr. Kolbe's second example was the engine diagnostics of C-5 transport aircraft. There is much less health monitoring instrumentation on the C-5, he said, than on an F-18 or F-35. When single-point solutions for improving the engine diagnostics are used—such as adding a sensor or other monitoring system component; improving the onboard computer that captures and preprocesses the sensor data; or making a single-point improvement in the ground system for receiving the engine data, doing the analytics, and preparing a report—these solutions typically run into a roadblock. There may be a bottleneck with transferring data off the aircraft because of hardware or security constraints, or there may be an operations bottleneck. To make a large enough difference in value to overcome these obstacles, he said, a total-system approach is needed.

Next, Dr. Kolbe discussed the analytic problems raised by "the curse of dimensionality" or having so much data that the number of possible data combinations to be analyzed becomes unwieldy. Techniques for reducing the amount of data that go into diagnostic analysis can greatly improve the value of that analysis because results can then be reported in a timely manner.

Another practical consideration, Dr. Kolbe said, is that the value of key performance indicators depends on the context of use. In some contexts, a health management system that reduces fuel and maintenance costs may be of greater value to the user, whereas another user may put far greater weight on ensuring that the personnel who are traveling get to their destinations within a high-priority time window. He also described why an "80 percent solution" in aircraft health monitoring may be a better value to the customer than a monitoring system that in principle should give "better" health information but that has much greater time and resource costs.

GE provides many of the health and usage monitoring systems (HUMSs) that are used for aircraft, and especially for rotorcraft, throughout the world, Dr. Kolbe said, particularly in the United Kingdom, Europe, and Asia. HUMSs became so popular, and are now frequently mandatory on rotorcraft, he said, because of several high-profile accidents that occurred. Before HUMSs, scheduled maintenance was the norm for rotorcraft fleets, but investigations of unexpected helicopter crashes were finding that bearings were failing. A system was needed that could detect bearing wear before failure occurred. The key benefits of a HUMS that could detect bearing wear before a transmission or gearbox failure were in cost avoidance—avoiding the loss of aircraft availability and avoiding the loss of the aircraft and potential loss of life—more so than the cost savings in replacing a bearing versus having to repair or replace a larger subsystem such as the whole transmission. Because of the high-profile incidents that had occurred, however, the HUMSs were accepted by customers independent of what could be quantified as maintenance cost savings for the system.

In response to a question about how much of the HUMS sensing and analysis could be done remotely, rather than locally, Dr. Kolbe said that these systems have been evolving. Initially almost all of the analysis had to be local, he explained, because a sensor had to be near the source of the vibration to make a successful determination. More recently, virtual sensor networks have replaced some of the need for a local in situ sensor, he said, and models that can simulate what an in situ sensor would detect are also coming into use. As an example of the latter, he cited the Virtual Twin methodology being developed by AFRL to assess the level of wear and potential damage that a particular aircraft has experienced.

There are many components and subsystems on an aircraft that have been identified as high-value areas for applying CBM or IVHM solutions, Dr. Kolbe said. In the propulsion/engine system, these include the controls and sensors of full authority digital engine control systems; gas-path components; and the gears, bearings, and shafts. In the airframe and structural components, monitoring for loads and usage and for environmental conditions can have high value. Flight controls and sensors are also high-value components worth monitoring, as are mechanical and hydraulic subsystems for landing gear and flight control systems, the electrical power generation and distribution subsystem, avionics, electrical and electronic interconnects, digital networks, and payloads.

In his summary, Dr. Kolbe described the holistic view of CBM or IVHM that his organization uses. It starts with data sources that include in situ sensors or virtual sensing via modeling and simulation. Data from these sources need to be acquired, transferred, and analyzed, and the results from the analysis need to be acted upon, whether that action involves a specific maintenance activity on one aircraft, a systemic change to a procedure, a supply chain or redesign change, or an input to subsequent system design. This sequence makes use of sensor/acquisition technologies, communications technologies, and analytic/decision support technologies, combinations of which are packaged into various "product" combinations to meet the specific needs and values of a customer, offering them a total CBM solution. It is this total solution, he emphasized, incorporating the entire chain from input data to decision support and user action, that provides the overall value that customers will accept and buy into.

Questions and Discussion

During Dr. Kolbe's discussion of engine diagnostics for the C-5 aircraft, Dr. Achenbach asked if the data transfer and data management problems could be mitigated by collecting data intermittently rather than with continuous system health monitoring. Dr. Kolbe agreed that continuous monitoring is not necessary;

the value objective should perhaps be to provide critical information at the critical time. He gave an example of how an interactive system that allowed human monitors to inquire about specific key parameters informed a reasoned decision that a temperature reading mismatch was most likely due to a sensor fault.

After the summary on what constitutes a total CBM or IVHM solution for a customer, Dr. Schafrik asked Dr. Kolbe to comment on the view that military customers were behind the commercial sector in embracing this holistic view. Dr. Kolbe replied that there seemed to be a general impression along the lines that Dr. Schafrik described. In his three principal customer categories—business/personal jets, commercial aviation, and military aviation—in general the growth in operational deployment and usage of this "total solution" approach has come first in the business/personal sector, then in commercial aviation, and then in military aviation. But, he said, there are a lot of caveats and exceptions to that generalization.

One reason for this difference in timing of acceptance and operational use, Dr. Kolbe continued, is the relative complexity, and the nature of the complexity, of operations in the three sectors. Transfer of a new concept into operations in the business jet world is more streamlined, he explained, in that the original equipment manufacturer (OEM) typically manufactures aircraft that will be bought and managed by a company that provides a total service package to its corporate (or personal) customers. That company has direct connections back to the OEM and engine manufacturer and forward to the end users, which makes adoption of these technology-based solutions easier. In the commercial aviation sector, transfer of new technology into operations has to navigate additional entities and interests such as mechanics and pilots' unions, supply chain diversity, and other impediments. Organizing and implementing the transfer is thus more difficult, he said; to make that transfer occur in the military aviation sector expands the complexity and the difficulty "by an order of magnitude." To illustrate, he listed the number of different databases of component information that exist in military supply and logistics chains, maintenance organizations, and financial systems. "None of those systems talk to each other," he remarked.

Dr. Achenbach referred to the 15-year strategic plan that Airbus has for introducing advanced system health monitoring in its commercial aircraft, which he had described at the end of his presentation, and suggested that it showed how an OEM, being a single company, could move forward in this direction on its own. He and Dr. Kolbe discussed whether there would still be problems with effective data acquisition, transfer, and analysis if the data generated by the embedded sensor systems during operational use were the property of the airline.

Mr. Lindgren of AFRL commented that for the military sector, an additional difficulty is adapting a new approach, such as the one Dr. Kolbe had discussed, for a fleet of legacy aircraft acquired in the 1960s and 1970s and the legacy maintenance systems that were acquired with them. Another difficulty is taking both platforms and operations that were systematized in the 1960s, for example, and reintegrating them into a new system construct. "There are a whole bunch of challenges there," he said, and he agreed with Dr. Kolbe that working the information flows among the different data systems and databases presents another huge challenge. Describing the military as being behind, he said, is not quite correct; it's that the complexity of the intrinsic hurdles due to the military's operational environment is much more challenging than, for example, in the business jet operational environment. Dr. Kolbe agreed with Mr. Lindgren's description of the problems in transferring these concepts into military operations. Mr. Lindgren added that the military can take some credit, as some of these concepts have originated in military R&D establishments; overcoming the implementation obstacles is the challenge.

The Emerging Role of ICME and ICSE in Airframe Design Analysis

Dale L. Ball, Lockheed Martin Aeronautics Company

Dr. Ball's presentation focused on the application of ICME and integrated computational structural engineering (ICSE) at the airframe level, particularly the design phase of an aircraft structures development program. In his introduction he emphasized that what the materials science community does with MSA has direct and important impacts on what is done in the structures community. He sees physics-based modeling as a key technology in the set of technologies whose further development will improve, directly or indirectly, the MSA capability of engineered systems throughout their operational lives. These technologies enable improved MSA capability insofar as they enable higher-fidelity definition of the initial state of a materials system, as this initial-state definition is a necessary precursor to viable prognostics capability during the system's operational life. Much of the technical information in his presentation, he noted, came from work done under the Metals Affordability Initiative (MAI) Consortium, particularly the contributions of the MAI BA-11 Team on large aluminum forgings and advanced techniques for measuring residual stresses in structural forgings. The MAI Consortium of 14 companies was formed in 1999,[14] and projects funded under it are required to have focused technical efforts, focused and defined implementation plans, and significant and realistic business cases (Bayha et al., 2002).

By way of an introduction to the ICME initiative, Dr. Ball said the vision for ICME was to (1) develop *computational* tools for materials discovery, design, development, and sustainment; (2) develop *experimental* tools for discovery, character-

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[14] Dr. Ball noted that the MAI Consortium includes the three major airframe OEMs—Lockheed Martin, Boeing, and Northrup Grumman—as well as engine manufacturers and major Tier 1 suppliers such as Alcoa and TIMET.

ization, validation, and verification; and (3) integrate these tools with information technologies, manufacturing-process simulations, and component design systems, to realize the ability to (a) develop and deliver optimized materials and manufacturing processes; (b) provide improved product performance, manufacturability, and sustainability; and (c) provide these capabilities at reduced cost and time.

The particular application of ICME on which his presentation focused included both the design and the manufacture of large aluminum forgings for advanced fighter aircraft and the sustainment of those aircraft structures. ICME is being used by Alcoa, Dr. Ball noted, to optimize the forging process, to predict process-induced bulk residual stresses, and to characterize intrinsic material properties. The focus of the BA-11 program within the MAI Consortium, he explained, is incorporation of residual stress modeling into the design, manufacture, and sustainment of advanced airframe structures. The specific objective is to account for residual stress in life cycle management (including design, manufacturing, and sustainment) of the F-35 Joint Strike Fighter, and, Dr. Ball said, the program is also intended as a demonstration of ICME capabilities. Box 3.4 lists Dr. Ball's set of projected benefits from the BA-11 program. He also discussed the published roadmap for MAI BA-11 program development and validation activities (Bucci et al., 2014, slide 10).

The next section of the presentation detailed how the computational capability of ICME is advancing the ability to design large aluminum forgings such as major airframe structural components. For a number of years, Dr. Ball began, Alcoa has been working on using forging process modeling to design and optimize for consistent and low residual stresses. The current generation of models can predict

BOX 3.4
Projected Benefits of the MAI Consortium's BA-11 Program

- Accelerate technology insertion and uncertainty management
- Accelerate design and build of first article(s)
- Link manufacturing process knowledge to mechanical behavior, life prediction, and sustainment
- Incorporate manufacturing and processing variability into next-generation design and life management processes
- Reduce testing (design allowables, certification)
- Reduce number and cost of design iterations
- Reduce cost of scale-up

SOURCE: Dale L. Ball, Lockheed Martin Aeronautics Company, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 8.

post-quench residual stress in a forging, post-cold-work residual stress in the forged part, and the residual stress in the final machined part. (Machining adds distortions and stresses in addition to those from the prior process steps.) This modeling is used to understand and mitigate bulk residual stress by the modification of quench practices and the use of a proprietary cold-work process called *Signature Stress Relief*™. The process model simulates four major processing steps: (1) heat treatment (elevating the forging to the heat treatment temperature), (2) rapid quench (which induces high tensile stresses in the core of the forging), (3) cold-work stress relief using Signature Stress Relief, and (4) machining of the forged part to the final part profile. Alcoa is using this modeling currently, he said, to optimize its processes and improve its products.

Modeling of each of the steps is fairly sophisticated, Dr. Ball noted, but especially the constitutive modeling of the first two steps, which must accurately simulate both the material's response to plastic deformation at temperature during forging and the material's elasto-thermal-viscoplastic behavior during rapid quenching. The detailed FEA modeling of the machining step currently simply simulates the removal of material from the worked shape; it does not simulate the action of the machining process on the material properties, including residual stresses. Dr. Ball talked through high-level features of the stress modeling in each of the four processing steps, using illustrations from Bucci and colleagues (2014, slides 12 through 17). The evolution of the residual stresses can be tracked across the steps in the fabrication process, starting with a wide distribution of substantial stresses and moving toward narrower and narrower distributions of lower stresses clustered within a narrow target zone of ±10 ksi (Bucci et al., 2014, slide 16).

The MAI BA-11 team is working on a business model, Dr. Ball said, for delivering a detailed residual stress map to the OEM for use in airframe design (Bucci et al., 2014, slide 17); this map will become part of the ICME product, or computational materials data, bought from the forgings supplier. Having this kind of knowledge, he emphasized, is the objective that allows design engineers to do a better job during the design stage of the system life cycle. Having a detailed map of the residual tensile stresses means not only that they can be accommodated in machining analysis calculations but also that these stresses are defined in the initial materials state in predictive modeling for fatigue and fracture calculations that are central to SLP.

Next, Dr. Ball discussed residual stress measurements used to validate the process model predictions. The BA-11 team wants to validate with experimental data the narrow distribution of relatively small residual stresses (±10 ksi, with most of the stresses within the ±5 ksi band) predicted by the processing model, he said. While noting that there are well-established NDE methods for estimating residual stress, such as x-ray and neutron diffraction techniques, he focused on a destructive technique called the *contour method* (Bucci et al., 2014, slides 19-28). Developed at

LANL, the contour method is based on the concept that residual stresses will result in deformations of the surface of a freshly cut cross section of the part in question (Prime, 2001). A detailed FEA model can be used to estimate the forces that would be required to "undo" the displacements and bring the surface of the cut back to a state with zero displacement anywhere on the surface.

Dr. Ball said that the structural design community likes this method because it can provide a measurement-based representation of the full two-dimensional stress field. He described tests done for the BA-11 team that computed the full-field residual stresses in a set of 7000-series aluminum coupon blanks machined from a quenched log of forged aluminum. In a further step, various coupons were then machined to add typical holes or pockets that might be present in an actual part, and the modeled stresses at the "design feature" in the simulated machined "part" were compared with the stresses measured by the contour method on an actual coupon machined to that design. Overall, Dr. Ball said, the simulated stress fields and the stresses determined by contour-method measurements have "compared very well, although the agreement is not perfect." The results have been encouraging enough that the team is continuing to pursue both the process modeling approach and the contour method validation approach.

He also presented some preliminary results from simulations of the processing of actual aircraft parts (7000-series aluminum bulkhead components) with contour-method residual stress measurements on physical specimens. With respect to a comparison of the simulated residual stress in a large forged bulkhead for the F-35 with results from sectioning an actual bulkhead and using the contour method to measure the stress field, Dr. Ball said the very good qualitative agreement between the complex modeling result and the measurement-based results was very encouraging. He also presented data showing that the contour method results were confirmable by more direct measures of residual stress such as hole drilling in an actual bulkhead.

The significance of this work, he emphasized, is that the process model together with the contour method validation provides the means to understand residual stresses and strains and to account for them properly in design. In the past, he said, there may have been mechanical property data derived from coupon blanks like those used in the contour method testing or design calculations that lacked appropriate representation of the part-specific bulk residual stresses.

The BA-11 team and Alcoa are also using the contour method to investigate the variability of residual stresses both in different locations in a component with a complex final structure and in different specimens (six to eight samples) of that component. Dr. Ball reviewed some of the results from this work that were presented at the 2013 Residual Stress Summit (James, 2013).[15] The contour data, he

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[15] Dale Ball, Lockheed Martin Aeronautics Company, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slides 23-26.

said, confirm there is good consistency across multiple forging samples of the same component in both stress field pattern and the tight distribution of stress values within the manufacturer's target zone of ±10 ksi (80% were within ±5 ksi for the six forgings tested by the contour method).

In the final section of his presentation, Dr. Ball supported the view that the ICME concept can and should be applied to structural development.[16]

By applying the ICME precepts to the structures domain we arrive at Integrated Computational Structures Engineering, or ICSE, which seeks to:

- Develop computational tools for loads, strength and life analysis (as required to support structural design), manufacture, test, and sustainment;
- Develop experimental tools for characterization, validation, and verification; and
- Integrate these tools with information technologies, manufacturing-process simulations, and component design systems.

Elaborating on the last point in the above list, he said the most important contribution of ICSE, in his view, was that it leads to the integration of engineering disciplines that heretofore have been separate and often "stovepiped" in isolation from each other: system life estimation, strength, weight management, dynamics assessment, and many others that come under the broad "structures" umbrella. Bringing these communities into an integrated environment will result in an improved design process and improved designs, he said.

The objective of the BA-11 team in using large aluminum forgings for aircraft bulkhead structures to demonstrate the feasibility and potential value of ICSE was to show that the residual stresses from the overall forging and fabrication process (from forging to final machining) could be explicitly represented, managed, and incorporated in the design process, rather than only being implicitly addressed. Dr. Ball characterized the legacy approach as addressing bulk residual stresses implicitly, when they are known to exist, by use of conservative material data for strength and life calculations. He contrasted this with the advanced approach (ICSE), which includes:

- Generating intrinsic, residual-stress-free, material property data on fatigue crack initiation, fatigue crack growth rate, and fracture toughness;
- Using the four-stage process simulation (forge, quench, cold work, and machining) to predict residual stresses and deformations in finished parts; and

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[16] Dale Ball, Lockheed Martin Aeronautics Company, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 28.

- Incorporating tensile residual stresses *explicitly* in strength and life analyses of affected locations.

To incorporate the residual stresses explicitly, they must be representable during design with respect to their spatial distribution and magnitude at each location within the part. The stresses were modeled by detailed FEA modeling, with validation of the model results through experimental testing by the contour method and by slitting and hole drilling.

The ICSE approach, he continued, was implemented in a prototype integrated structural analysis tool that incorporates the intrinsic material property data with the residual stress generated by the fabrication process. The analysis tool has an auto-zoning capability, with a predefined residual stress for each zone, and uses location-dependent fatigue stress spectra to compute fatigue-crack-initiation-based and fatigue-crack-growth-based allowable stresses. These allowable stresses are then used to size the structure to accommodate the residual stresses represented in the simulation. This tool was applied to the design of four to six bulkheads from each of three design variants (a total of 15 bulkheads) for the F-35 Strike Fighter, with 800 to 2,000 control points per bulkhead (7,000 control points per design variant).

The ICSE design analyses were compared with the legacy design approach at each control point with respect to the design-allowable stress. Dr. Ball presented data for one bulkhead for which the ICSE analysis indicated 49 control points (from a total of 1,113 control points for the bulkhead) where additional material was needed to satisfy a decreased design-allowable stress (decrease from the legacy design analysis) and 25 control points where the ICSE analysis indicated the allowable stress could be increased and the forging could potentially be made lighter (less material). The ICSE analysis for a second bulkhead indicated 85 control points (out of 1,443 total) where greater thickness was needed to satisfy a decreased design-allowable stress and 300 control points where the bulkhead thickness could potentially be reduced. Dr. Ball described the first bulkhead as appearing to be fairly well optimized already, based on the advanced analysis compared with the legacy approach, whereas the comparison for the second bulkhead indicated significant opportunities to avoid problems, improve damage tolerance and service life, and reduce the overall bulkhead weight by 5 percent. These kinds of data, he noted, are valuable for optimizing the aircraft structure with respect to residual stresses, strength, and service life requirements.

In his closing summary, Dr. Ball said that the exposure of the airframe community to ICME up to this point has been limited. Now, with the availability of sophisticated models to simulate the forging and fabrication effects on materials state and the increased use of ICME in the design of new materials, he anticipates that the airframe community will begin turning more frequently to ICME-informed applications. He added that, although he had not addressed MSA during operational life directly, both ICME and ICSE are critical to providing high-fidelity representation of the initial state of a fabricated article as it enters operational life. Having ICME capability improves our knowledge of the initial state, he said, and that in turn will be paramount in proper implementation and realization of MSA applications (such as the Digital Twin and Digital Thread programs), in which success requires probabilistic prognostics of the effects of operational experience on that initial material state.

Questions and Discussion

Dr. Schafrik asked if experience with the ICSE analysis tool had reduced the time required to design a structural part such as a bulkhead. He said that a similar approach had cut the number of prototype forging die designs for a jet turbine blade from three prototypes to just one. Dr. Ball replied that it was too early to say whether the specific ICME/ICSE activity he had discussed was going to shorten the design cycle. Thus far, he said, it has not reduced the time required; the technology needs to mature and produce enough confidence in it before it will significantly affect the design cycle time. He described the history of bulkhead forging decisions for the F-35 and ascribed the trend toward acceptance of "less fat" designs (bulkhead "right-sizing" decisions) to growing confidence in both the aircraft system requirements and the final configuration of the part. If the ICSE technology he described had been in place in 2004-2006, he speculated, the cycle for right-sizing the bulkheads might have been shortened by several years. But, he added, since it didn't happen back then, he does not know for sure.

Dr. Hemker asked about the status of the material models. If a designer asked, for example, about using an aluminum alloy with smaller grain size, higher strength, but lower creep resistance, would that lower creep resistance show up in lower residual stresses in the simulations? Or if designers thought a thinner structure could have better heat-shedding behavior, would that flow down into the design simulations? Dr. Ball replied that those were excellent questions to ask. The hitch is that Alcoa keeps confidential the details about the material and forging process parameters used for the development of its proprietary alloys. If they were asked for explicit data specifications used in these models, he guessed they would be unwilling to release that information. He and Dr. Hemker discussed further the practical value of enabling designer-initiated options to feed back to the materials supplier/developer. Dr. Ball added that Alcoa had been an outstanding partner on the BA-11 team's work and had worked closely with the team, even though some proprietary details had been closely held.

Dr. McGrath described a case study by the Massachusetts Institute of Technology of the design decision by the Swiss in their version of the F-18 to use titanium rather than aluminum for the bulkheads. Several hundred engineering changes rippled through the design from that material change decision, he said, including changes to the flight control software. He suggested that the coupling of the feedback loop, enabled by ICSE, from design changes in materials to system-wide consequences, would have major implications. Dr. Ball agreed with the point and mentioned similar issues that have come up concerning the performance trades with substituting titanium for aluminum in one or another bulkhead in a CTOL (conventional take-off and landing) version of the F-35. The substitution changes internal load distribution and a lot of other structural characteristics, he said.

Dr. Bayoumi commented that a group led by John Bell at North Carolina State University began the modeling of residual stresses from forging and fabrication processing in the late 1970s and 1980s. Mr. Lindgren asked if the OEMs or the BA-11 team have thought about using this process modeling capability to simplify the certification processes for replacement materials and/or parts as part of service life extension for an airframe, when the aircraft's operational life is extended beyond its original design life. Dr. Ball replied that there is not an easy answer to the question. Numerous researchers have studied the impact of life-extension technologies on life analysis, including work done at Lockheed Martin on the beneficial impact on service life of compressive residual stresses. However, those benefits are generally not counted toward service life when doing component design; instead, they are taken as balanced against unplanned-for realities of operational life, such as more severe than anticipated usage or increased stresses or loads. With respect to use of the models, he added, the fatigue crack initiation and crack growth models and other modeling of stress-related material state behavior would be the same for the certification of replacement materials or components.

Measurement of Material State Change and Physics-Based Prediction

Prasun K. Majumdar, Department of Mechanical Engineering,
University of South Carolina

Dr. Majumdar's group at the University of South Carolina has ongoing activities in nanocomposites, material state evolution and life prediction, multiphysics and multifunctionality, and 3D image–based analysis. The range of applications to which this work contributes is illustrated by the research centers at the university with which his group is affiliated, including the Ronald E. McNair Center for Aerospace Innovation and Research, the Center for Multiphysics of Engineered Functional Materials and Structures, the Solid Oxide Fuel Cell Center, and the HeteroFoaM Center (a U.S. Department of Energy [DOE]–funded Energy Frontier Research Center specializing in heterogeneous functional materials for energy systems, including fuel cells, batteries, and membranes).

In the introduction to his first topic, the role of material state evolution in life prediction, Dr. Majumdar pointed out that although composites are not new (there are now more than 60 years of performance history in multiple disciplines), life prediction for composites is still an ongoing research area. The reason why life prediction research is ongoing, he believes, is that the target has been evolving: the problems to be addressed are increasingly complex. He defined "material state" as the constituents of a material and their arrangement at the atomic and at the nano-, micro-, meso-, and macroscales. Changes in material state can happen at all of these scales, and material state change is typically a multiscale process. These scale-specific processes occur continuously at their respective "local levels," he continued, but one may not observe the ultimate macro effect (e.g., the effect on global properties and service life) of these processes immediately. The as-manufactured material state of a structural composite or other heterogeneous material is changed by the system's operating conditions, and the durability and remaining life of the system depend on the details of these local (scale-specific) changes. And that, Dr. Majumdar said, is why life prediction for these materials is so challenging.

A life prediction framework for a material system always incorporates a set of key ingredients, Dr. Majumdar said, including knowledge of the initial material state of the system (how it was made, its microstructure and nanostructure), how the material state has evolved, knowledge of property degradation changes, the constitutive law for the relevant physics affecting the system, and a failure theory (including continuum damage mechanics and discrete damage mechanics) to follow how material state changes will eventually lead to failure. All of these ingredients feed into the last key ingredient, a rate equation for the remaining service life of the system. The goal of his presentation, Dr. Majumdar said, was to provide information to help understand how the first set of key ingredients (specifically, the relationship between material state evolution and property degradation) contributes to the final step of deriving a rate equation for remaining life.

Because composite materials are, in effect, designed to survive the development of defects or to sustain damage at multiple locations distributed through the material, he said, finding a single defect or point of damage is not the goal when predicting remaining life, as it may be for a homogeneous metallic material. The material state evolution of a composite is not a problem of damage propagation for the majority of the composite's service life. Rather, he explained, the state evolution involves a distributed accumulation of defects, then increasing interaction among these defects, and finally a much shorter but rapid "propagation" phase that occurs near the end of life, just prior to the final failure of the composite material. Thus, the goal in composite design, he concluded, is not to remain defect-free but to design for damage tolerance, substantially delaying that final phase of fracture path propagation leading to material failure. Dr. Majumdar illustrated this general principle of damage-tolerant design with diagrams of the stages of damage evolution from damage/defect initiation through the extended stage of gradual damage accumulation and growth, followed by interaction among damage/defect locations and then the final, relatively rapid stage of fracture propagation (Reifsnider and Case, 2002).

During the extended stage of gradual damage accumulation, he said, the global (or bulk) properties of the composite system do not change. For example, strength and stiffness do not change quickly or substantially during this stage. But the ability to predict an incipient fracture path is very important. Within this broad framework, Dr. Majumdar said, there are many complementary approaches to material state and life prediction with similarities and differences. He stressed that no single approach is (or needs to be) better than all of the others in all metrics; the aim is to use them collectively to serve the major objective of reliably predicting remaining service life prior to catastrophic system failure. Efforts that have produced significant recent progress include postmortem NDE, detection methods (which are relatively mature at the macroscale but an ongoing R&D activity at smaller length scales), and two-dimensional and 3D ex situ visualization techniques, including those described in other workshop presentations (see section above on “The State of the Art in Applied MSA”).

The current challenges, he said, include areas in which there has been limited effort to date or areas that are yet to be explored. Challenge areas he mentioned were in situ NDE at multiple length scales; techniques to identify mechanisms, capture anisotropy, and follow interactions among locations in the evolving material state; 3D in situ (not ex situ) visualization methods; and predictive formulations that incorporate variables representing the directly measured information on extent and distribution of damage, anisotropy, and other relevant elements of current material state. Furthermore, these predictive formulations also have to achieve reliability without requiring so many empirical inputs that they are impractical to use—a capability that Dr. Majumdar called “reduced empiricism.”

The challenge of reduced empiricism, he said, is echoed in the Digital Twin program, which is a joint DOD and National Aeronautics and Space Administration (NASA) effort to reduce expensive experiments and speed up certification. But the program’s objective of “model before flying” may not be achieved, he cautioned, without an appropriate description of the defect/damage-producing mechanisms and knowledge of their relation to available empirical measurements. Durability cannot be understood without identifying material state changes in response to the operational environments and conditions experienced. A successful predictive formulation, he said, will have to incorporate representation of engineered local features so that the effects of those features on interaction and propagation can be captured.

Beyond these current challenges for MSA, Dr. Majumdar highlighted multifunctional composites and multiphysics as emerging challenges. He cited NASA’s 2012 space technology roadmaps as listing innovative multifunctional concepts as top-priority technical challenges, and he noted that an NRC review of the draft NASA roadmaps stated that "multifunctional structures concepts, such as those involving thermal-structural and electrical-structural functionality, are likely to find broader applications" in addition to the spaceflight applications in the roadmaps (NRC, 2012, pp. 53-54). How does one understand and model the material state evolution and modes of degradation, Dr. Majumdar asked, when the physics of electrical current flows and of electrical/electronic device performance, for example, are factors in system life, in addition to the physics of mechanical stresses and loads that have been the focus of life prediction frameworks? Life prediction of multifunctional material systems, he emphasized, cannot be done unless the material state evolution of those synergistic and interacting property domains can be successfully modeled. He identified the following components of an approach to address these emerging challenges:

- Material state change due to multiphysical effects should be represented.
- Interactions should be captured so that evolution into emergent properties can be understood.
- Representation should be usable in predictive formulations.
- In situ visualization (contact or noncontact method) is needed to provide experimental input, insights, and verification of predictions.
- Predictive formulations also need to account for multifunctionality and synergistic multiphysical effects.

Next, Dr. Majumdar presented the ongoing work by his research group to address the current and emerging challenges and opportunities in system life prediction (SLP). This work is based on the concept that the extent of damage in a material system affects the polarization of charge as electrical voltages are applied across the material. The changes in polarization provide a measure of the level of damage via these electrical characteristics. His group is using AC impedance spectroscopy (and a similar technique named Broadband Dielectric Spectroscopy, which uses different hardware) to follow the evolution of damage in heterogeneously conductive composites such as woven and laminated carbon- and glass-fiber reinforced composites, particularly during the intermediate, precatastrophic stage of fracture path formation, and to quantitatively estimate remaining life (Reifsnider et al., 2009; Fazzino et al., 2009; Reifsnider and Majumdar, 2011; Majumdar et al., 2013).

In an undamaged sample of glass/epoxy composite (which is predominantly insulating), he explained, there is an inverse relationship between measured impedance and the AC frequency of the applied voltage. In a fully damaged sample, where a fracture path extends through the thickness of the composite, a conductive response is observed (i.e., no change in impedance with frequency). He then gave examples of how the graph of impedance versus frequency changes as fatigue damage increases. Because the material response is anisotropic, he said, the measured variable of interest must be captured and analyzed as a tensor property. The size, shape, and distribution of charge conduction sites (i.e., damage sites) determines the dielectric characteristics of the material, and the increasing interaction among the sites as the average distance between them decreases can be captured by observable field effects.

The research group is accumulating data on the material response of carbon/epoxy and glass/epoxy systems to both mechanical and electrical damage. They can measure and predict anisotropic tensorial damage in these systems, including the directional dependence of damage and how the volume distribution of damage affects directional properties.

Questions and Discussion

Dr. Gerhardt asked about the experimental procedure used to determine the remaining service life of the material samples at the specific percentages of service life indicated in the impedance versus frequency graphs presented by Dr. Majumdar. She commented that the impedance response as a function of frequency would be very sensitive to the temperature and humidity of the samples, based on her 35 years of experience using impedance spectroscopy. She questioned whether the response differences observed in the testing were associated with material state evolution as closely as implied by the presentation.

Dr. Majumdar assured her that the observed responses were indeed due to the evolution of damage as validated by 3D x-ray images and that these measurements were performed at conditions with no substantial variation of temperature or humidity. The methodology and confirming experimental data have been published in peer-reviewed articles (Reifsnider et al., 2009; Majumdar et al., 2013; Reifsnider and Majumdar, 2011). In relevant unpublished work done by Dr. Reifsnider's group at the University of South Carolina, material state changes were captured in situ while the specimen was loaded in tension, evidence that further validates the position that such dielectric characteristics are due to an evolving damage state. In principle, environmental conditions can change material state, he agreed, and hence an assessment technique should be sensitive to that. The sensitivity to environmental changes depends on material type, he said, adding that detailed discussion was beyond the scope of the current presentation. He noted that investigations of the effects of relative humidity and temperature on the methodology had been studied separately by members of the research group for a polymer composite (Fazzino and Reifsnider, 2008) and also investigated in other material systems (e.g., ceramics). In addition, the methodology is designed to produce a 3D tensor measurement of anisotropic response utilizing different variables, not just a single impedance spectroscopy curve. Dr. Majumdar stated that his research teams have successfully applied the technique, in situ and ex situ, to measure damage due to multiphysical inputs and electrical currents.

A participant asked Dr. Majumdar if his group was planning to explore at the atomistic level the damage accumulation effects that they are following at the macroscale with impedance spectroscopy. He replied that related work is in fact being done by his collaborating colleagues at the University of South Carolina, using modifications of atomic force microscopy to measure the electrical properties across heterogeneous microstructures—for example, damaged and undamaged areas. He emphasized that remaining service life and strength characteristics are global (macroscale) properties of the materials system, so a top-down approach is needed to quantify material state evolution as it affects those global properties.

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

James A. Warren, NIST

Dr. Warren noted in his introductory remarks that the objectives of materials informatics he would be discussing represent a paradigm shift for materials science and that these objectives are meant to achieve *workable* results rather than perfect solutions. He reminded the participants that the motivation for the MGI, which is now more than three years old, was to speed up the insertion rate of new materials into manufactured products. Among its concrete objectives are to cut in half the average time from new material development to practical application and to reduce the costs of new material applications. With respect to the name itself, he said that "materials genome" should be taken as a metaphor for the computational, experimental, and data infrastructures of materials science. An ideal that the MGI embraces is open access to both data and models, preferably with open-source community model development. Although some of these ideas may seem alien to the defense world, Dr. Warren said, he considers them to be extremely relevant.

An innovative notion being developed with the MGI is the funding of teams of theorists and experimentalists, rather than individuals, because of the inherently collaborative nature of developing multiscale, validated computational software bridging the innovation pathway from materials discovery to manufactured products. Another MGI characteristic is emphasizing the potential for engineering impact by identifying partnering entities in industry, government, and academia who are willing to commit to taking computational methods and materials discovery results and applying them.

Direct funding of programs and projects linked to the MGI totaled $63 million in fiscal year 2012, Dr. Warren said, with more than $100 million requested for 2013-2014. These totals include funding for NIST, DOD, DOE, and National

Science Foundation (NSF) programs. NIST is currently funding MGI-oriented programs at $13 million per year, plus another $5 million per year for the Chicago-based Center for Hierarchical Materials Design. In April 2012, a National Science and Technology Council (NSTC) Subcommittee on the MGI was formed (under the NSTC's Committee on Technology), with representation from NIST, DOD (including DARPA), DOE (including the National Nuclear Security Administration), NSF, NASA, National Institutes of Health, U.S. Geological Survey, and Office of Management and Budget. In June and November 2013, NIST and DOE sponsored two MGI Grand Challenges Summits to seek stakeholder input on critical industrial problems that the MGI should target. Half of the nonfederal participants were from industry, half from academia. The input from these summits led to the formulation of nine Science and Technology Grand Challenges, which were included in the *Materials Genome Initiative Strategic Plan*, which was released in December 2014 by the NSTC subcommittee (NSTC, 2014). The materials areas covered by the MGI Grand Challenges are indicated by their titles: Biomaterials, Catalysts, Lightweight and Structural Materials, Polymer Composites, Energy Storage Systems, Electronic and Photonic Materials, Correlated Materials, Polymers, and Organic Electronic Materials.[17]

The remainder of Dr. Warren's presentation focused on the NIST role in pursuing the third National Strategy Goal of four presented in the MGI Strategic Plan: "Facilitate Access to Materials Data." After a brief overview of NIST's mission and high-level organization, he said that NIST's traditional role in providing standard reference data has defined a niche role for NIST with respect to this third MGI goal. After recounting the history of how this role for NIST has evolved, Dr. Warren presented some conceptual issues related to what data are, the relationship between models and data, what it means to measure something (take a measurement), the role of simulation in data creation, and the nature and role of metadata[18] in describing the measurement process. He views these issues as foundational questions (he used the term "ontology" to characterize them) that need to be addressed to facilitate access to materials data. Among the many points Dr. Warren made with respect to these issues and how one should think about them are the following:[19]

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[17] Additional information about the MGI is available on the NIST MGI website at http://www.nist.gov/mgi/.

[18] Expressed in simple terms, metadata in this context are data about (i.e., data describing or defining) the data that constitute the measurements. For example, if the datum is "the bolt is 4 and 3/8 inches long," then metadata might be "the parts were measured with a 25-foot flexible steel tape measure, Stanley Model 483629, acquired in June 2012 and ruled in 32nds of an inch."

[19] Editorial insertions indicated by square brackets are the rapporteur's additions to clarify or interpret a point as expressed by Dr. Warren.

- Examples of metadata for measurements include (1) the descriptions of the experimental setup and instrumental settings used when a measurement was taken and (2) the virtual, explicit, or underlying model that informs the understanding of what is being measured.
- A simulation is just an instantiation of a model on a computer.
- The software through which a computer-based model is instantiated is metadata for the simulations performed with that model. If one has the software [and more importantly, if one has the source code for the executable software and the run input data] used in a simulation, then one has a lot of information about how the simulation was done.
- In traditional experimental methodology, the technical publication of how experimental measurements were taken is a form of high-quality metadata.
- In most cases, the values measured for a parameter or quantifiable characteristic of interest make sense only in the context of an equation or other form of "model" within which that parameter or characteristic has meaning. Since the equation or model is typically, at some level, only an approximation of the reality being measured, the measured value is, in an ultimate sense, "false." (In support of this point, Dr. Warren quoted a maxim attributed to George Edward Pelham Box: "All models are wrong, some are useful."[20])
- If a model is really well tested and accepted as fact, we call it a theory. Sometimes the model is put forward explicitly as a hypothesis to be tested. But sometimes it is an unacknowledged assumption, "and that gets us into really deep trouble."
- The "experiential knowledge" that comes from acquiring data using models that are unacknowledged assumptions can be really valuable [most of the time] but at the same time can be really dangerous because of "black swan" events [i.e., statistically infrequent exceptions to the model's explicit or implicit assumptions].
- If you are doing an experiment, essentially what you are doing is testing a model that you happen to have [or think you have] in vivo, in the real world.
- The comparison of the simulation with the experiment is [the process of] validation. The convergence of the two [the computer-based simulation and the experiment] is validation [as a result of the validation process].
- Data come out of both simulations and experimentation. How well the data resulting from computational methods apply to reality depends on

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[20] According to Wikipedia (http://en.wikipedia.org/wiki/George_E._P._Box), the exact quotation is "Essentially, all models are wrong, but some are useful." It appears in print in Box and Draper (1987, p. 424). See also Box (1979), where a section is entitled "All models are wrong but some are useful."

how well the computational algorithm instantiates the [underlying conceptual] model, as well as how well the model represents reality.

- "You need the model to make sense of the data." The magnitude of credible data reduction attainable from experimentation depends on how reliably the model [that informs the experimentation] captures reality [under those experimental conditions].
    - —In physics—for example, with data obtained from the Large Hadron Collider—there can be many orders of magnitude of data reduction because the model (the Standard Model of particle physics, which is widely accepted in the high energy physics community) is [accepted as] highly reliable.
    - —For current biological methods, there are few good models with this level of certainty of application [community acceptance] for complex systems, so much more of the data must be retained.
    - —Computational methods for complex materials are somewhere in between these two extremes. Dr. Warren said that, although he previously believed that understanding materials meant turning materials science into physics, his work over the past several years on the MGI has convinced him that materials science and facilitating access to materials data have much to learn from both sides: physics and biology.
- If the goal is to disseminate a lot of information, which is the aim of the MGI, then a dissemination "package" should include the measured quantities, the associated quantifying models, all of the raw data, the protocols used to obtain the data, the specification of the equipment used, and all relevant environmental conditions [conditions external to the experimental setup that, under the model, might affect the results].
    - —The more of this metadata that is included with the measurement data, the more likely that someone will be successful in reproducing the results.
    - —For practical reasons, one has to stop somewhere in specifying potentially relevant metadata, but "you should do your best."
- The bottom line: a change is needed in the way [technical and scientific] information is published [disseminated].
    - —If one set out to define a publication system to meet today's data-communication requirements, it would not be the system of journal article publication inherited from the Royal Society of London [and other seventeenth-century institutions, including the French Academie des Sciences and other European science societies, for formal and informal communication within and between then-nascent science communities].

—"We don't know the correct model yet, but it's unlikely to be the one that evolved so long ago."

Dr. Warren said the barrier to adoption of new ways to disseminate methods and results is "pretty high," with a lot of duplication of effort and missed opportunities (missed because the data needed to disseminate methods and results usefully are gone). To illustrate common data-sharing barriers in science, he played the cartoon video "Data Sharing and Management Snafu in 3 Short Acts," originally created by Karen Yacobucci, Alisa Surkis, and Karen Hanson for the NYU Health Sciences Libraries.[21] In light of these barriers and related problems in current scientific practice, Dr. Warren posed the question, "What should we do, and in particular what should NIST do?"

New federal requirements on making research data and results accessible and shareable are "beginning to trickle down" through federal agencies, he said, adding that he expects these requirements will in time be applied to all federally funded research. A selling point he uses in talks about the MGI is to ask his audience of researchers, "Can you find your own data?" and "Can you duplicate exactly a simulation run you did 6 months ago?" But there are tools now, he continued, that can change the way researchers do their work and that make collaboration and data sharing more practical and efficient.

Dr. Warren then discussed how the MGI is intended to work, in principle, to enable effective collaboration on multiscale modeling approaches applied to designing and using new materials. Data from simulations and experiments need to get into the shared repository system somehow, but in ways that overcome all of the barriers and challenges to using what someone else has done. One area that NIST is focusing on, he said, is enabling the exchange of information not only into and out of the multiple data repositories that are being established but also along the R&D progression from initial research investigations to practical applications. He described a variety of NIST activities for working with specific industry, academia, and government partners to develop standards, tools, and techniques for the acquisition, representation, and discovery of materials data; for interoperability of computer simulations of materials phenomena across multiple length and time scales; and for quality assessment of materials data, models, and simulations.[22] NIST has set up an open-access data repository, which is beginning to accumulate

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[21] A YouTube version of the video cartoon is available from the website of the Institute for Health Technology Transformation at http://ihealthtran.com/wordpress/2013/01/youtube-data-sharing-with-bears-great-video-by-nyu-health-sciences-libraries/, accessed December 2014.

[22] For more on NIST activities with specific partners, see "The Materials Genome Initiative at NIST," available at http://www.nist.gov/mgi/overview.cfm, accessed December 2014.

data sets in various topical categories.[23] Along with these efforts, Dr. Warren noted, there are a lot of "straightforward standards questions" of the types that NIST has traditionally addressed through interactions with standards-setting bodies in the various scientific and technical communities with domain expertise. He also listed and briefly described a wide range of NIST activities related to information technology, applications of informatics to materials data curation, and data access and retrieval infrastructure.

Questions and Discussion

Dr. Kolbe asked how NIST deals with privacy concerns (individual-identifiable data) associated with the data in its repositories. Dr. Warren replied that the data sets and data types that have been entered into the repositories thus far have not involved human subjects or individual-identifiable data elements. He agreed that there are complex legal issues that arise when data sets contain identifiable personal data.

In response to a comment from Dr. McGrath about data access restrictions in defense-related materials R&D, Dr. Warren agreed that the International Traffic in Arms Regulations represent another whole set of data-access and data-sharing questions, but he believes those issues are much more tractable than are the privacy and consent issues related to identifiable data. Dr. McGrath and Dr. Warren discussed the extent to which compatibility issues would be a problem for users interested in working with both defense-related materials data repositories and the open access repositories that are the objective of the NIST programs.

A New Statistical Method for Assuring Mechanical Reliability

Stephen Freiman, Freiman Consulting, Inc.

Dr. Freiman acknowledged the contributions of three NIST scientists—Jeffrey Fong, James Filliben, and Alan Heckert—to the research work he presented. Although the statistical methods he discussed were developed to assess the mechanical reliability of brittle materials—particularly glasses and ceramics—he emphasized that they are equally applicable to a wide variety of materials. Like Dr. Warren, he quoted George Box's comment about models being wrong (not perfectly true representations of the reality to which they are applied) but useful, saying that it is important to remember that the models used in place of data are mostly just

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[23] For the current status of NIST-led data repository efforts, see http://nist.matdl.org/ and http://www.nist.gov/mml/msed/thermodynamics_kinetics/materials-informatics.cfm, accessed December 2014.

empirical models and that one needs to exercise caution about believing that they are "100 percent correct" all of the time. One of his themes, he said, would be uncertainty, and uncertainty in the model (as a representation of reality) is of equal importance with uncertainty (i.e., measurement imprecision) in the data that are used to fit the model.

Dr. Freiman explained that this statistical work on mechanical reliability began with a request to NIST from a commercial company for a testing method to meet the FAA's requirement of 90 percent survival probability, with 95 percent confidence, for aircraft inner windows that were all glass rather than a glass-polymer laminate.[24] The results were reported in a 1994 technical publication (Fuller et al., 1994). A particular challenge for an adequate testing methodology, he said, is that, in addition to measuring the initial strength of the windows, strength degradation over time has to be measured because small surface cracks in glass grow over time and can lead to delayed failure. In this context, Dr. Freiman said, a measure of mechanical reliability should answer the question, "With what confidence can we say that a component under known stresses will survive for a specific time?" The reference to confidence is important, he explained, because we can make predictions about time to failure, but how well do we know that those predictions are accurate?

This problem of the degree of confidence in the estimate of strength over time, expressed in statistical terms, was the challenge that the query about testing airplane windows raised for Dr. Freiman and his NIST colleagues. For brittle materials such as ceramics and glasses, he said, there was at that time—and probably still is today—no nondestructive test method that could pick out the most severe flaw: the flaw that with some confidence could be used to predict time to failure. Proof testing was another option, but the team ruled it out because it is very complex and expensive; it requires that stresses be applied to the component exactly as they would be in operational service; and rapid unloading from the proof stress is crucial but difficult to achieve in controlled conditions. The remaining option was to carry out fracture testing on a subset of the entire population of specimens of the component and then to extrapolate the test results to the universe of components that might be built. Specimen testing of this sort, he noted, requires statistical analysis of the fracture test results to determine a minimum failure stress and the time to failure given that stress. To ensure that their statistical approach gave an accurate measure of reliability, the NIST team set requirements (i.e., the team had to be able to reasonably assume) that (1) all test specimens of the component (the glass window) had to be

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[24] During the questions and discussion session following his presentation, Dr. Freiman clarified that the aircraft fuselage windows in question were "double windows" with an outer window designed to sustain high impacts and particulate/precipitation erosion over the aircraft's operational life. His presentation focused on the all-glass inner windows proposed for the aircraft.

BOX 3.5
Expression for Estimating Time-to-Failure from Empirical Strength Parameters and Crack Growth Constants

$$t_f = \frac{\lambda}{N'+1}\left(\frac{S}{S_v}\right)^{N'-2} \sigma^{-N'}$$

S is the initial strength
S_v is the strength of an indented reference set of specimens
σ is the tensile stress in the component
λ and N' are crack growth constants

SOURCE: Stephen Freiman, Freiman Consulting, Inc., presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 8; Fuller et al. (1994).

manufactured and finished exactly like the components to be used in operational service and (2) no flaws would be created during operational use.

The equation in Box 3.5 is the expression used by the NIST team to estimate time to failure for the component population based on testing of the reference set of specimens. Dr. Freiman emphasized that the parameters and constants in this expression are empirically derived and that, although the community “thinks they are right,” they are not necessarily fundamental (i.e., mathematically derived from or exactly expressing the underlying physics of component failure).[25] He also pointed out that the tensile stress in the component, σ, is typically derived from an FEA, which also carries a degree of uncertainty. Reviewing the empirical methods typically used to obtain values for each of the parameters and constants, he stressed that there are uncertainties in each of them. The next question, then, is how to combine these uncertainties to derive an overall confidence level, or measure of uncertainty, in the estimate of time to failure.

At this point, Dr. Freiman said, the NIST team began deviating from the traditional method for estimating probability of failure. That traditional approach uses the two-parameter Weibull model, shown in Box 3.6, for deriving the probability of failure by fitting experimental fracture data to the model. The problem with this model, said Dr. Freiman, is that the model assumes that the minimum strength in an instance of failure can be zero; that is, the model allows for the possibility of failure at zero strain. This very conservative assumption,

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[25] With respect to the “fundamental” versus “heuristic” nature of the time-to-failure equation, also see the summary, below, of Dr. Freiman’s response to Dr. McGrath during the questions and discussion session.

he explained, would be a problem when designing airplane windows, because a crack that would cause failure at even a small stress would be clearly visible to the naked eye. Instead, what is required is a more realistic way of setting the lower limit to the strength distribution in the set of measured specimens. Even so, the reliability prediction for the universe of components must account for the possibility of a difference in probability of a severe flaw between the universe of components and the set of tested specimens. The two-parameter Weibull model assumes that strength scales inversely with the area under stress. For the original airplane window problem, the team computed the total area of the windows in the universe of built windows and the total area of the windows in the set of tested specimens. They then used this inverse relationship between strength and area to derive an estimated minimum strength in the universe of components, given the minimum strength found in the specimen set.

Although that approach satisfied the FAA requirement for window survival probability with a statistically determined measure of confidence, Dr. Freiman's team did not consider it a fully satisfactory solution for this kind of mechanical reliability estimation. First, comparing total areas in the component universe and the tested specimen set was not a reasonable approach when the maximum number of components that might be built was not determinable. Second, on a more fundamental level, the two-parameter Weibull model seemed (and still seems) overly conservative and, as Dr. Freiman illustrated with the test data from the original airplane-window study, a two-parameter Weibull distribution does not provide the best fit to experimental data. Other models—for example, a three-parameter

BOX 3.6
Two-Parameter Weibull Model for Probability of Failure

$$P = 1 - \exp\left[-\int \left(\frac{\sigma}{\sigma_0} \right)^m dV \right]$$

P is the probability of failure
σ is the fracture stress
σ_0 is a scaling parameter
m is the Weibull modulus, or slope of the probability-strength curve
V is the volume (or area under stress)

SOURCE: Stephen Freiman, Freiman Consulting, Inc.,presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 10.

Weibull model, which establishes a nonzero minimum stress at which there is nonzero probability of fracture—provide a better fit of the data.[26]

The more sophisticated (and presumably more realistic) approach that the team has subsequently developed for determining mechanical reliability incorporates the following steps, which Dr. Freiman presented and explained:

- *Step 1:* Establish the minimum initial strength and standard deviation for the set of test specimens, which must be finished identically to the final component (i.e., the universe of final components that will be used operationally).
  - —There are a number of methods to establish the location parameter σ_u, the lowest value in the three-parameter Weibull distribution. Dr. Freiman illustrated this point with the strength test data from the airplane window specimens and listed 54 different distributions that could be used as models against which one could test the goodness of fit of strength data from a given set of test specimens. “Let your data determine which [distribution model] gives the best fit to your data,” Dr. Freiman advised, “and from that select [the model] to use to make your predictions.”
  - —Based on their analysis of the goodness of fit, the NIST team chose to fit the strength data from the test set of airplane window specimens to a three-parameter Weibull distribution.
- *Step 2:* Instead of using the inverse ratio of areas to estimate failure probability, as suggested by the two-parameter Weibull model, use the concepts of “tolerance limit” and “coverage” to determine the uncertainty in the lower limit to the initial strength of the universe of components.
- *Step 3:* Determine the uncertainty in the lifetime prediction calculated from the data on all of the specimens (apply the probability-of-failure equation in Box 3.5). To determine the uncertainty in the time-to-failure estimate calculated using the formula in Box 3.5, Dr. Freiman noted, one must combine the measurement uncertainties associated with determining the values of the five parameters in the probability-of-failure equation.
  - —If the uncertainty in the value of each parameter is less than 10 percent, then a *propagation of errors* approach can be used to combine them (Ku, 1966).
  - —There are other methods for combining the uncertainties if any exceed

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[26] In the three-parameter Weibull model, the numerator in the integrand of the equation in Box 3.6 becomes $\sigma - \sigma_u$, rather than just σ. The third parameter, σ_u, is the minimum stress at which fracture occurs in the tested specimens.

10 percent, he added, but then the cross-terms in the uncertainties need to be considered.

Following this three-step approach, the team calculated the minimum lifetime of the population of windows from which they had selected their test set to be 11.2×10^6 hours, with a 90 percent confidence level. This was sufficient to meet the FAA requirements, and the plane with the windows in question was approved for flight.

In concluding his presentation, Dr. Freiman highlighted the following summary points:

- Based on this three-step approach for estimating mechanical reliability, all data necessary for a failure probability prediction can be obtained from fracture strength measurements.
- For any statistical prediction of the reliability (time to failure) of brittle materials such as ceramics, strength is the best measure of flaw severity. But the strength data must be obtained under the most severe conditions expected in service.
- Strength distributions are not always straight lines. Bimodal strength distributions—for example, from two different sources of failure—and outliers must be addressed. Fractographic analysis of test specimens is recommended because it indicates where the failure originated.
- Scale-up makes use of the concepts of tolerance limits and coverage. Although this may be a new concept in the ceramics-testing world, it is of value as a better alternative than is comparing the total area of the tested specimen set to an estimate of the total area of the population in the universe of components.
- Although a two-parameter Weibull distribution often works well for modeling strength data from the test set, it may not be the best fit to the experimental data. *Let the* [goodness of fit to the] *data determine the distribution used.*
- The statistical methodology is applicable to a wide variety of materials—not just the brittle materials (glasses and ceramics) discussed in this presentation. To apply it, all that is needed is an established functional relationship between failure and one or more measurable parameters. This relationship can be:
  —Based on data for a sample space within the population of all items to be estimated;
  —Based on a model fitted to data for the population space;
  —Based on a model assumed to apply to the population space (for product design done before test specimens exist); or

—Established through validation in both the sample space and the population space (to ensure that reliability predictions made on one or more of the above bases are accurate).

Questions and Discussion

Dr. Warren asked if an automated algorithm had been used to explore the goodness of fit of a range of statistical distributions to the test set data in the case discussed by Dr. Freiman. Dr. Freiman replied that he did not know whether that approach to determining functional fit had been used by the statisticians on the NIST team, but the algorithm that the team used for measuring goodness of fit for a range of model distributions is to be included in one of the technical articles being written on this work.[27]

In response to a question from Dr. Wadley on the basis of the final prediction of minimum lifetime at a 90 percent confidence level, Dr. Freiman noted that the time-to-failure equation (Box 3.5) uses the tensile stress in the component, which is derived from an FEA of a given window geometry. There were different predictions made for windows with different geometries, he explained, and these predictions were only for the glass interior windows of the aircraft, not the exterior windows. The latter were subject to dust and rain erosion and other impact stresses, for which other time-to-failure methods were used.

Dr. Freiman, Dr. Wadley, and other participants discussed options that could have been used if the estimated lifetime of the windows had not met the FAA requirement. In response to the suggestion of using a sensor on the windows in operational conditions to provide data for CBM, Dr. Freiman noted that the failure mode of the glass windows would not have allowed time to replace them after crack growth was sensed but before the window failed. The participants and Dr. Freiman discussed alternatives to other simplifying assumptions in this case, such as the assumption that the maximum stress was applied constantly during operating conditions.

Dr. McGrath noted that other statistical approaches to estimating probability of failure, such as Bayesian statistics, might affect the results obtained using Dr. Freiman's methodology, and he noted that there was not an underlying physical model of failure ("physics of failure") involved. Dr. Freiman responded that the time-to-failure model (i.e., Box 3.5) is based on the physics of crack growth, which engineers think they understand. The expression used to fit the data (e.g., the two-parameter Weibull distribution in Box 3.6 or an alternative distribution equation) is in question, he said, but the data on crack growth and the physics of why cracks grow are known extremely well. What we can't do, he continued, is take

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[27] As of May 2015, this technical article was still undergoing internal technical review within NIST.

the data about crack growth in one material and use it to predict accurately the crack growth behavior of a different material.

AFRL Perspective on Damage/Materials Characterization, CBM+, and Life Prediction

Eric Lindgren, Materials State Awareness and Supportability Branch, Materials and Manufacturing Directorate, Air Force Research Laboratory

Mr. Lindgren began by acknowledging the contributions, to his presentation and to AFRL's MSA efforts, from his colleagues in the Materials State Awareness and Supportability Branch of AFRL and from other AFRL personnel engaged in relevant projects and programs, including the Digital Twin and Digital Thread programs, which had been mentioned by others during the workshop. As requested by the workshop committee, his presentation focused on how MSA could affect the Air Force's capabilities for CBM, in the context of fleet sustainability rather than new materials development. Mr. Lindgren emphasized the importance of ensuring that the Air Force's fleet is ready to meet all mission requirements, despite the advanced age of most of the fleet. For example, the precision flight team, the Thunderbirds, has been flying the same model of F-16 since 1983.

Mr. Lindgren characterized the objective of MSA in the Air Force context as enabling the move from damage detection to characterization of current material condition (i.e., material state) as the basis of gathering the data used in maintenance decisions, using model-centric technologies. The definition of MSA used by the Materials State Awareness and Supportability branch, he said, is "reliable *nondestructive* quantitative materials/damage characterization regardless of scale." In that definition, "reliable" means there are some statistical metrics of performance that can be delivered to the users of MSA information; "quantitative" means there are numerical methods of characterization. There are two life prediction teams in the Materials and Manufacturing Directorate: one deals with life prediction for metals, the other with life prediction for organic- and ceramic-matrix composites. However, from his research team's perspective, there is a difference between awareness (the diagnostic focus of MSA) and prediction (as in life prediction), and he recommended against defining diagnostics and prediction (prognostics) as one thing, saying that they should be kept as distinct and separate sciences. In this context, he defined "life prediction" as predicting behavior based on current materials state and anticipated use—hence it is materials dependent (e.g., life prediction for metals is different than for composites) and application dependent (e.g., life prediction is different for a propulsion subsystem versus fixed-wing structures versus rotary-wing structures).

Mr. Lindgren described how the current requirements for ensuring the safety of flight systems depend on (1) the approach of the cognizant organization (the Air Force uses damage tolerance assessment, the Navy uses a "safe life" approach, the FAA uses a hybrid of the two); (2) the material involved (e.g., there are predictive methods for metals but currently only reactive requirements for composites); and (3) the damage mode (e.g., fatigue crack propagation versus corrosion). One element of commonality, he noted, is that the requirements for damage sensing capability are generated from each organization's integrity community—for instance, the Air Force's Aircraft Structural Integrity Program and Propulsion System Integrity Program—because the safety of the system is those communities' responsibility ("they own the safety of the system").

The current damage tolerance assessment method used by the Air Force under Military Standard 1530C provides three options: slow crack growth modeling, fail-safe multiple load path modeling, and fail-safe crack-arrest modeling. However, inspection of composite materials is still event driven, Mr. Lindgren explained, because slow crack growth modeling for composites is not yet mature. Service life extension decisions use a risk management methodology, and periodic inspection is still the preferred approach. Air Force propulsion systems have their own safe life approach, codified in Military Standard 3024. A key point, he stressed, is that the Air Force is currently meeting the safety metrics set by the requirements from the integrity community.

The maintenance community performs the NDE assessments on which the damage tolerance assessment options depend, along with other factors, to determine the overall risk. A probability of detection curve is used for the risk calculation, and Mr. Lindgren explained how NDE inspection intervals are set to provide crack detection redundancy before cracks reach critical size. Although availability of aircraft and cost are concerns, he said, safety trumps those concerns. What the maintenance community is seeking, he added, is less burdensome (either faster or cheaper) NDE technology/methods of equivalent quality (with respect to ensuring safety) to the technology/methods now in use.

Next, Mr. Lindgren described AFRL efforts to move from the current focus on detecting damage (including age- and use-related cracking, corrosion, etc.) to characterization in support of CBM+. The current Department of Defense Instruction (DODI) 4151.22, dated October 2012, includes the following definition of CBM+:

> CBM+ is the application and integration of appropriate processes, technologies, and knowledge-based capabilities to achieve the target availability, reliability, and operation and support costs of DOD systems and components across their life cycle. At its core, CBM+ is maintenance performed based on evidence of need, integrating RCM [reliability centered maintenance] analysis with those enabling processes, technologies, and capabilities that enhance the readiness and maintenance effectiveness of DOD systems and components. CBM+ uses a systems engineering approach to

> collect data, enable analysis, and support the decision-making processes for system acquisition, modernization, sustainment, and operations (DOD, 2012, p. 9).

The policy section of DODI 4151.22 states that "CBM+ shall be implemented in accordance with [the CBM+ definition quoted above] and guidance detailed in Enclosure 2." Furthermore, CBM+ shall be "[u]sed as a principal consideration in the selection of maintenance concepts, technologies, and processes for all new weapon systems, equipment, and materiel programs based on readiness requirements, life cycle cost goals, and reliability centered maintenance (RCM)-based functional analysis formulated in a comprehensive reliability and maintainability (R&M) engineering program" (DOD, 2012, pp. 1-2). Mr. Lindgren emphasized that the guidance for implementing CBM+ contained in Enclosure 2 of DODI 4151.22 is not prescriptive of the technologies and business processes that must be used; how the objectives of CBM+ are to be achieved is left to the implementer's discretion.

For Mr. Lindgren's branch at AFRL, determining the "condition" on which maintenance decisions are based requires quantitative characterization of any flaws (flaw presence, location, size) and a statistically validated capability to make a risk determination, always bearing in mind the importance of putting safety first. Unlike instant and complete damage state characterization capabilities portrayed in some science fiction movies, Mr. Lindgren said, the "sensing physics" of currently available primary condition interrogation methods is limited to the electromagnetic spectrum in the frequency range from a hertz to gigahertz (or higher), stress waves in the range from hertz to gigahertz, and thermal diffusion phenomena. For field and depot applications, he added, the ionizing radiation methods discussed in many of the workshop presentations are inspection methods "of last resort" because of the cost and safety issues they entail. They are great tools in the laboratory, he said, where these factors can be controlled, but applying them to an entire aircraft in maintenance inspection brings into play many challenges.

A consequence of these limitations, Mr. Lindgren continued, is that condition characterization of Air Force operational systems is probabilistic in nature and requires attention to the propagation of measurement errors and determination of the uncertainty in condition assessments. Although there have been some successful demonstrations of the detection capability for specific damage modes in controlled environments, he said (Mr. Lindgren showed current estimates of the Technology Readiness Level for several crack and corrosion damage modes when inspection/sensing is performed at the depot, in the field, or "onboard" an operational system), sufficiently reliable structural damage characterization with statistical metrics for a typical aerospace system is not now available for any approach; the current Technology Readiness Level is only around 3. Instead, the current state of the art is manual estimation based on individual interpretations of available sensor data and inspections.

Against this problem-framing context, Mr. Lindgren described the strategic approach his branch is taking to find a CBM+ solution. To address the complexity of the challenge presented by condition characterization of entire aircraft, as directed by DODI 4151.22, they have worked at decomposing the "problem space" of condition characterization by breaking out issues of the complexity, variance, and other attributes of the problem. Mr. Lindgren said that they expect modeling, particularly forward models for virtual parametric (i.e., sensitivity) studies, to play a key role in their effort, but this will require validated models that integrate realistic structures. They will be trying to identify the key characteristics of fatigue cracks that can be linked to sensing modality responses and to extract those response signals even when they are buried in noise. The aim is to provide reliable condition characterization with statistical metrics. One of the software tools they are using to track metadata across multiple data sets is the DREAM.3D software architecture, which Mr. Lindgren had discussed with Dr. Withers after Dr. Withers's presentation at the beginning of the workshop.

To illustrate the complexity of the condition characterization challenge, Mr. Lindgren presented and discussed a list developed in 2006 of more than 20 factors affecting the NDE of a two-layered structure (Lindgren et al., 2007). The list of factors includes three factors related to the NDE method, ten factors related to structure (part geometry, material, and condition), and eight factors related to characteristics of the flaw to be detected.

He said that the three NDE inspection-system parameters can generally be captured and assessed with minimal variance. They are relatively easy to understand and to quantify and control in the laboratory environment. For these reasons, Mr. Lindgren said, they have typically been the focus of research. He suggested that getting caught up in characterizing these factors too precisely has diminishing returns for the larger characterization problem.

By contrast, the structure parameters have a high degree of variance, are extremely hard to capture, and typically, he said, have not been a focus of research because they are challenging to simulate in a laboratory environment. The structural variability of Air Force aircraft is high, he explained, because they were originally assembled one at a time, like a custom-built automobile, and the tolerances on parts and assembly procedure were fairly loose (since they were not anticipated to be in service as long as they have been). Their service lives have been and continue to be extended, and operational stresses, combined with variable modes of operation and new operational parameters, have further exacerbated that original variability in structural details that are relevant to flaw modes such as fatigue crack initiation and growth. To illustrate, Mr. Lindgren described the variability one finds in hole geometry around the fasteners in an aircraft wing assembly. All of this variability, he noted, will influence the response from that structure to NDE sensing.

The parameters of the flaw characteristics, Mr. Lindgren continued, also have a high degree of variance, are hard to capture in real aircraft, and are typically simplified or truncated by researchers because these details are challenging to extract from actual systems and then simulate in a controlled environment. However, the details of these factors can substantially alter the probability of detection of a flaw condition, as he illustrated with data from an analysis of the effect of sealant condition on the probability of detection of fatigue cracking at fastener holes in wing assemblies. He described the implementation of an ultrasound detection method that overcame the crack-detection challenges by incorporating dual transducers (for sending and receiving the sensing signal) and using multiple ultrasonic wave modes to interrogate fastener holes and detect cracks at locations distant from the signal source. This successful approach included automating the analysis of the data while maintaining human review of the positive indications from the automated analysis results to minimize false calls.

Next, Mr. Lindgren presented an example of model-assisted characterization: quantifying the depth of corrosion at the faying surfaces of a multilayered structure (Aldrin and Knopp, 2005). Ultrasound sensing was used to map the upper layer; multifrequency eddy-current analysis was used to characterize the surface of the lower layer. Model-based inversion of simulated/representative data was used to enhance the signal in the eddy-current response that indicated localized features of particular interest in the lower layer, such as corrosion pitting. Mr. Lindgren emphasized that once sufficient data are collected to populate the model, which is done using destructive analytic methods on samples of the characteristics of interest, model-inversion analysis can be used to achieve reasonable fidelity in the NDE characterization of operational structures. If one is looking for distinct locations of microstructural orientation that differ from the surrounding material structure and that can influence life-determining parameters, he said, these examples give hope that useful NDE characterization of multilayer components can be done.

Mr. Lindgren used Figure 3.9 to summarize this overall approach to the use of NDE methods for both the CBM of existing systems and for generating new materials properties and new performance characteristics. A model-driven quantitative representation of material/damage state, including statistical metrics (middle of Figure 3.9), is produced by applying signal analysis and uncertainty quantification techniques as well as a method for discerning for 3D representation and validating microstructure to the data from the NDE sensing technologies (top row of Figure 3.9). This quantitative representation of material state / damage state contributes both to efficient, effective maintenance and to improvements in materials design, processing, and performance (bottom row).

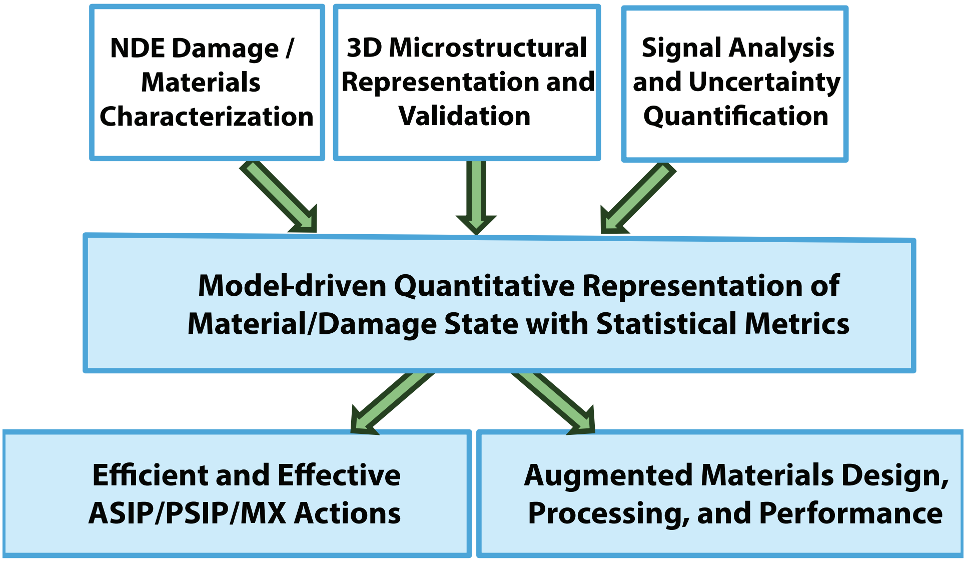

FIGURE 3.9 Model-assisted characterization of material state. SOURCE: Eric A. Lindgren, Air Force Research Laboratory, presentation to the Workshop on Materials State Awareness, August 6-7, 2014, slide 27. Distribution Statement A. Approved for public release; distribution is unlimited. Case Number 88ABW-2014-3560.

With respect to research directions in MSA being followed by his branch and the directorate of AFRL, Mr. Lindgren said that the current projects build on this model-based (or model-assisted) approach:

- They started with inversion on propulsion components that have been removed from engines of operational systems because the geometric tolerances of these components at the macroscale are very tight. This limited variance at the macroscale makes it easier to do an inversion (from the NDE data) to the quantitative representation of the crack structure of the component within the reliability parameters important for making decisions to return to operation, repair, or replace. The model-based outputs are being confirmed with data from actual turbine engine systems.
- The first step in working on a multilayered structure is to understand the complexity of the structure well enough to locate the damage.
- The next step for complex structures is developing image-based methods for understanding and interpreting the scattering and complexity of the response signal from different modes of NDE interrogation. Mr. Lindgren developed this point with an example of immediately determining the

extent of a fatigue crack at a fastener hole using an eddy-current probe, rather than taking a series of corrective action steps, requiring multiple days, to determine what level of corrective action is sufficient. The NDE characterization data, interpreted through the model-driven quantitative representation of material/damage state, can inform the repair action at the first instance of structure interrogation.

- They are examining ways to characterize variance in tailored microstructures and new resonance methods to explore localized characterization of material/damage state, particularly localized perturbations in the resonance signal that indicate nucleation sites associated with crack initiation and/or crack growth. Mr. Lindgren noted some research work that was funded by AFRL to determine which localized perturbations correspond to microstructural characteristics that need to be detectable and identifiable to guide MSA-related decisions (e.g., when maintenance/repair actions are indicated).

Summarizing the above points, Mr. Lindgren said that, for this part of AFRL activities, "the future is characterization regardless of scale."

He then highlighted some recurring challenges, or common attributes of the problem, for pursuing this future. These challenges include (1) the geometric complexity of structural components/parts; (2) the variability that occurs at all scales and in all structure-relevant processes from initial manufacturing through sustainment; (3) the complexity of the material parameters that characterize microstructures and composites; (4) the variability in the time dependence of material/damage state changes, particularly for changes affected by irregular intervals and magnitudes of operational stresses; and (5) the stochastic nature of material/damage behavior, which renders inversion of the response to NDE interrogation to characterize current state quantitatively an "ill-posed problem" for the mathematics of inversion modeling. Tying these challenges back to points that other workshop presenters had made about the probabilistic nature of MSA, Mr. Lindgren noted several points:

- The ill-posed nature of inversion yields probabilistic answers (from the model-driven representation of current state).
- To enable informed risk-based decisions (about CBM, system life extension versus system retirement, etc.), probabilistic answers require quantification of the uncertainties.
- System integrity (i.e., safety) always trumps other considerations.

In closing, Mr. Lindgren summarized the key messages from his presentation as follows:

- He believes that NDE-based characterization will enable realization of CBM+ and new materials with tailored properties. But to ensure safety and cost/time savings, this characterization requires statistical metrics of accuracy for ill-posed inversion.
- The research strategy of AFRL's Materials State Awareness and Supportability Branch to realize NDE-based characterization is model centric. Demonstration projects have shown the feasibility of this strategy.
- The branch has a multiyear plan to realize these objectives.
  - —Skilled, structured research will be needed to realize these objectives, and the branch is looking for interaction and collaboration with others.
  - —They are starting with the end in mind, which means acknowledging up front and addressing the challenges of geometric complexity, stochastic variability, and stochastic time-based change.

Questions and Discussion

Dr. Achenbach described Mr. Lindgren's presentation as an outstanding enumeration of all of the problems that must be dealt with. Given the successes highlighted by Mr. Lindgren in the face of the difficult challenges, he asked, what are the specific areas, particularly in the modeling domain, where further improvement would provide the most value? He described an approach to introducing probabilistic considerations into a model by perturbing the model to see how the perturbations affect model outcomes. Mr. Lindgren agreed that there was room for that approach and that some researchers in his community are doing parametric virtual sensitivity studies to examine how perturbations in model-based methods affect results. They are also running multiple models to try to assess the variability, to begin putting statistical metrics of performance on how the structural/material variability influences NDE response and the inversion from that response to the representation of state. Although the challenge is significant, Mr. Lindgren continued, he does think it is addressable by what the AFRL community is trying to do. His confidence comes from the feasibility of the concept that the demonstrations have shown. But, he added, the strategy will take an extended effort; it is not going to be realized in a 3-year window.

Mr. Lindgren added some remarks about prior presentations, based on notes he had made during the workshop. First, he noted that a HUMS is focused on MSA and CBM+ for rotorcraft, rather than fixed-wing aircraft systems. The HUMS community has been very successful, and there are probably some valuable "lessons learned" for other applications, he continued, but some of the material state signatures and features being sought and used in HUMSs are not as relevant or as available in fixed-wing systems. So there is some distinction between the two communities and their CBM issues. Second, with respect to the Digital Twin and Digital

Thread programs, he said there is "probably room for improvement in what we are doing." He described a program that started out with a substantial false-positive rate in its first year but is now showing a downward trend in its false-positive rate. This and other examples show the potential of the approaches, he concluded, but implementation will not be easy, especially for legacy systems.

DISCUSSION SESSIONS ON CROSSCUTTING TOPICS AND ISSUES

The final session on each day of the workshop was an open discussion led by members of the Workshop Planning Committee. These discussions cut across the specific topics of the individual presentations to bring together (1) implications of MSA, as discussed in the preceding sessions, for qualification of new materials, processes, and products (the Day 1 closing session) and (2) implications of MSA for CBM and life extension decisions (the Day 2 closing session). As with all of the workshop sessions, the points, judgments, and suggestions made during these discussions and reported here reflect only the views of the individual participants who expressed them and do not represent a corporate position or consensus of the workshop as a group, the Workshop Planning Committee, or the Defense Materials Manufacturing and Infrastructure Standing Committee.

Day 1 Closing Discussion: Implications of MSA for Qualification of New Materials, Processes, and Products

Dr. Schafrik, the facilitator of this discussion section, began by stressing that this topic is important because the cost and time required to qualify a new material, process, or product is a major barrier to the use of promising new materials in operational systems. He began by developing a working definition or characterization of qualifying a new material, process, or product and then asked how the ideas and views on MSA and NDE that had been expressed during the day's sessions might influence qualification timing and cost. With respect to the cost of qualification, he distinguished between the cost of qualifying a new material, the cost of requalifying after making a "tweak" or adjustment in a previously qualified material, and the cost of qualifying a new supplier. When Dr. Schafrik examined the actual cost of such qualifications for an employer several years ago, he reported, the amounts ranged from a low of $10 million to more than $100 million, with an average cost of approximately $50 million. Not only were the costs substantial, he said, but there were also risks that the qualification might not succeed due to the changes that invariably happen when a process is scaled up—some process changes greatly affect required material properties. When the development and qualification timelines are extended, Dr. Schafrik added, there is a risk that the requirements will change and thus that the qualification testing could fall short of what is needed.

In response to Dr. Schafrik's request to Dr. Ball for the latter's experience with qualification costs and challenges, Dr. Ball replied that, in his almost 30-year career, he knew of no instance where an entirely new material had been introduced. He did know of several successful attempts at the introduction of incremental advances to metallic materials. In one high-profile case, a new material (an aluminum-lithium alloy) was selected during the design phase for the F-35 fighter but was subsequently rejected because undesirable material properties emerged during system development. Dr. Ball recounted some of the technical details and political impasses that arose in this case and suggested it would make an excellent case study for the challenges of introducing a new material as a primary structural material in a man-rated flight system with stringent safety requirements. He contrasted this attempt at a new material with making incremental improvements to a material, such as incremental improvements in aluminum alloys and titanium alloys. In response to a question about the cost of the ICME methodology for the large aluminum structural forgings that he had described during his presentation, Dr. Ball said that the team was unable to demonstrate a cost savings for manufacturing cost alone, but if life cycle costs were included, the estimated cost savings with the ICME approach were "huge." The large disconnect between manufacturing cost savings and sustainment / life cycle cost savings, he added, was "incredible."

Dr. Luscher commented on qualification issues as they affect life extension programs for nuclear weapon systems. When a replacement is needed for a material, he said, it is typically necessary to go back and develop a heightened understanding of the original material and its associated processing to ascertain critical aspects of the material state and the role the material played in the system as originally designed.

In his notes drawn from these and other comments from the participants, Dr. Schafrik listed four categories of "new material qualification": (1) qualifying a new class of material, such as intermetallics; (2) qualifying a change to a current material, such as using different precursor materials or different sources in its production; (3) qualifying a change in processing (of a current material); and (4) qualifying an existing material in a new application (or for new requirements). He then discussed his outline of elements in qualifying a new material in any of the four categories listed (Box 3.7) and the challenges for such qualification (Box 3.8).

Dr. McGrath commented that the entire process of new material qualification was probably too large a topic to address in this workshop, and he suggested that the participants focus the discussion more on the theme of what MSA could contribute to qualification. This theme remained more or less at the center of the diverse comments that followed during the remainder of the session, as indicated by relevant highlights abstracted below.

BOX 3.7
Elements of Qualification of a New Material

- Demonstrate that the material meets necessary performance requirements—but not all requirements may be known at the beginning of qualification. It is likely that the requirements will evolve over time (example: aircraft engine requirements).
- Understand the effects of variations in chemistry, morphology, and processing, and then prepare the Material Specification and associated Processing Specification.
  —Specifications based on a sufficient understanding of variations allow for the reproducibility of the material in scale. (For metals in the aircraft engine world, a minimum of a million pounds of material; for composites it would be less.)
  —Material has to meet minimum (e.g., –3 sigma) properties of the Specifications for the entire lifetime of the system.
  —How can the tools and techniques for MSA discussed at the workshop help address this part of qualification related to service life?
  —Participant Question: Who owns the performance requirements and the Material and Processing Specifications? Sometimes the OEM, sometimes the supplier, sometimes a technical association (consensus standard), sometimes the government, etc.
- Demonstrate that the material is scalable to production quantities.
  —This may require an investment in process equipment.
  —The material must meet the supplier ROI based on volume and profitability.
  —The *ideal* is to be able to measure the qualification properties using material samples that were processed via the full-scale production process.
- Demonstrate that the material is inspectable to ensure it was properly made; you need to have criteria for acceptance/rejection.

SOURCE: Adapted from Robert E. Schafrik, GE Aircraft Engines (retired), presentation to the Workshop on Materials State Awareness, August 6-7, 2014.

BOX 3.8
Challenges for Qualification

- Must assess the long-term material performance based on relatively short-term testing.
- Must ensure service life. (How would MSA impact this risk?)
  —How does the intrinsic material state affect the end product performance?
  —MSA would provide knowledge of intrinsic material details.
- Must assess what information is really important. In some cases, can the qualification activity be “drowned in too much detail”?
- Must assess when the qualification process starts. Also, what amount of precursor work is required?
- Must have suppliers ready to scale up. Examples: a new aluminum alloy, graphene suppliers.

SOURCE: Adapted from Robert E. Schafrik, GE Aircraft Engines (retired), presentation to the Workshop on Materials State Awareness, August 6-7, 2014.

- As an example of his suggested theme, Dr. McGrath asked, if service life is a consideration in qualifying a new material, how can some of the tools and techniques discussed during the Day 1 sessions contribute to the qualification process?
- Mr. Lindgren suggested that material state assessment techniques could be of particular value in cases where a material's performance-critical characteristics depended on "tailoring" into it a particular microstructure and only a small production run was envisioned. Standard sampling and destructive testing techniques might be prohibitively expensive in such a case, he added, opening the way for MSA techniques. Dr. Ball agreed with the point that knowledge of microstructure could be crucial and illustrated its relevance with an example where better MSA might have uncovered a microstructure problem earlier in development.
- Building on these comments, a participant noted that some manufacturers have attempted to use NDE techniques and modeling to monitor microstructure during manufacturing, to try to steer a process with variability to the desired material state in the end product.
- Dr. Majumdar said that OEMs are interested in reducing cost by reducing the amount of material scrapped during production processes. He suggested that having in-process material state assessment (which is not available now) could have value in this regard, to go beyond just having accept/reject decisions based on testing the product after a process step is completed. As an example, he described how production-scale autoclaving to cure composites might be adjusted in situ through the use of material state monitoring during the process. In short, he said, could we do corrective processing by adjusting processing conditions in real time? Dr. McGrath agreed that this is an important topic for MSA and noted that the only current sensor-based control on powder-casting of titanium parts is for the temperature of the melt pool. Dr. Majumdar suggested, as another application, in situ corrections in real time to variations from design in laying down the fiber pattern in an embedded fiber composite.
- Dr. Gerhardt suggested that further elaboration is needed of the different senses in which something could be a "new material" in need of qualification. One might need to qualify a new (different) precursor material or qualify a different source (vendor) of the same material, she explained, or there might be issues or changes in the impurities in the precursor material. Any changes in the manufacturing process can potentially change the properties of the product material. Nonetheless, she noted, one can get lost in the details of variations in source materials. She agreed with Dr. Ball's point on needing a way to categorize what information is important for qualifying a type of material for a given application. That is where the

challenge and the cost come in, Dr. Gerhardt said. Dr. Ball added that "the beauty of ICME" is that it can allow thousands of simulations to be done during the design/development phase, whereas in the past perhaps only 10 experiments were affordable. Another participant spoke about the potential value of being able to assess the likely degree of impact of a minor processing change in the manufacture of commodity plastics.

- Dr. McGrath said that sometimes the need is to qualify an existing material in a new application. His example was the use of existing adhesives in bonded composite structures as a way of reducing aircraft weight. "I'm not sure I'm ready to fly in an aircraft that has been glued together, especially when it was glued together 20 years ago," he remarked.
- Dr. Majumdar said that for a heterogeneous material such as an organic composite, every change in composition changes the structural heterogeneity. As a result, users want the entire qualification process repeated. He recounted a statement he heard from Boeing's Chief Technology Officer at a conference: it takes, on average, 10 years for a technology change [in organic composites] to go from a university laboratory's published results to use in Boeing aircraft. Mr. Lindgren added that this point also applies to metal alloys, and he thought the average lag between academic publication and new metal technology insertion in aircraft was closer to 15 years. If ICSE and ICME techniques can truncate that time lag, Mr. Lindgren said, and MSA plays a role in understanding the material variability and evolution in qualification testing, then there is a very powerful place for MSA in new material qualification processes.
- Dr. Schafrik said that often the developmental history for a new material is much longer [than 15 years], as the technology for its production evolves and new versions of the material emerge. It's often much later in this process before "we get serious about qualification" of the material, he said. Dr. Wadley agreed, saying that the evolution of newer versions of a material raises the question of when (and therefore on what version) qualification should start. Using graphene as an example, he said that the versions of graphene being manufactured today will probably no longer be made when the need for certification/qualification of graphene in applications gets serious. He posed the question, "With what version of [an evolving] material should qualification start?"
- Dr. Hemker asked about external drivers that provide an impetus for use of a new material—for example, if one were developing a new aircraft engine. Should the question be, he suggested, "Assuming we are going to need this new material, what does it take to get it qualified?" Dr. Schafrik commented, in answer to the point about external drivers, that the main driver for change in a material [in the aircraft industry] is competition.

- Dr. Wadley asked if qualification of a material [at least in its present form] would still be necessary "if we had perfect MSA." Dr. Schafrik replied that qualification would still be necessary because the manufacturer has to warrant the performance of the product under specified conditions. Perfect MSA would mitigate some of the risk to be managed in making such warranties, he opined, but monitoring material state would not provide an alternative to qualification testing. Nevertheless, the perfect MSA would improve confidence in going forward with a material alternative into the design and development stages.
- Dr. Luscher suggested, "If we had full MSA, then material specifications might be cast in terms of that material state, as opposed to [being stated in terms of] a property that we are using as a proxy for the response that we anticipate will occur throughout the design life of the component." Several other participants thought that this was a good way to formulate the issue.
- Dr. Plummer said that, from a physicist's point of view, the discussion seemed to be about incrementally changing an existing material, rather than discovering a new material. He feared that the concept of "discovering" new materials with a computer, as the federal government was promoting with the MGI, would destroy what he saw as "real creativity" in the discovery process. "You can design something where you know the rules," he said, "but discovery of a new material is not where you know the rules." He expressed concern that a reliance on computer-based design in the United States would allow foreign competitors to outperform the U.S. R&D community.

In wrapping up this discussion session, Dr. Schafrik said that the discussion had shown that there is a lot of opportunity for MSA knowledge to have a real impact on the qualification process. He thought that, if MSA provided alternative ways to specify design and performance requirements to deal with challenges such as resistance to corrosion or residual and load-induced stresses, it could have important benefits. Dr. McGrath suggested that the question "If we had perfect MSA, what would we do differently?" and Dr. Luscher's response to it (see final comment above by Dr. Luscher) would be worth further discussion by the participants on Day 2.

Day 2 Closing Discussion: Implications of MSA for CBM and Life Extension Decisions

Dr. Wadley of the University of Virginia and Jesus M. de la Garza of Virginia Polytechnic Institute served as facilitators for the Day 2 closing discussion. To initiate the discussion, they presented a list of potential responses to the question, "What are the implications of perfected MSA?" Dr. Wadley said this preliminary list (consisting of the first six items in Box 3.9) was intended to stimulate ideas

BOX 3.9
Some Implications of Perfected MSA for Condition-Based Maintenance and Life Extension Decisions

- Changes to the way materials are specified
- Vehicle design consequences
- Materials manufacturing consequences
- Digital certification implications
- Implications for the time and costs of flight certifications
- Implications for global supply chains
- Physics-based understanding of the degradation modes in the operational environment and techniques for correlating those modes with methods of characterization such as sensory data
- Knowledge of what happens to functionally important properties as the material state changes
- Life cycle cost implications
- Implications for DOD: cost, availability, tactics, strategy, readiness, design implications for capability
- There is more to a material state than properties; what constitutes a material state? Physics-based models are needed to define a material state
- Better property-processing-structure relationships are needed for a perfected MSA
- Programs for education/training in CBM+ are needed in universities

SOURCE: Adapted from Haydn N.G. Wadley, University of Virginia, and Jesus M. de la Garza, Virginia Polytechnic Institute and State University, presentation to the Workshop on Materials State Awareness, August 6-7, 2014.

and thoughts from the workshop participants. MSA is here, he said, but it is not perfect, and the previous two days of presentations raise the question, "Will we end up with a satisfactory system for MSA, one that gives us the information we want?" He also posed the question, "Can we envisage a future with a perfected MSA, first for homogenous, anisotropic materials in components without geometric complexities, then in environments like those Mr. Lindgren has just shown us, with much more geometric complexity, and then for nonhomogenous materials like the composites that are beginning to be used in the skins and bodies of aircraft and ships?" Furthermore, multifunctional materials pose challenges for MSA beyond just structural failure, he said.

Dr. Schafrik suggested that "physics-based understanding of the degradation modes in the service environment" be added to the list, and Dr. Malas noted that several presentations had highlighted the need for the correlation of that physics-based understanding with available methods of characterization, such as sensors. Dr. Majumdar suggested adding that a perfected MSA would include knowing what happens to [functionally important] properties of the material as the material state changes. In response to Dr. McGrath's comment that the list did not include using MSA to do better CBM, Dr. Wadley explained how he interpreted the title of the list to include that as an overarching objective of perfecting MSA. Their exchange led to other comments on whether to include the different techniques for finding out about the health of a system (system/structural health monitoring).

Mr. Lindgren pointed out that the AFRL is not involved in any organizations seeking to provide guidance on how to do SHM because that role is owned by the Air Force system integrity community, not the research community. "The integrity community sets the requirements for what we [the research community] need to do," he noted, adding that a perfected MSA would have life cycle cost implications important in the Air Force research community. Another participant suggested a number of implications (cost, availability, tactics, etc.) that could apply to DOD broadly.

Box 3.9 shows the final version of the list of implications of a perfected MSA as suggested by various participants. With respect to the first item in the list, Dr. Wadley asked the participants if they thought a "better and better" capability for assessing material state would lead to changes in how materials are specified (e.g., in specifications for major DOD systems and platforms). One participant thought that a specification in terms of the required material state might "give everyone a common language" and a shared understanding of a requirement. Dr. Ball described how improved MSA would have a direct impact on the prognoses of future performance capability and (remaining) system life that his organization makes at various stages in managing an aircraft during its operational life.

In response to a question about whether his first bullet (on changing the way materials are specified) meant a performance-based specification, Dr. Wadley described how a component or subsystem might be specified in terms of a set of material properties determinable by MSA techniques. This description led another participant to ask if such a specification could mean that different materials might meet the specification in different production runs, based on factors such as cost or availability, as long as the alternative materials met the state-based specification. The extended discussion of this hypothetical approach to meeting specifications led one participant to sum up the issues raised as "there is more to a material state than properties," given that, as Dr. Warren had pointed out in his presentation, what a property is depends implicitly on a conceptual model. (This became the 11th bullet in the list shown in Box 3.9.) Perhaps, this participant said, the objective should be to define what "material state" is for a specific context. There was further discussion around the interplay among concepts of material state, material properties, and physics-based models of the material. Dr. Gerhardt suggested that a key prerequisite for a perfected MSA is better property-processing-structure relationships (the next-to-last bullet in Box 3.9).

At this point, Dr. Wadley directed the discussion to a second, related topic: Given that the goal of "perfect MSA" is still a long way off, he asked, how does CBM,

BOX 3.10
How Might Condition-Based Maintenance (Prognostics and SHM) Change as MSA Improves over Time?

- The premature “failure” rate may change (decrease)
- Costs of false positives may become more problematic
- False negatives may become as problematic as false positives
- Cost-benefit analysis may move against doing CBM
- Overloads that stress material state, such as chemical and thermal environments encountered during operational life, may become identifiable with material state monitoring
- Unknown unknowns (and “black swan” low-probability events) may continue to challenge CBM applications
- Enhanced prognosis of future capability at different points in the life cycle (a tighter uncertainty range on the predicted remaining life) may occur; also, the use of prognosis of end-of-life to support system end-of-life and replacement planning decisions may occur
- Maintenance activities may become optimized to minimize time and cost
- Frequency of inspections may be reduced
- Improvements may occur in sensing and other assessment technologies and in modeling material state and remaining life from these assessments
- CBM assessment and decisions may need to be applied not only to materials but to parts, components, and systems in their operational context
- Incremental improvements in understanding current material state may accelerate and simplify maintenance planning and repair processes, even if inspection intervals cannot be decreased due to other factors
- Usability conditions from material state monitoring may be used as an input into the design of next-generation systems

SOURCE: Adapted from Haydn N.G. Wadley, University of Virginia, and Jesus M. de la Garza, Virginia Polytechnic Institute and State University, presentation to the Workshop on Materials State Awareness, August 6-7, 2014.

understood in terms of both SHM and prognostics, change as MSA capabilities gradually improve over time? He then explained an initial sample of such changes that he and Dr. de la Garza had thought about (these are the first five bullets in Box 3.10).

- *System failures decrease.* The frequency of premature system failures should decrease, provided there are no other “unaccounted for” variables.
- *Cost of false positives.* As material state is better understood, the rate of system failures decreases. Assuming that the probability of false positives is constant, at some point the cost of false positives exceeds the benefits of a CBM approach. Therefore, decreasing false positives is important. Presenters at the workshop had given examples where false positives were

high initially and trended downward over time. Dr. Wadley asked, "Can that 'induction period' before false positives decline to an acceptable rate be shortened?"

- *False negatives may also increase.* Dr. McGrath noted that, if MSA is used to determine maintenance/replacement decisions instead of a fixed-interval preventative maintenance approach, then false negatives may also become problematic for CBM.
- *Adverse cost-benefit analysis.* Dr. Wadley suggested that, as system failures decrease, the cost of rigorous assessment to support CBM may become an issue, if systems are seen as being "too good to fail." Dr. Ball described a real-life example of adverse cost-benefit during the cost modeling for the application of CBM techniques to a large aircraft system. If a CBM approach increased the time between inspections for one key failure point, he said, then some other failure mode/point would become the critical driver for the inspection interval. So a sufficient cost savings for introducing CBM was not demonstrable. This experience suggests, he added, that big gains in CBM application may not occur until it can be applied to the entire system (e.g., an entire aircraft).

The comments and discussions related to the above points, plus other points raised by various participants, are summarized in Box 3.10 as "possible changes in CBM as MSA capabilities improve over time."

Noting the broad range of practical experience and expertise represented by the participants, Dr. Wadley next asked if any participants had additional thoughts to offer to the workshop that had not been covered in the presentations and discussions.

- A participant suggested that the density of monitoring points in a distributed monitoring system might increase in the future, as design improvements reduced the relative criticality of just a limited number of "hot spots" where fatigue, impact damage, etc. were most likely to occur. A second participant "strongly seconded" this suggestion, adding that "hot spots" monitoring tends to focus on known problems, whereas distributed monitoring improves the capability to manage risks from "unknown unknowns." A third participant added that distributed monitoring could help with sensor reliability issues by providing some degree of built-in redundancy in the monitoring system. Dr. Majumdar suggested that distributed monitoring systems would become an essential feature of the emerging area of variable-stiffness composites because they are designed for greater damage tolerance by distributing impact effects on material structure.

- Dr. Bayoumi suggested that a series of workshops or training sessions on CBM and CBM+, as understood by DOD, would be valuable to stakeholders and the academic community. This suggestion led to discussion of current course offerings and postgraduate programs in CBM and related areas.

In his closing comments before adjourning the workshop, Dr. McGrath spoke about the summary report of the workshop and said that the lists of implications and potential consequences, for both the long-term goal of a "perfected" MSA and the interim improvements in MSA capabilities, would be of value for communicating the advances in the field, the trajectory toward future capabilities, and what can be reasonably anticipated if that trajectory continues to receive support. Jeffrey Zabinski of the Army Research Laboratory spoke of the workshop's value for informing the process by which DOD prioritizes technology investments to give U.S. forces advanced capabilities at reduced cost while ensuring the safety of personnel. After closing comments from the participants representing the Project Reliance partners and an expression of thanks to all of the participants from Dr. Schafrik, chair of the National Materials and Manufacturing Board of the NRC, Dr. McGrath adjourned the workshop at 3:00 p.m.

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Appendixes

A

Workshop Statement of Task

An ad hoc committee will convene a series of three 2-day public workshops to discuss issues in defense materials, manufacturing and infrastructure including: (1) Globalization of Defense Materials and Manufacturing; (2) Big Data in Materials Research and Development; and (3) Materials State Awareness. The committee will develop the agendas for the workshops, select and invite speakers and discussants, and moderate the discussions. The workshops will use a mix of individual presentations, panels, and question-and-answer sessions to develop an understanding of the relevant issues. The workshop topics will highlight some recent developments in the fields. Key stakeholders will be identified and invited to participate. Individually-authored workshop summaries will be prepared separately by a designated rapporteur after each workshop in this series.

Materials state awareness seeks to quantify the current state of a material and/or damage with statistical metrics of accuracy located in individual systems, structures, or components, and is the heart of condition-based maintenance strategies. In principle, such quantitative evaluation should be based on knowledge of the initial state, damage or failure processes, operational environment, and nondestructive evaluation (NDE) assessment of state. However, most frequently the initial state is not known and the assessment must be done from an unknown reference state. Achieving this goal requires the integration of information from a variety of disciplines, including the mechanics of materials, materials science, engineering mechanics, and NDE engineering. Data interpretation and analysis will play a key role, including the integration of advanced analytics and statistical measures of accuracy and precision. This workshop on materials state awareness will focus around three topics:

Topic 1: Advances in Metrology and Experimental Methods
Topic 2: Advances in Physics Based Models for Assessment
Topic 3: Advances in Databases and Diagnostic Technologies

B

Workshop Participants

DEFENSE MATERIALS MANUFACTURING AND INFRASTRUCTURE STANDING COMMITTEE AND WORKSHOP PLANNING COMMITTEE MEMBERS

Michael F. McGrath, McGrath Analytics, LLC, *Workshop Chair*
Robert E. Schafrik, GE Aircraft Engines (retired), *Chair, National Materials and Manufacturing Board (NMMB)*
Jesus M. de la Garza, Virginia Polytechnic Institute and State University
Rosario Gerhardt, Georgia Institute of Technology
E. Ward Plummer, Louisiana State University
Haydn N.G. Wadley, University of Virginia

SPEAKERS

Jan D. Achenbach, Northwestern University
Dale L. Ball, Lockheed Martin Aeronautics Company
Abdel E. Bayoumi, University of South Carolina
Joannie W. Chin, National Institute of Standards and Technology
Stephen Freiman, Freiman Consulting, Inc.
Kevin J. Hemker, Johns Hopkins University
Dashiell Kolbe, General Electric Aviation
Eric Lindgren, Air Force Research Laboratory
D.J. Luscher, Los Alamos National Laboratory

Prasun K. Majumdar, University of South Carolina
James Malas, Universal Technology Corporation
Susan B. Sinnott, University of Florida
James A. Warren, National Institute of Standards and Technology
Philip Withers, University of Manchester, U.K.

OTHER ATTENDEES

Julie Christodoulou, Office of Naval Research
Kevin Curtis, General Dynamics
Robert Dowding, Army Research Laboratory
Rick Everett, Naval Research Laboratory
Natalie Gluck, Institute for Defense Analyses
Joycelyn Harrison, Air Force Office of Scientific Research
Charles Lee, Air Force Office of Scientific Research
Ignacio Perez, Office of Naval Research
Robert Rapson, Project Reliance
Jocelyn Seng, Institute for Defense Analyses
Lewis Sloter, Office of the Assistant Secretary of Defense for Research and Engineering
Jennifer Wolk, Naval Surface Warfare Center, Carderock Division
Jeffrey Zabinski, Army Research Laboratory
Marc Zupan, University of Maryland, Baltimore Campus

WORKSHOP STAFF

Robert J. Katt, Rapporteur
Erik B. Svedberg, Senior Program Officer, NMMB
James Lancaster, Acting Board Director, NMMB
Joseph Palmer, Senior Project Assistant, NMMB

C

Workshop Agenda

DAY 1, AUGUST 6, 2014

8:00 a.m. Working Breakfast
8:30 Welcome
8:45 Meeting Objective

Introduction

9:15 James Malas, Universal Technology Corporation
Presentation title: *The DOD/NRC Materials State Awareness Collaboration*

Topic 1: Advances in Metrology and Experimental Methods

9:40 Philip Withers, University of Manchester
Presentation title: *Correlative Tomography in Materials Science*

10:20 Break

10:40 Jan Achenbach, Northwestern University
Presentation title: *QNDE and SHM for State Awareness of Materials and Structures*

11:20	Kevin Hemker, Johns Hopkins University Presentation title: *Supporting the Development of Physics-Based Models: An Experimentalist's Perspective*
12:00 p.m.	Lunch

Topic 2: Advances in Physics-Based Models for Assessment

1:00	D.J. Luscher, Los Alamos National Laboratory Presentation title: *Physics-Based Mesoscale Modeling of Materials in Extreme Environments*
1:40	Joannie Chin, National Institute of Standards and Technology Presentation title: *Predicting the Service Lives and Durability of Engineered Materials and Systems*
2:20	Prasun Majumdar, University of South Carolina Presentation title: *Measurement of Material State Change and Physics-Based Prediction*

Implications for Qualification of New Materials, Processes, and Products

3:00	Dale Ball, Lockheed Martin Aeronautics Company Presentation title: *The Emerging Role of ICME and ICSE in Airframe Design Analysis*
3:40	Discussion on Qualification of New Materials, Processes, and Products Lead: Robert Schafrik and Valerie Browning
4:40	Adjourn
5:30	Working Dinner

DAY 2, AUGUST 7, 2014

8:00 a.m.	Working Breakfast
8:30	Welcome, What We Heard Yesterday

Topic 3: Advances in Databases and Diagnostic Technologies

8:40 Abdel Bayoumi, University of South Carolina
Presentation title: *CBM+: A Smart Predictive Approach*

9:20 Susan Sinnott, University of Florida
Presentation title: *Advanced Approaches for Material Design and Discovery*

10:00 Break

10:20 James Warren, National Institute of Standards and Technology
Presentation title: *The Materials Genome Initiative, Data, Open Science, and NIST*

11:00 Ed Hindle, General Electric Aviation
Presentation title: *Implications for Condition-Based Maintenance and Life Extension Decisions*

11:40 Lunch

Implications for Condition-based Maintenance and Life Extension Decisions

12:40 p.m. Steve Freiman, Freiman Consulting Inc.
Presentation title: *A New Statistical Method for Assuring Mechanical Reliability*

1:10 Eric Lindgren, Air Force Research Laboratory
Presentation title: *AFRL Perspective on Damage/Materials Characterization, CBM+, and Life Prediction*

1:40 Discussion on Condition-Based Maintenance and Life Extension Decisions
Lead: Jesus de la Garza and Robert Latiff

2:40 Adjourn Workshop
2:40 Planning
3:00 Full Adjourn

D

Abbreviations and Acronyms

3D	three-dimensional
AFRL	U.S. Air Force Research Laboratory
ASR	alkali-silica reaction
CAMS	Cyberinfrastructure for Atomistic Materials Science
CBM	condition-based maintenance
CBM+	Condition Based Maintenance Plus Prognostics (a DOD program/initiative)
COMB	Charge Optimized Many-Body (potentials)
CT	computed tomography, x-ray computed tomography
CTOL	conventional take-off and landing
DARPA	Defense Advanced Research Projects Agency
DFT	Density Functional Theory
DMMI	Defense Materials Manufacturing and Infrastructure (Standing Committee)
DOD	U.S. Department of Defense
DODI	Department of Defense Instruction
DOE	U.S. Department of Energy
DVE	design volume element

EAM	Embedded Atom Method (potentials)
EBSD	electron backscatter diffraction analysis
FAA	Federal Aviation Administration
FEA	finite element analysis
FIB-SEM	focused ion beam scanning electron microscopy
FLAIR	Fine Lightweight Aggregates as Internal Reservoirs
HUMS	health and usage monitoring system
ICME	integrated computational materials engineering
ICSE	integrated computational structural engineering
IDIQ	Indefinite Delivery/Indefinite Quantity
IVHM	Integrated Vehicle Health Management
LANL	Los Alamos National Laboratory
MAI	Metals Affordability Initiative (Consortium)
MGI	Materials Genome Initiative
MSA	materials state awareness
MVE	microstructural volume element
NASA	National Aeronautics and Space Administration
NDE	nondestructive evaluation
NIST	National Institute of Standards and Technology
NRC	National Research Council
NSF	National Science Foundation
NSTC	National Science and Technology Council
OEM	original equipment manufacturer
PROF	Probability of Fracture
PVE	property design volume element
PZT	lead zirconate titanate
QNDE	quantitative nondestructive evaluation
R&D	research and development
RCM	reliability centered maintenance
ReaxFF	Reactive Force Field (potentials)
RVE	representative volume element

S&T	science and technology
SEM	scanning electron microscopy
SHM	structural health monitoring
SLP	service life prediction, system life prediction
SPHERE	Simulated Photodegradation via High Energy Radiant Exposure (chamber)
SPS	Smart Predictive System
STEM	scanning transmission electron microscopy
SVE	statistical volume element
TATB	triaminotrinitrobenzene
USAF	U.S. Air Force
UV	ultraviolet
VERDiCT	Viscosity Enhancers Reducing Diffusion in Concrete Technology (NIST program)