The National Academies of Academies of

ENGINEERING THE NATIONAL ACADEMIES PRESS

This PDF is available at http://nap.edu/18345





Novel Processes for Advanced Manufacturing: Summary of a Workshop

DETAILS

82 pages | 7 x 10 | PAPERBACK ISBN 978-0-309-28591-9 | DOI 10.17226/18345

CONTRIBUTORS

GET THIS BOOK

Maureen Mellody, Rapporteur; Standing Committee on Defense Materials, Manufacturing and Infrastructure; National Materials and Manufacturing Board; Division on Engineering and Physical Sciences; National Research Council

FIND RELATED TITLES

Visit the National Academies Press at NAP.edu and login or register to get:

- Access to free PDF downloads of thousands of scientific reports
- 10% off the price of print titles
- Email or social media notifications of new titles related to your interests
- Special offers and discounts



Distribution, posting, or copying of this PDF is strictly prohibited without written permission of the National Academies Press. (Request Permission) Unless otherwise indicated, all materials in this PDF are copyrighted by the National Academy of Sciences.

Copyright © National Academy of Sciences. All rights reserved.

Novel Processes for Advanced Manufacturing

SUMMARY OF A WORKSHOP

Maureen Mellody, Rapporteur

Standing Committee on Defense Materials, Manufacturing and Infrastructure

National Materials and Manufacturing Board

Division on Engineering and Physical Sciences

NATIONAL RESEARCH COUNCIL OF THE NATIONAL ACADEMIES

THE NATIONAL ACADEMIES PRESS Washington, D.C. **www.nap.edu**

Copyright National Academy of Sciences. All rights reserved.

THE NATIONAL ACADEMIES PRESS 500 Fifth Street, NW Washington, DC 20001

NOTICE: The project that is the subject of this workshop summary was approved by the Governing Board of the National Research Council, whose members are drawn from the councils of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine.

This study was supported by Contract/Grant No. W911NF-10-C-0098 between the National Academy of Sciences and the Department of Defense. The views presented in this publication do not necessarily reflect the views of the organizations or agencies that provided support for this project.

International Standard Book Number-13:978-0-309-28591-9International Standard Book Number-10:0-309-28591-7

This report is available in limited quantities from:

National Materials and Manufacturing Board 500 Fifth Street, NW Washington, DC 20001 nmmb@nas.edu http://www.nationalacademies.edu/nmmb

Additional copies of this workshop summary are available for sale from the National Academies Press, 500 Fifth Street, NW, Keck 360, Washington, DC 20001; (800) 624-6242 or (202) 334-3313; http://www.nap.edu/.

Cover: The image depicts the juxtaposition of established industrial processes such as sand-casting of metals. It shows the novel uses of additive manufacturing, which is capable of creating objects of intriguing complexity in many dimensions, voxel by voxel, and represents a case of modernization and rejuvenation, perhaps even a revolution, of established industrial processes. Artist: Erik Svedberg, 3D image generated computationally, pixel by pixel.

Copyright 2013 by the National Academy of Sciences. All rights reserved.

Printed in the United States of America

THE NATIONAL ACADEMIES

Advisers to the Nation on Science, Engineering, and Medicine

The **National Academy of Sciences** is a private, nonprofit, self-perpetuating society of distinguished scholars engaged in scientific and engineering research, dedicated to the furtherance of science and technology and to their use for the general welfare. Upon the authority of the charter granted to it by the Congress in 1863, the Academy has a mandate that requires it to advise the federal government on scientific and technical matters. Dr. Ralph J. Cicerone is president of the National Academy of Sciences.

The **National Academy of Engineering** was established in 1964, under the charter of the National Academy of Sciences, as a parallel organization of outstanding engineers. It is autonomous in its administration and in the selection of its members, sharing with the National Academy of Sciences the responsibility for advising the federal government. The National Academy of Engineering also sponsors engineering programs aimed at meeting national needs, encourages education and research, and recognizes the superior achievements of engineers. Dr. C. D. Mote, Jr., is president of the National Academy of Engineering.

The **Institute of Medicine** was established in 1970 by the National Academy of Sciences to secure the services of eminent members of appropriate professions in the examination of policy matters pertaining to the health of the public. The Institute acts under the responsibility given to the National Academy of Sciences by its congressional charter to be an adviser to the federal government and, upon its own initiative, to identify issues of medical care, research, and education. Dr. Harvey V. Fineberg is president of the Institute of Medicine.

The **National Research Council** was organized by the National Academy of Sciences in 1916 to associate the broad community of science and technology with the Academy's purposes of furthering knowledge and advising the federal government. Functioning in accordance with general policies determined by the Academy, the Council has become the principal operating agency of both the National Academy of Sciences and the National Academy of Engineering in providing services to the government, the public, and the scientific and engineering communities. The Council is administered jointly by both Academies and the Institute of Medicine. Dr. Ralph J. Cicerone and Dr. C. D. Mote, Jr., are chair and vice chair, respectively, of the National Research Council.

www.national-academies.org

Novel Processes for Advanced Manufacturing: Summary of a Workshop

PLANNING COMMITTEE FOR NEW AND NOVEL PROCESSES THAT ARE ON THE VERGE OF INDUSTRIAL MODERNIZATION: A WORKSHOP

ROBERT E. SCHAFRIK, GE Aviation, *Chair* ROSARIO A. GERHARDT, Georgia Institute of Technology GEORGE T. GRAY III, Los Alamos National Laboratory ROBERT H. LATIFF, R. Latiff Associates MICHAEL F. McGRATH, Analytic Services, Inc. GREGORY B. OLSON, Northwestern University PRABHJOT SINGH, GE Global Research SONYA T. SMITH, Howard University DENISE F. SWINK, Private Consultant HAYDN N.G. WADLEY, University of Virginia

STANDING COMMITTEE ON DEFENSE MATERIALS, MANUFACTURING AND INFRASTRUCTURE

ROBERT H. LATIFF, R. Latiff Associates, *Chair* ROBERT E. SCHAFRIK, GE Aviation, *Vice Chair* VALERIE BROWNING, ValTech Solutions, LLC JESUS M. de la GARZA, Virginia Polytechnic and State University GEORGE T. GRAY III, Los Alamos National Laboratory MICHAEL F. McGRATH, Analytic Services, Inc. E. SARAH SLAUGHTER, Built Environment Coalition DENISE F. SWINK, Private Consultant A. GALIP ULSOY, University of Michigan HAYDN N.G. WADLEY, University of Virginia STEVEN G. WAX, Private Consultant

Staff

DENNIS I. CHAMOT, Acting Director ERIK B. SVEDBERG, Senior Program Officer TERI G. THOROWGOOD, Administrative Coordinator HEATHER LOZOWSKI, Financial Associate ANN F. LARROW, Program Associate, until May 2013 JOSEPH PALMER, Senior Project Assistant, from June 2013

NATIONAL MATERIALS AND MANUFACTURING BOARD

ROBERT E. SCHAFRIK, NAE, GE Aviation, Chair PETER R. BRIDENBAUGH, NAE, ALCOA, retired LAWRENCE D. BURNS, NAE, University of Michigan JIM C.I. CHANG, National Cheng Kung University STEPHEN H. DAVIS, Northwestern University GEORGE T. GRAY III, Los Alamos National Laboratory JENNIE S. HWANG, H-Technologies Group SUNDARESAN JAYARAMAN, Georgia Institute of Technology ROBERT H. LATIFF, R. Latiff Associates MICHAEL F. McGRATH, Analytic Services, Inc. CELIA MERZBACHER, Semiconductor Research Corporation EDWARD MORRIS, National Center for Defense Manufacturing and Machining ROBERT C. PFAHL, JR., International Electronics Manufacturing Initiative VINCENT J. RUSSO, Aerospace Technologies Associates, LLC HAYDN N.G. WADLEY, University of Virginia BEN WANG, Georgia Tech Manufacturing Institute ALBERT R.C. WESTWOOD, Sandia National Laboratories

Staff

DENNIS I. CHAMOT, Acting Director ERIK B. SVEDBERG, Senior Program Officer TERI G. THOROWGOOD, Administrative Coordinator HEATHER LOZOWSKI, Financial Associate ANN F. LARROW, Program Associate, until May 2013 JOSEPH PALMER, Senior Project Assistant, from June 2013 Novel Processes for Advanced Manufacturing: Summary of a Workshop

Acknowledgment of Reviewers

This workshop summary has been reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise, in accordance with procedures approved by the National Research Council's (NRC's) 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 workshop summary:

Peter R. Bridenbaugh (NAE), ALCOA, retired, Rosario A. Gerhardt, Georgia Institute of Technology, Paul S. Peercy, University of Wisconsin, Madison, and Prabhjot Singh, GE Global Research.

Although the reviewers listed above have provided many constructive comments and suggestions, they did not 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. Appointed by the NRC, he was responsible for making certain that an independent examination of this 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. Novel Processes for Advanced Manufacturing: Summary of a Workshop

Contents

OV	VERVIEW	1
1	WORKSHOP INTRODUCTION: WELCOME AND MEETING OBJECTIVES	11
2	 ADDITIVE MANUFACTURING—SESSION SUMMARY Introduction to Additive Manufacturing and Current and Future Applications, 12 Additive Manufacturing at GE, 16 Center for Innovative Materials Processing Through Direct Digital Deposition, 19 Open Discussion: Additive Manufacturing, 23 	12
3	ELECTROMAGNETIC FIELD MANIPULATION OF PROPERTIES— SESSION SUMMARY High-Magnetic-Field Processing and Synthesis to Develop the Next Generation of Structural and Functional Materials, 25 Materials Processing at the National High Magnetic Field Laboratory, 30 Field-Assisted Sintering Technology, 34 Open Discussion: Electromagnetic Manipulation of Properties, 37	25

4	DESIGN OF MATERIALS—SESSION SUMMARY Materials Genomics Past and Future from CALPHAD to Flight, 39 Some Steels on the Verge of Industrialization, 45 Data-Driven Materials Codesign, 48 Open Discussion: Design of Materials, 51	39
5	WORKSHOP WRAP-UP	54
REFERENCES		56
APPENDIXES		
А	Workshop Statement of Task	59
В	Workshop Participants	60
С	Workshop Agenda	64
D	Acronyms	68

Overview

The Standing Committee on Defense Materials, Manufacturing and Infrastructure (the DMMI standing committee) convened a workshop on December 5 and 6, 2012, to discuss new and novel processes that are on the verge of industrial modernization. The standing committee is organized under the auspices of the National Materials and Manufacturing Board of the National Research Council (NRC) and is sponsored by Reliance 21, a 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 increase coordination among the DOD services, components, and agencies.

The workshop was conducted as a convening activity. In accordance with NRC procedures, all participants provided individual opinions at the meeting, and no consensus findings, conclusions, or recommendations were developed at the workshop or as an outcome of the workshop. This report is a record of the workshop event prepared by the workshop rapporteur, and any statements or views summarized in the report must be considered an opinion expressed by an individual participant at the workshop, not a consensus view.

To organize its workshop on new and novel processes, the DMMI standing committee first organized a workshop planning group to identify workshop topics and agenda items, speakers, and invited guests. The workshop planning group consulted with Reliance 21 and members of the community to develop and organize the workshop. The workshop was held at the Keck Center of the National Academies, in Washington, D.C. Approximately 55 participants, including speakers, members of the DMMI standing committee, Reliance 21, invited guests, and mem2

bers of the public, took part in the 2-day workshop. The workshop was organized into three sessions, focusing on the following topics:

- Additive manufacturing,
- Electromagnetic field manipulation of materials, and
- Design of materials.

Additive manufacturing is defined as the process of making three-dimensional (3D) objects from a digital description or file; it is considered an additive process because the materials are deposited in successive layers. Electromagnetic field manipulation of materials is the use of electric and/or magnetic fields to change the mechanical or functional properties of a material or for the purposes of sintering. "Design of materials" refers to the application of computational and analytic methods to materials to obtain a desired material characteristic.

To assist the reader, recurring themes from the workshop discussion are summarized below, organized by session topic. These recurring themes represent discussion items that were addressed by multiple speakers or participants during the course of the workshop; they were identified for this report by the rapporteur, not by the workshop participants. The recurring themes are as follows:

- Additive manufacturing
 - -Qualification and certification
 - —New materials for additive manufacturing
 - -Access to manufacturing capabilities and resources
 - —Surface finish
 - -Unlawful uses of additive manufacturing
- Electromagnetic field manipulation of materials
 - -Understanding the physical phenomena
 - -Research prioritization
 - —Permanence of the material changes made
- Design of materials
 - -Materials databases
 - -Balancing experiment and modeling
 - -Model fidelity
 - -Materials qualification

After briefly describing each recurring theme in this overview, the report goes on to summarize the workshop presentations and discussions. Appendix A contains the statement of task for the workshop, Appendix B lists the workshop participants, and Appendix C contains the workshop agenda.

ADDITIVE MANUFACTURING THEMES

Qualification and Certification

It was noted by multiple participants and speakers that qualification and certification is a significant challenge in additive manufacturing. The qualification and certification process in its current form is not well suited to additive manufacturing. With traditional bulk manufacturing techniques, by way of contrast, all of the initially produced parts manufactured are certified; then, a sampling (perhaps 2 percent) of subsequent manufactured parts is certified. In additive manufacturing, where parts are individualized, the small sample size will not allow for statistical analysis. It was noted that perhaps the process should be certified, not the part. It was important to connect the additive manufacturing community with certification experts.

Each of the three speakers was asked about the impact of certification on additive manufacturing during the question-and-answer period following his presentation. Prabhjot Singh was asked to describe the certification process in general. He spoke of a very involved process, where the specification is written for each materials processing step. He pointed out that the current certification process takes 10-12 years, whereas he would like it to take 1-2 years. In response to a question from the audience, David Bourell noted that while from a research perspective it may make sense to develop new materials that would be better suited to the additive manufacturing process, DOD may not be interested in a new material because of the lengthy and tedious certification process associated with its use. Richard Martukanitz, in response to a question following his presentation, pointed out that the welding industry might be a good qualification model for the additive manufacturing industry; a welded structure has a design code to provide guidelines, qualified materials, qualified operators, processes, and repeatability within a range of process parameters.

New Materials for Additive Manufacturing

Several participants questioned whether it would be either needed or desirable to develop new materials that would be optimized for the additive manufacturing process. On the one hand, it could be useful to have materials optimized to this new manufacturing technique. On the other hand, however, new materials might add complications of their own that outweigh their potential benefits. Dr. Bourell pointed out that while most of the materials currently used in additive manufacturing are polymers and plastics, there is much interest in the development of new metals and new ceramics for additive manufacturing. He went on to say that there is a need to develop new metal alloys with characteristics appropriate for additive 4

manufacturing; however, because of the certification concerns noted above, new metal alloys might not be considered desirable by either DOD or industry.

In the session on the design of materials, Gregory Olson spoke of research interest in investigating metals for additive manufacturing. He described research in the use of design tools to create new alloys optimized for the capabilities of the additive manufacturing process. Researchers are particularly interested in new alloys with relatively fast solidification rates for additive manufacturing. Dr. Olson specifically mentioned the Open Manufacturing project of the Defense Advanced Research Projects Agency (DARPA) in collaboration with Honeywell, in which laser-based additive manufacturing is being considered.

During the open discussion following all three presentations, participants agreed that materials in production today are not specifically tailored to additive manufacturing and thus might be somewhat deficient. Further, participants noted that designers are not very involved in the materials process; they are the ones who should be giving materials scientists the specifications for the new materials.

Access to Manufacturing Capabilities and Resources

The lack of access to processing equipment, raw materials, and appropriate modeling tools was consistently noted as a potential handicap for the additive manufacturing community. Several participants pointed out that because both the electron beam and the laser system used in additive manufacturing are primarily made by companies that are not based in the United States, access to these manufacturing processes can be difficult. Both systems use a closed architecture, where the processes and materials used to service the equipment are known only to the manufacturer. Several participants discussed the need to have machines supplied by more companies and to have a more open, collaborative environment. Dr. Singh, who discussed this in particular during his presentation, was asked about access to machines in his question-and-answer session. He responded that no U.S. companies make electron beam machines and only one Swedish company does, which makes the supply quite limited. While six companies manufacture laser machinery, electron beam processing is 4-5 times faster than laser processing. Dr. Martukanitz also discussed the access to processing equipment in his talk: He pointed to the need for an open architecture for the equipment system used to allow everyone to have full access to the processes. The powder bed electron beam system currently used is a closed system—that is, the parameters and the materials used to service the equipment are held closely by the equipment manufacturer.

During the open discussion period it was noted that, in general, there are more manufacturing capabilities in Europe than in the United States. This led to a discussion on how the United States could stimulate its own manufacturing capabilities. Some participants noted that research in Europe tends to be more applicationspecific, or at least more project-specific, and that European governments award more grants for additive manufacturing processes. The European Union also builds on a more traditional approach to technology transfer, which tends to lead to more manufacturing. Other participants responded that research in the United States is more fundamental, and when it proves useful, the hope is that it will work its way into industry by market forces.

During the open discussion period, participants noted that while there is a U.S. source for most materials feedstocks, some manufacturers for niche applications may have more difficulty sourcing their material.

Another resource discussed was the modeling tools needed for additive manufacturing. Dr. Martukanitz's presentation focused heavily on the modeling and simulation tools for virtual experimentation that are being developed at Penn State University. During the open discussion period, participants discussed the lack of a standard modeling tool set for additive manufacturing. They noted that the current tools are better suited for the mechanistic models than for the process or materials structure and composition models.

Surface Finish

While not discussed in detail, surface finish was brought up as a research area that would benefit from additional research and development. Dr. Bourell noted that research into surface finish has tended to lag behind research into other areas and was in need of technical advancements. During the general discussion participants agreed that surface finish is consistently recognized as needing more technical research and development.

Unlawful Uses of Additive Manufacturing

The group discussed the potential dangers associated with putting additive manufacturing technology in the wrong hands. Participants discussed how additive manufacturing could be used to make unlicensed weapons, unlawful versions of copyrighted material, and substandard copies of goods at a lower cost. In each of these cases, however, there are circumstances that may make the application of additive manufacturing less attractive to a potential criminal. In the case of unlicensed weapons, for example, the weapons could only be made of plastics using current technology, and thus the weapons would not be practical. In the case of copyrighted material, the issues that arise for 3D designs are not substantially different from those for two-dimensional (2D) designs and can be addressed in the same way. In the case of substandard copies, the costs associated with the small production runs in additive manufacturing are high enough to deter criminals.

6

These topics were discussed by Dr. Bourell in his presentation and by the group as a whole in the discussion that ensued.

ELECTROMAGNETIC FIELD MANIPULATION OF MATERIALS THEMES

Understanding the Physical Phenomena

Overall, participants noted that processing with electromagnetic fields offers a wealth of opportunities. However, participants also noted the need to better understand the underlying phenomena that explain the physical changes caused by processing with electromagnetic fields. Rosario Gerhardt began the open discussion period by remarking on how thoroughly the presenters were sold on the ability of high magnetic fields to improve mechanical and magnetic properties of the materials, as well as the ability of electric fields to enable sintering capabilities. However, researchers do not always understand the physics behind the technologies. For instance, Robert Dowding explained in his presentation that the mechanisms to describe electric field-assisted sintering technology (FAST) are not well understood and discounted the most popular explanations, particularly any relationship to plasmas, sparking, or even sintering, despite the fact that the most popular name for the technology is spark plasma sintering (SPS). Despite the poor understanding of the underlying physics, Mr. Dowding pointed out that the process is still a very useful one, with lowered sintering times and temperatures, increased production rates, and lower energy costs. There were also several examples of processing in a high magnetic field in which the underlying mechanisms are currently being explored.

Research Prioritization

A number of applications of electromagnetic field processing techniques and applications were described in this session. While some participants noted that high magnetic fields offer several intriguing possibilities for further exploration, others wondered what research idea(s) the community should investigate in detail next. The workshop goals did not include focusing on or prioritizing research ideas, and several participants remarked on the vast array of examples provided. Examples of magnetic field processing techniques and applications given in the session on electromagnetic field manipulation included these:

- High and thermomagnetic processing (H&TMP),
- Examining creep life in metal alloys,
- High-temperature superconductors,
- Compaction and sintering of commercial magnet materials,

- Next-generation composites,
- Point defects,
- Oxidation reactions,
- Polymeric and organic materials,
- Magnetoplasticity and reduction of residual stress,
- Functional material applications (nanomaterials for magnetic storage, nanostructures, superconducting materials, and magnetic control of hydrogen storage),
- Electromagnetic acoustic transducer (EMAT) solidification/casting technology,
- Single crystal growth of iron-nickel-cobalt alloys,
- Crystallizing biological macromolecules,
- Changing the structural properties of high-strength steels,
- Processing and aligning nanotubes,
- Improving rare earth magnets, and
- High-magnetic-field annealing.

During the open discussion period, Dr. Gerhardt said that there were many examples but not many details in the presentations in this session. She said that while the presenters clearly advocated the technology and the ability to change the material microstructure at will, she wanted to get a sense of priority among the many applications. Dr. Gerhardt asked the presenters which area(s) would have the highest priority if only one or two areas of research were possible. Gerard Ludtka responded by saying that industry would not be interested in high-temperature superconductors. Industry would be most interested in changing the mechanical properties of materials. DOD would want to push the envelope for performance, so they might be more interested in the high-temperature superconducting magnet technologies. Ke Han noted that industry would probably want to get the most value for the smallest investment. For instance, manufacturers would like to use a low-performance material but find a way to get a 20-30 percent improvement from it. A 1 T magnet is cheap enough and can be built large enough to contain an entire truck for processing. This type of practical application might be useful to industry.

Permanence of Material Changes Made

Participants asked the speakers whether the changes to a material brought about by an electromagnetic field are permanent, and what aspects of the material can or cannot be relied upon. During the open discussion, Dr. Gerhardt asked the group if, once a field is used to induce a particular change, the resulting material is in a metastable state. Would the treated material revert to its original state at different temperatures? Or could it change its properties in some other way? Dr. Han replied that it depends on what property has been changed. If a material's texture is changed and the material is in a solid state, the texture will not be lost. If the solubility is affected at a high temperature, that effect will not be lost. But if a material is processed at a certain temperature and then subjected to a higher temperature, the effect that had been achieved could be lost. The issue of metastability was also discussed during the question-and-answer period following the presentation of Gregory Boebinger and Dr. Han, who were asked if the material property changes were permanent. Dr. Han responded that at ambient temperatures, the changes are permanent in the examples presented. However, the materials would reanneal at different temperatures, which could further change material properties. Another participant said that high-temperature solution treatments tend to be stable, but it is important to understand what has changed and what has been manipulated in the microstructure.

DESIGN OF MATERIALS THEMES

Materials Databases

A recurring theme of several presentations in this session was the need for a national fundamental materials database. Dr. Olson opened his presentation by restating one of the goals of the Materials Genome Initiative, which is to expand the database of materials' properties.¹ He also detailed a recommendation from the 2004 NRC study Accelerating Technology Transition: Bridging the Valley of Death for Materials and Processes, advocating the construction of a fundamental database for materials and suggesting that the White House Office of Science and Technology Policy (OSTP) lead the effort. The idea would be to promote the science-based engineering of materials instead of empirically based engineering, which was common then (and still largely is). While implementation of this recommendation began with formation of the Materials Genome Initiative, Dr. Olson reiterated his belief that focused support is necessary to make significant progress. Other participants asked what was needed to make significant progress in federal support for fundamental materials databases, as six NRC reports have discussed this need in the last 15 years. Dr. Olson responded that the database project is taking place but that additional force and energy must be brought to bear.

In his presentation Dr. Olson also described a vision for design and databases. One area of opportunity, he said, is a large-scale public database system, which could reside at the National Institute of Standards and Technology (NIST). He recommended that such a database consist of protodata below the assessed genome level: raw information on experimentally measured phase relations, thermochemi-

¹ See http://www.whitehouse.gov/mgi/goals. Accessed March 8, 2013.

O V E R V I E W

cal measurements, and DFT calculations.² The data could be pooled and periodically assessed to generate usable databases for public and private development channels. The website http://www.tms.org, which is maintained by The Minerals, Metals, and Materials Society, for example, stores 3D microstructural information. The standard database for materials selection is the set of discrete properties of materials searchable by the Ashby materials selection system. The opportunity exists to use the same architecture to search all databases at all levels, even to select atoms and components the same way as higher-level systems. Another opportunity is to hand off the material plus the associated information system for adapting to future manufacturing/field experience; this would allow moving beyond discrete properties into a system based on microstructural state variables.

Krishna Rajan also discussed materials databases in his presentation and said that his goal is to retrieve such data from their repositories and transmit them to laboratories where users can make new and unexpected discoveries.

Balancing Experiment-Based and Modeling-Based Design Approaches

A second recurring theme during this session was the appropriate balance between experimentation and modeling to develop new materials. During the open discussion period, Haydn Wadley, a committee member, framed this balance by asking the group to consider how they would design a new material, first, purely through experiment, and second, purely through modeling, and then to conduct this design process 30 years ago, in the present, and in the future. Respondents generally agreed that experiments would always be necessary for a material to be accepted for use, even a material designed purely by modeling. However, the future is likely to see materials design driven by models, followed by experiments to validate the new product. Participants also noted that experiments do not quantify uncertainty well; for that, computational tools are necessary.

Dr. Olson was asked during his presentation what types of models should be used—data-driven or physics-based. He responded that the most successful projects use a mechanistic, modeling-based approach rather than a data-driven one. Data-driven models tend to be superficial and to have too much empirical data to provide useful solutions. Modeling-based approaches can also point the way to experiments and lead to new discoveries.

Dr. Rajan also discussed the balance between experimentation and modeling, though he framed it as part of the strategy of informatics. Informatics integrates information of all types (including experiments, modeling, data, and theory) in an environment where there is no preexisting model. Informatics in this context is the computational strategy to integrate information associated with a mate-

 $^{^2~}$ Density functional theory (DFT) is a method for modeling the chemical bonding between atoms.

rial's structure, chemistry, and performance to extract patterns for its behavior at multiple scales.

During the open discussion period, Dr. Wadley asked participants for challenge problems—important capabilities that are currently out of reach—in this field. Several people spoke of instances in which fabrication produces a material with predictive approaches, and they recommended that data should be kept on such failures. Others pointed out that the Materials Genome Initiative may result in new experimental protocols that will generate new data, rapidly expanding fundamental materials databases.

Model Fidelity

There was some discussion of the DFT as the basis for calculation of phase diagrams (CALPHAD) modeling. In the open discussion period, some workshop participants questioned the resolution of the DFT calculation, which is about 0.1 eV at an ambient temperature of about 0.05 eV.³ Others defended the use of the DFT, pointing out that it was not inhibiting the design process and that the relative uncertainties were already well known. During the question-and-answer period following Dr. Olson's presentation, a participant asked about the accuracy of the DFT as well, and Dr. Olson replied that in surface thermodynamics, techniques are almost always DFT-based, and the accuracy is very good for grain boundary cohesion.

Materials Qualification

One of the goals of the design of materials approach is to reduce the amount of time needed to qualify materials. In his presentation, Dr. Olson described the qualification process for S53 and M54, the two landing gear steels QuesTek has developed. It took 8 years from material design through qualification for S53, and QuesTek is on track to get M54 qualified within 5 years. This computation-based qualification is much faster than a standard 10- to 20-year development cycle. Dr. Olson noted that the accelerated qualification of the stainless steel allowed QuesTek to share necessary inventory costs with the supplier because there was shared confidence in model accuracy.

10

³ One electron volt is a unit of energy equal to approximately 1.6×10^{-19} joule. In this case, it is customary to express the temperature in electron volts.

Workshop Introduction: Welcome and Meeting Objectives

Robert Schafrik welcomed participants to the Workshop on New and Novel Processes on the Verge of Industrial Modernization, an activity of the National Research Council's (NRC's) Standing Committee on Defense Materials, Manufacturing and Infrastructure (DMMI). The DMMI committee, which is under the auspices of the NRC National Materials and Manufacturing Board (NMMB), meets at the request of its sponsor, Reliance 21, a Department of Defense (DOD) group of professionals established in the DOD science and technology (S&T) community to increase awareness of DOD S&T activities and increase coordination among the DOD services, components, and agencies. Dr. Schafrik explained that this workshop would focus on three topics: additive manufacturing, electromagnetic field manipulation of materials, and design of materials. He explained that the workshop is an open meeting, that the publication produced from the workshop will be publicly available several months after the workshop concludes, and that no classified, proprietary, or For Official Use Only information was to be presented or discussed during the workshop. The workshop publication summarizes the discussions and presents the views of individual participants. There are no conclusions or recommendations that reflect a corporate or consensus position of the DMMI, the NMMB, or any other entity of the NRC. The report will serve as record of the activity, not a consensus report.

2

Additive Manufacturing— Session Summary

INTRODUCTION TO ADDITIVE MANUFACTURING AND CURRENT AND FUTURE APPLICATIONS

David Bourell, Temple Foundation Professor, Mechanical Engineering and Materials Science and Engineering Departments, University of Texas at Austin

Dr. Bourell began his presentation by defining additive manufacturing as the ability to print three-dimensional (3D) objects. The technology has been in existence for 20 or 30 years and is undergoing a rapid transformation. As with 2D printers, the quality and cost of 3D printers can vary dramatically. They range from low-quality, homemade printers costing several hundred dollars to elaborate printers that can cost a million dollars or more.

Dr. Bourell said that a primary challenge in 3D printing is the lack of standards in the community, including a lack of common terminology. ASTM International is developing standards for terminology, machines, and processes for 3D printing. Current ASTM standards have identified seven types of additive manufacturing machinery, as well as specific processes or technologies supporting each type of machinery. The seven types of machinery are these:

- Binder jetting, in which a binder glues the material together;
- Directed energy deposition, in which a laser or electron beam joins material not in a powder bed;

Copyright National Academy of Sciences. All rights reserved.

- Material extrusion, in which a polymer is melted and extruded;
- Material jetting, in which material (usually a polymer) is sprayed in droplet form;
- Vat photopolymerization, an older technique including stereolithography;
- Powder bed fusion, in which an energy beam is used to melt powder in a bed; and
- Sheet lamination, a cut-and-stack approach.

To date, at least 35 different companies are involved in developing additive manufacturing machinery, processes, and supporting technologies worldwide.

Interest in additive manufacturing is developing around the world, particularly in Europe. Lower-cost machines tend to be located in the United States, while the higher-end capabilities tend to be in Europe or Japan. Dr. Bourell reported that the value of the machinery and parts is approximately \$1.7 billion, and the industry is growing at 15-20 percent per year (Wohlers Associates, 2012). He also reported a rise in patents and patent applications, with between 600 and 800 patent applications per year.

Dr. Bourell then discussed the cost basis of additive manufacturing. In standard injection molding manufacturing, the cost is inversely proportional to the quantity of parts produced. For example, it may cost approximately \$10,000 per part to produce tens of 2 lb nylon parts via injection molding but less than \$10 per part as the production quantity increases to tens or hundreds of thousands. With additive manufacturing, however, the cost to produce one part is the same as that of producing 100,000 parts (in the case of the 2 lb nylon part, the price is fixed at roughly \$100 per part). Figure 2.1 shows a sample schematic comparing the cost per piece as a function of quantity for additive manufacturing and injection molding.

Additive manufacturing is an attractive option for low-volume production, but it is not a viable alternative for large-scale production. Additive manufacturing is also able to produce very complicated geometries that standard injection molding may not be capable of. Thus, Dr. Bourell shared his "mantra" for additive manufacturing: low production runs, complicated geometry.

Dr. Bourell then listed a number of industries and areas that could benefit from additive manufacturing technology:

- Automotive industry: Not for large-scale production pieces but for support items, such as jigs and tooling, and for custom automobiles, such as Bentleys.
- Aerospace industry: Additive manufacturing may be well suited to this industry, as the number of parts produced is quite small (for example, the Boeing 747 had 1,524 orders).

14



FIGURE 2.1 Economics of additive manufacturing showing the price per part as a function of quantity for a 2 lb nylon part manufactured via additive manufacturing and via injection molding. SOURCE: David Bourell, University of Texas, Austin, presentation to the Standing Committee on Defense Materials, Manufacturing and Infrastructure on December 5, 2012, slide 15.

- Tooling for injection molding.
- Medical implants and prosthetics: Each item must be custom-fit, so items are individually produced.
- Game avatars: Each item is customized to the consumer.
- Art and jewelry: Each piece can be custom-made and can include complex geometry.
- Architecture: These include scale models and custom pieces, including those with high levels of geometric detail.
- Prototyping: Additive manufacturing could be used in the design process, enabling a more efficient process through rapid prototyping.

A roadmapping effort was conducted in 2009 by the additive manufacturing community, funded by the Office of Naval Research and the National Science Foundation. The document that resulted from the roadmapping effort (Bourell et al., 2009), identified the following topics as the most critical research areas:

- Consistency and repeatability;
- Process standards;
- Closed-loop feedback control;
- Predictive analysis and modeling;
- Material property data generation;
- Exploitation of unique features of additive modeling;
- Design rules and tools (uniformity used to be critical, but additive manufacturing has changed this); and
- In-build considerations, such as inspection and sensors.

Dr. Bourell noted that work on process standards was completed in 2009: ASTM International has formed a technical committee and produced three or four standards. In addition, ASTM and the International Organization for Standardization (ISO) have agreed to fast-track efforts between ASTM and ISO.

Dr. Bourell predicted an increase in the near term in research emphasis on manufacturing in general, and on additive manufacturing specifically, pointing to the National Additive Manufacturing Innovation Institute (NAMII) as an example. He said that he anticipates more widespread consumer acceptance of additive manufacturing through the standard-setting efforts of ASTM. In addition, he said that he believes there will be more low-cost printers entering the marketplace from do-it-yourself enthusiasts, as well as easier access to libraries of parts, such as the Shapeways library (http://www.shapeways.com), where manufacturers sell their parts online. In the mid-term, Dr. Bourell stated that he foresees the community moving toward easy-to-use consumer software for 3D applications, driven by the need to print 3D objects. He also could envision a "Kinko's-style" additive manufacturing capability, where the consumer designs his or her part and sends it to a neighborhood printer to be printed and retrieved. He believes that the lower costs of 3D printing will drive the higher-cost technology along and that the experience base will foster new applications and spur competition among different additive manufacturing technologies.

Dr. Bourell described several potential challenges facing additive manufacturing processes. Surface finish and tolerances have been continual research challenges for the community. There is also a question of liability. There are many people involved in creating a part (designers, standard setter, downloader, printer, etc.), making it difficult to identify where the responsibility lies if a part fails. There is also the question of copyright: A 3D printer provides the ability to print copyrighted material. However, copyright concerns are no different in 3D than they are in 2D. Finally, there is the question of terrorism and unlicensed weapons. There is the potential for an explosive device to be implanted into an additively manufactured part. It is also conceivable that someone could use additive manufacturing to build a weapon that is not licensed, though Dr. Bourell pointed out that the weapon would have to be made of plastic at this point (he described a case where this had occurred). However, such a capability still poses a safety concern.

During the question-and-answer session, Dr. Bourell said that most of the materials used in additive manufacturing are polymers and plastics, and that there is currently much interest in developing metals as well as ceramics. There is a need for new metal alloys with characteristics appropriate for additive manufacturing; however, certification considerations are one major concern. The Air Force is likely to reject an altered metal because it would not be able to incorporate parts made from such a metal without a lengthy and tedious recertification process.

In response to a question, Dr. Bourell noted that separating the information content from the part content is a great advantage to the additive manufacturing process. Hod Lipson's research group at Cornell University has developed a programming language to capture the information content of a part, such as color, gradient, and features.

In closing, Dr. Bourell was asked about the costs of additive manufacturing. He pointed out that, historically, machine cost dominates the costs of 3D-printed parts, not the material itself. If machine cost could be reduced or productivity increased, then the cost of additive manufacturing (the horizontal line on Figure 2.1) would decrease. As patents expire, competition will increase and machine costs will decrease. Dr. Bourell also noted that additively manufactured metals have made great inroads recently, but not in the consumer market.

ADDITIVE MANUFACTURING AT GE

Prabhjot Singh, Manager, Additive Manufacturing Laboratory, GE Global Research

Dr. Singh began his presentation with a broad overview of GE and a description of its manufacturing research activities. He then moved on to the more specific area of additive manufacturing research, and said that there are two primary uses for additive manufacturing:

- Rapid prototyping to compress the design cycle from a few years to a few months (for example, an engine part could undergo 50-60 iterations in less than 6 months) and
- Manufacturing previously difficult-to-produce high-performance components at a lower cost.

Dr. Singh divided additive manufacturing research into three size scales: micro (tens to hundreds of microns), macro (hundreds of microns), and large (500

16

microns and above). At the microscale, GE is developing processes to print ceramics and is printing sensors atop existing turbomachinery components. At the macroscale, GE has a range of machines that are being commercialized for turbomachinery applications, as well as for direct metal laser melting and electron beam processes. Large-scale features are created with existing conventional technologies such as laser and electron beam cladding and spray technologies. Parts repaired with those techniques are currently used on aircraft. Most of GE's efforts are focused on macroscale additive manufacturing, Dr. Singh said, although it has a small effort in microscale technologies. He described research efforts at each size scale in more detail.

In microscale additive manufacturing, Dr. Singh explained that the technologies under development at GE are focused on digital microprinting with a thin layer (20-100 μ m) of ceramic slurry and a UV-cured photopolymer. Using this low-cost, highly adaptable manufacturing method, GE has created high aspect ratio shapes with lateral dimensions of less than 30 μ m. The technique has been demonstrated in materials including polymers, alumina, piezoceramics, platinum, and phosphors. Dr. Singh described how this microscale technique could be used to create novel ultrasound transducers. Using microscale additive manufacturing, piezoelectric elements can be placed into unique ultrasound transducer architectures instead of a standard rectilinear arrangement. This can change the acoustic response of the device built, allowing GE to produce a high-frequency ultrasound probe with an improved signal-to-noise ratio.

Dr. Singh then discussed macroscale additive manufacturing, including both direct metal laser melting (DMLM) and electron beam melting (EBM). In each case, an electron beam moves over a metal powder and melts it locally, stitching the metal powder together, layer by layer, until a fully manufactured part is created. GE has over 20 DMLM systems in place and collaborates with other entities on EBM systems. Dr. Singh reported that the material properties of the resulting parts are reasonable, with tensile strength and fatigue somewhat comparable to wrought and cast iron. The two primary advantages to the macroscale additive manufacturing technique are the ability to create novel shapes (many flanges can be eliminated from GE's original engine design) and reduced mass (GE's stated goal is to shed 500-600 lb from its engine). In addition to structural benefits, additive manufacturing process to create parts optimized for reduced emissions or heat transfer properties; the freedom of this technique lies in the ability to develop new geometries optimized for specific purposes.

Dr. Singh then briefly described large-scale additive manufacturing, in which a laser beam or an electron beam is used to heat the metal powder. The technology is 20+ years old. Dr. Singh described an example where large-scale additive manufacturing is being used—the leading edge of a fan blade approximately 2 ft long.

The primary advantage of the technique is in material savings; using conventional techniques, significant amounts of material would be machined away.

Dr. Singh went on to describe the path forward for additive manufacturing. Machines are improving, both increasing in size and decreasing in price. However, one primary drawback is that the machines capable of this type of processing are all based in Germany, and acquiring a custom machine is expensive and difficult. He would like to see more machines made by multiple producers. Also, the qualifying of materials is a big problem; some materials developed in the late 1980s (such as materials for the composite fan blade) are only now qualified for flight. There are long development times for all kinds of materials processing; this is in part due to rigorous aviation certification procedures. The same is true for materials processing qualification. Inspection is also a problem: Additive manufacturing can create unique, complex shapes that are difficult to inspect. New inspection methods will be necessary to qualify these new parts.

Dr. Singh would like to see materials databases developed collaboratively, so that everyone can benefit from the technology development. He would like to see accelerated materials qualification. Dr. Singh envisioned an "ecosystem-like" R&D environment in which government, industry, universities, and national laboratories cooperate to develop a range of technologies to support additive manufacturing. Additive manufacturing makes the most sense and will have the greatest impact when there exists a unique design, a qualified materials system, and a mature manufacturing technology.

During the question-and-answer session, Dr. Singh was asked about the access to electron beam and laser processing machines. He answered that no U.S. companies make electron beam machines; only one Swedish company makes them, which is a restrictive situation for U.S. users. About six companies manufacture the laser machinery, but electron beam processing is 4-5 times faster than laser processing.

It was pointed out by a member of the audience that the examples given in the presentation were all mechanical; the person asked whether integrated electronic circuits could be manufactured by additive processing methods. Dr. Singh replied that GE is interested in flexible electronics, and there is active research in that area at GE and in academia as well. Hence, rapid prototyping is also relevant to circuits.

Dr. Singh was asked to elaborate on parts that are difficult to produce. He explained that some parts can take as many as 15-20 steps to process conventionally, as opposed to one single step with additive manufacturing. Additive manufacturing would also eliminate joints, which provides a performance advantage. As it takes less time to develop the manufacturing techniques in additive manufacturing, it provides a cost savings as well.

Dr. Singh also said that combining materials with different properties, growing parts onto one another, and embedding structures are all areas that will likely take off in the near term.

Dr. Singh was asked to describe the certification process. He said it starts with the material, which must have a composition that meets the specification. The machine being used must be qualified. The laser has to be within the right operating window, and additive layers must be produced at the right thickness. The heat treatment steps must produce the part to the right dimensions, material properties, and microstructure. The specification gets written for the material, for each step. It is a very involved process. The current process takes 10-12 years, and he would like it to take 1-2 years.

In response to a question about the application domain in which to invest, Dr. Singh pointed out that it is important to consider the game changers and to think about where industry may be willing to pay the premium for high-performance parts. For instance, the manufacture of prosthetics is far ahead of the aerospace industry in additive manufacturing because each piece needs to be custom-made. Indeed, biomedical applications in general would be another application to consider. Printing cells is a long-term goal (perhaps something to consider in our grandchildren's lifetime).

CENTER FOR INNOVATIVE MATERIALS PROCESSING THROUGH DIRECT DIGITAL DEPOSITION

Richard Martukanitz, Assistant Director, Applied Research Laboratory, Pennsylvania State University

Dr. Martukanitz began his presentation by briefly describing the additive manufacturing process. Additive manufacturing uses a digital description, or digital file, to drive the manufacturing process: The digital description generates a "build path" that consolidates material in an additive manner using a laser, electron beam, or other concentrated energy source. The energy source can be scanned over a powder bed or can be directed along the build path with the addition of new material. Additive manufacturing techniques are applicable to a range of materials, including polymers, metals, and ceramics. Dr. Martukanitz described three primary advantages to additive manufacturing:

- The ability to reduce costs through decreased material usage and machining;
- The ability to create complex designs and features that would be difficult to manufacture with traditional manufacturing methods; and
- The ability to use multiple materials or graded materials to locally tailor a component's functionality and performance.

With these advantages, additive manufacturing can both produce new components and repair or remanufacture existing parts.

20

Dr. Martukanitz described how additive manufacturing processes can provide benefits in three primary areas:

- *Production of unique materials.* The high solidification rates and high cooling rates allowable with additive manufacturing can produce materials with unique properties. Examples include bulk metallic glass and eutectic ceramics.
- *Modification of the surface*. Additive manufacturing can allow local changes to the surface of the material (e.g., repairing turbine blades in the aerospace industry).
- *Production of a component.* This is the most interesting goal of additive manufacturing today: creating 3D components.

Dr. Martukanitz then described the requirements for ensuring process and product reliability in the design, process, and product phases of development. He said there first must be a certified material source; the whole material supply chain should be defined for this process, which is not true today. Next, there should be an open architecture for the equipment system used to allow everyone to have full access to the processes. The powder bed electron beam system currently used is a closed system: The parameters used and the materials used to service the equipment are closely guarded by the equipment manufacturers. Dr. Martukanitz believes it is important to have an open architecture and full access to the process and materials. Next, he stated the process requires quality control and assurance. Finally, he said that there needed to be more significant data sharing within the industry. He expressed this as follows: "Everyone is making bricks, but no one is building houses."

Dr. Martukanitz then went on to describe the capabilities at Penn State University in the Center for Innovative Materials Processing through Direct Digital Deposition (CIMP-3D) laboratory, a university-wide initiative designed to become a world-class facility for developing and implementing additive manufacturing technology for critical metallic components. CIMP-3D was scheduled to break ground in January 2013 on a new 10,000 ft² manufacturing and demonstration facility with state-of-the-art additive manufacturing capabilities as well as ancillary capabilities.

CIMP-3D is divided into two areas: the Advanced Manufacturing Laboratory and the Advanced Design and Prototyping Studio. The Advanced Manufacturing Laboratory contains three primary pieces of equipment: an Optomec LENS MR-7 laser-based powder-fed system for complex geometries, an EOS M280 laser-based powder bed system, and a large Sciaky wire-feed electron beam system. The laboratory can interrogate and inspect final parts and reverse-engineer parts and can design and prototype parts.

The Advanced Design and Prototyping Studio consists of several models being

developed for virtual experimentation. Dr. Martukanitz described five submodules, which are interoperable (Figure 2.2). The first model is the process submodule, which can be refined and engineering and economic metrics assessed for their suitability to additive manufacturing. That submodule drives the coupled thermal-mechanical submodule, which simulates the thermal-mechanical response of the material during processing. That information drives two areas: (1) the micro-structural evolution submodule, developed primarily for titanium alloys, and (2) the phase identification submodule, which ascertains the best mixing of materials and material grading. That information drives the resultant mechanical properties



FIGURE 2.2 The five basic modeling tools of the Advanced Design and Prototyping Studio. SOURCE: Richard Martukanitz, Penn State University, presentation to the Standing Committee on Defense Materials Manufacturing and Infrastructure on December 5, 2012, slide 15.

model, which is currently the weakest link in the modeling process and considers such features as dynamic properties, fracture properties, fracture propagation, and fatigue. These tools will be available on the Shared Information and Data Network.

Dr. Martukanitz then provided some examples applying the modeling techniques to the microstructural evolution of a titanium alloy; these examples reflected an understanding of the processes based on their advanced modeling tools. He showed the ability to analyze fairly complex geometries, simulating such variables as distortion, residual stress, and thermal history.

CIMP-3D, which was established in 2011, has been actively involved in the more rapid acceptance of additive manufacturing technology. It is hoping to cultivate a national network committed to the advancement and implementation of direct digital manufacturing technology.

In response to a question about qualification, Dr. Martukanitz said that the welding industry would be a good model to follow. Welded structures have a design code to provide guidelines, qualified materials, qualified operators, processes, and repeatability within a range of process parameters. This makes welding a good model for additive manufacturing. An audience member pointed out, however, that welding might make sense because it is formed by attaching two well-defined end structures instead of using powder. Dr. Martukanitz replied that we do need to look at the feedstock. He said that the specifications that cover injection molding and sintering do not apply to additive manufacturing. He does believe that ASTM is moving in the right direction.

In response to several questions regarding repair, Dr. Martukanitz clarified that additive manufacturing is used to repair jet engine turbine blades, not replace them. A limited number of jet engine blades are in use today that were repaired using laser-based additive manufacturing repair techniques. In response to a more general question about repair compared to manufacturing, Dr. Martukanitz agreed that the processes for qualification for additive repair and additive manufacturing are similar. The codes are separate, but the processes are similar. Thus, the qualification for repair compared to qualify additive manufacturing.

Dr. Martukanitz was asked about the size of parts that can be manufactured additively. He said that a modified electron beam welding system by Sciaky, Inc., has a build envelope of 4 m; this system works by adding material to a plate. This shows that directed energy systems can be quite large in extent. Powder bed systems are quite different: There, because the bed size sets the limit, the system is much more constrained in size.

22

OPEN DISCUSSION: ADDITIVE MANUFACTURING

Discussion Leaders: Denise Swink, Private Consultant, and Robert Latiff, Chair, DMMI Standing Committee

Ms. Swink began the discussion by noting that the major effort in additive manufacturing appeared to be taking place in the United States and Europe; she then asked the group to describe the differences between the research efforts in the two arenas. She noted that there were more manufacturing capabilities in Europe and asked if that was tied to any research efforts. She also asked how the United States could stimulate more manufacturing capabilities here. Some participants noted that the research in Europe is more applied, or at least more project-specific, and that Europe has more grants in additive manufacturing. Europe also builds on a more traditional approach, technology transfer, which tends to lead to more manufacturing. Other participants responded that research in the United States is more basic, and when it proves itself to be useful, it will work its way into industry. The more basic U.S. research tends to be more innovative and a little more high risk; the United States is more tolerant of failure. A participant noted that the Manufacturing Innovation Institutes under President Obama could be very innovative, though potentially short-lived.

Dr. Latiff asked if there were any standard model and simulation packages used throughout the community. Participants replied that there are mechanical models that have been well verified for design. Process models and materials models are less standardized, and less validation and verification has been performed on those models.

The group then discussed sustainment and performance capability. Ms. Swink noted that this is the opportunity for additive manufacturing to get sustainment right—by including, for example, processes and principles that ensure that a part's complete digital history is accessible to all users. Participants then also briefly discussed performance capability, or making sure that a part meets specification. Someone pointed out that a sequence of rudimentary tests for reliability and performance or quality can be built into the process. When one participant asked whether there would be problems caused by suppliers printing poor-quality goods, other participants noted that the incentive would not be very great, as the cost of doing so would be high.

Participants then brought up the issue of qualifying the process rather than qualifying the end product. To take an integrated computational approach to materials qualification, it may be necessary to qualify all the interrelationships among the materials and processes. The certification processes would then need to change. Multiple participants discussed the need for change in the certification process used by the Federal Aviation Administration, which is currently designed for bulk
manufacturing, where the first 100 parts are built and certified, and subsequently 2 of every 100 parts are certified. It was noted that that style of certification does not make sense if the process to create individualized parts is certified.

Ms. Swink asked whether new materials would be needed for additive manufacturing. She also asked if there is a challenge in that the manufacturing and design communities are not well integrated. Other participants agreed that materials in production are not specifically tailored to additive manufacturing and may be somewhat deficient. Further, designers are not much involved in the materials process even though it is they who should be providing specifications to the materials scientists.

Surface finish was mentioned as an area where technical advances could be made.

Ms. Swink pointed out that the United States lacks an industrial base for additive manufacturing machine systems and for some materials supply to the DOD community and wondered if this posed a problem. Some participants pointed out that part production for the machinery is done in the United States, although the machines may come from overseas; since DOD is a relatively minor player in this area of additive manufacturing, this scenario is unlikely to change. There is an industrial base for some materials feedstock in the United States; nonetheless, some niche applications may have a hard time sourcing their material in this country.

3

Electromagnetic Field Manipulation of Properties— Session Summary

HIGH-MAGNETIC-FIELD PROCESSING AND SYNTHESIS TO DEVELOP THE NEXT GENERATION OF STRUCTURAL AND FUNCTIONAL MATERIALS

Gerard Ludtka, Distinguished Research Staff, Materials Processing and Manufacturing Group, Materials Science and Technology Division, Oak Ridge National Laboratory

Gerard Ludtka began his presentation by noting that high-magnetic-field processing affects all materials. While people think of iron and steel when they think about magnetic fields, magnetic fields can impact all metallic systems, covalently bonded systems, and polymeric systems. He mentioned examples as diverse as graphite, copper, and chocolate. He said one advantage to being at Oak Ridge National Laboratory (ORNL) is the access to supercomputing capabilities that allow sophisticated modeling to explain some of the physics being observed. ORNL also has a spallation neutron source, allowing for in situ, real-time materials characterization.

Dr. Ludtka then discussed how high and thermomagnetic processing (H&TMP) can improve the performance of materials. The approach used at ORNL couples induction heating within a superconducting magnet, with H&TMP for rapid throughput, part-by-part heat treatment processing. ORNL also has experimented with applying this process without the induction heating for a "heat-free" heat-treating method. The processing technique provides accelerated kinetics, novel

microstructures within the material, and the possibility for enhancing material performance. This technique is a new synthesis-catalysis tool for overcoming reactionactivation barriers, and it has the potential to reduce processing energy and costs.

Dr. Ludtka then went on to describe numerous material properties that strong magnetic fields affect, including these:

- Phase stability;
- Diffusion barriers;
- Dislocation cores;
- Fault energies;
- Phonons and magnons;
- Kinetics, by raising temperatures and by affecting the critical stable nucleus for precipitate formation; and
- Catalysis and synthesis, by affecting activation energy barriers.

Dr. Ludtka described a workshop conducted in 2005 by the National High Magnetic Field Laboratory to understand the needs of industry in X-ray and neutron effects. The workshop, Probing Matter at High Magnetic Fields with X-rays and Neutrons, resulted in a long list of material families and impact areas, including biological materials, synthesis of proteins, composite systems, and many, many others (Granroth et al., 2005). ORNL researchers are working to extend and realize some of these ideas.

Dr. Ludtka then very briefly described magnetic field processing at ORNL as a commercial-scale, synthesis-catalysis processing tool designed to impact phase equilibria and accelerate phase transformation kinetics. It is designed to simultaneously impact material properties such as strength, toughness, and phase equilibrium. The magnetic field processing facility at ORNL uses 9 T superconducting magnets with a vertical, 8 in. diameter bore.

Dr. Ludtka then explained why a high magnetic field shifts the phase boundaries of a material. There is a term in the free energy equation that is correlated with the external magnetic field (the integral expression in the equation below), although it is not traditionally considered to play a significant role:

$$\Delta G_{\rm Fe}^{\gamma \to \alpha} = RT \Big[\ln \Big(a_{\rm Fe}^{\alpha} \Big) - \ln \Big(a_{\rm Fe}^{\gamma} \Big) \Big] + \int_{0}^{H} \Big(M_{\rm Fe}^{\gamma} - M_{\rm Fe}^{\alpha} \Big) dH$$

 ΔG represents the change in free energy, α represents the ferrite fraction, and γ represents the austenite fraction in the *Fe* phase diagram, where *a* is the free energy for either ferrite or austenite. *R* is the gas constant and *T* is the temperature. In the integral *H* is the magnetic field and *M* the magnetization. Contrary to the assumption that the magnetic field term is unimportant, research at ORNL has shown that high-magnetic-field processing does have an impact on microstructure,

phase transformation kinetics, and materials performance. The effect of the magnetic processing on any of these parameters scales with the applied magnetic field.

Dr. Ludtka showed that H&TMP processing provides typical improvements of 10-15 percent in strength, ductility, and/or toughness, with maximum gains of 30 percent in these parameters. H&TMP also provides shorter tempering times (by up to 80 percent) and lower tempering temperatures (by up to 30 percent) while still achieving performance gains of 20-30 percent in yield strength and ultimate tensile strength with no loss of ductility. He also described how inexpensive alloys that do not contain cobalt can be used in steel to improve toughness. The sample sizes processed to date range up to 75 mm in diameter by 200 mm in length. Dr. Ludtka also pointed out that it is important to think about scaling up to commercial applications; this processing has been successfully demonstrated on several commercial prototype systems. He emphasized that the H&TMP technology is a transformational breakthrough that has the ability to significantly impact phase equilibria and kinetics, and it is a new synthesis and catalysis tool that can influence the behavior and performance of all materials.

Dr. Ludtka then said that understanding creep life remains an important unresolved question. Creep life improves significantly—up to 600 percent—in some alumina-forming austenitic steel alloys (Brady et al., 2008) after magnetic field annealing as compared to as-processed alloys that have not undergone magnetic field annealing. In experiments, however, when titanium and zirconium were added, creep life did not change or became worse after magnetic field annealing compared to as-processed samples, and the mechanism for this is not well understood. This is something ORNL is trying to understand through modeling. Dr. Ludtka also discussed the need to understand the impact of the interaction of the magnetic field, temperature, and alloying elements. In particular, he described a collaborative effort with Toyota Motor Engineering & Manufacturing North America to increase the strength of magnesium alloys. It seems like magnetic processing during aging increases the strength of the alloy.

Dr. Ludtka then addressed another set of experiments with high-temperature superconductors. The goal of this project is to develop processing technologies for rare-earth-element-free superconductors using high magnetic fields to increase the critical current density by two orders of magnitude while also improving material strength by 30 percent over conventionally processed material. The approach incorporates H&TMP techniques along with carbon nanomaterials and powder metallurgy processing to develop the superconductor. The high-magnetic-field processing allows the critical current of the Josephson junctions to increase without decreasing the size of the devices. Superconductor synthesis using high-magnetic-field reaction sintering has yielded microstructural features typical of a high-pressure phase fabrication process.

Dr. Ludtka then described a project in compaction and sintering of commercial

magnet materials under high magnetic fields. The goal of this project is to reduce the rare earth content and improve the performance of rare-earth-element permanent magnets. The research uses cold powder compaction in a high magnetic field, followed by high-magnetic-field sintering, to process materials for maximum efficiency by aligning their microstructure. The expectation is a reduction of more than 30 percent in rare earth element usage using the magnetic field assisted powder consolidation and sintering techniques without loss of magnet performance.

Dr. Ludtka then described research in the next generation of composites. Using techniques based on H&TMP, the next generation of carbon fibers is expected to yield 100 percent improvements in strength and a 50 percent increase in stiffness modulus. Polymeric matrix (epoxy) materials are expected to gain improvements in tensile stiffness of 300 percent in the direction of the applied magnetic field. These changes to strength and stiffness would allow for revolutionary changes in the weight of aircraft and other vehicles.

Dr. Ludtka then very briefly described three additional applications of magnetic fields. The first application is defects, where the defect interacts with the magnetic field and effectively acts as a localized magnetic field source, producing a pseudo-field of up to 300 T at the point defect location. The next application is oxidation, where magnetic fields can accelerate a radical oxidation reaction. The third example was polymeric and organic materials, where magnetic fields have the potential to impact the orientation of polymeric and organic materials.¹

Dr. Ludtka spent some time discussing the benefits of magnetoplasticity and the reduction of residual stress. Magnetic fields afford the ability to improve fatigue life and deformation behavior, thus extending component life by up to 30 percent. The assumption is that magnetic fields can be used to break main domain walls, preventing (or delaying) the formation of persistent shear bands and their migration, as well as crack formation. Similarly, residual stress reduction via magnetic processing during or after component fabrication also extends component lifetimes and allows for design stresses to be higher, enabling smaller, lighter-weight, moreenergy-efficient components.

Dr. Ludtka then mentioned potential functional material applications of magnetic field processing to produce. The functional materials research topics included nanomaterials for magnetic storage, nanostructures, superconducting materials, and magnetic control of hydrogen storage.

He also described the electromagnetic acoustic transducer (EMAT) solidification/casting technology. The goal of this project is to achieve wrought-like microstructure and properties in as-cast materials. This would mean the elimination of micro- and macrosegregation, a reduction in grain size, an overall increase in strength, and improved creep performance. Dr. Ludtka showed examples of cast

¹ Including, for example, controlling the solidification and crystallization of sugar and chocolate.

29

iron successfully processed using this technology, with a 51 percent improvement in hardness.

Dr. Ludtka then showed some results of single crystal growth of an iron-nickelcobalt alloy, where the molten alloy is subjected to a high magnetic field and then solidified. This allows for single crystal growth in a low-energy process. He also described crystallizing biological macromolecules in a high magnetic field; the magnetic field can control the growth kinetics and structure.

Dr. Ludtka then showed the magnet capabilities at ORNL, where there are four separate superconducting magnet processing facilities:

- A commercial-scale superconducting 9 T magnet with a vertical 8 in. bore and 9 in. uniform field strength, designed for large-scale experiments;
- Two continuous-feed H&TMP systems with two horizontal 5 in. bore superconducting magnets with a 9 in. uniform field; and
- A 9 T, 5 in. vertical bore superconducting magnet with a 9 in. uniform field, designed for solidification processing.

All systems have a cryogen recondensing cooler, eliminating the need for replenishing the cryogens.

During the question-and-answer session, Dr. Ludtka was asked if anisotropy could be causing local strain, causing strain hardening when a sample is put into the magnet. Dr. Ludtka said that while magnetostrictive forces can be significant, the dislocation dynamics tend to be normal. A participant suggested that the sample be removed and put in again with the opposite orientation as a test.

A questioner noted that the potential improvements reported by Dr. Ludtka (100 percent in tensile strength and 50 percent in stiffness modulus in carbon fibers) are amazing increases and asked if this information had drawn the attention of carbon fiber producers. Dr. Ludtka responded that today's economy is such that industry is discouraged from funding this type of research, but that DARPA might be interested.

Another questioner asked if ORNL has conducted any research in carbon nanotube growth in a magnetic field. Dr. Ludtka responded that several years ago researchers at the laboratory took carbon precursors and made graphene sheets and nanotubes in a magnetic field.

In response to a question about research in China, Dr. Ludtka said that Chinese researchers are publishing aggressively in many areas related to high-magnetic-field processing. The government of China hired Bruce Brandt, former director of the National High Magnetic Field Laboratory DC Magnet User Program, to help build a high-magnetic-field facility in China. In general, China lags about 5 years behind the United States in developing high-magnetic-field processing.

Dr. Ludtka was asked what was on his wish list. He responded that he wished

for sustained funding. DOD is more apt to fund an industry-led proposal; however, developments made possible by DOD may not be shared outside DOD. He would like to see a situation where research is sustained and the information is publicly available. From the perspective of funding agencies, there are also challenges in finding the right balance between modeling and application.

MATERIALS PROCESSING AT THE NATIONAL HIGH MAGNETIC FIELD LABORATORY

Gregory Boebinger, Director, National High Magnetic Field Laboratory, and Ke Han, Scholar/Scientist, National High Magnetic Field Laboratory

Dr. Boebinger began the presentation by describing the National High Magnetic Field Laboratory (MagLab). Most of the facility resides at the Florida State University campus site, with smaller campuses at Los Alamos National Laboratory and the University of Florida. The laboratory was formed in 1990 as the result of an NRC study and the ensuing national competition. It is recompeted periodically, and the next recompetition is in 5 years. It is funded primarily by the National Science Foundation (NSF), with substantial contributions from the state of Florida as well. Since 1990, NSF has contributed roughly \$500 million and the state of Florida has contributed roughly \$350 million, which is a unique national-state financial partnership. The Department of Energy also supports the laboratory, especially the Los Alamos site. In 2011, the MagLab's user program hosted over 1,200 scientists from more than 200 institutions in the United States and around the world. The user community is ever changing, as every year roughly 20 percent of the principal investigators on proposals to use the facility are first-timers. To use MagLab facilities, there is a competitive proposal process for magnet time. Successful proposals receive no-cost access to magnet facilities and time. Experimental results obtained using the facility must be published. MagLab usage results in approximately 400 journal publications per year; about half of the research activity at the laboratory is concentrated in condensed matter physics and materials science, and the remainder is distributed across geochemistry, chemistry, biology, biochemistry, and other engineering. MagLab currently holds the world records in magnet strengths in all categories and also holds records in short-pulse magnets (101 T), long-pulse magnets (60 T), hybrid magnets (45 T), resistive magnets (36 T), and superconducting magnets (35 T in a demonstration test coil). Figure 3.1 shows how magnet strength has evolved over time for the various types of magnets.

Dr. Boebinger described the status of the 35 T all-superconducting magnet project. At the MagLab, researchers have taken a wide-bore resistive magnet and dropped a high-temperature superconducting magnet into it to create a proof-of-



FIGURE 3.1 Maximum magnetic field strength as a function of year for different types of magnets. SOURCE: Presentation by Gregory Boebinger and Ke Han, National High Magnetic Field Laboratory, presentation to the Standing Committee on Defense Materials, Manufacturing and Infrastructure on December 5, 2012, slide 6.

principle 35 T demonstration. In superconducting magnets, the superconducting materials used constrain the magnet. Because of the current-carrying capacity limitations of the material, niobium-3 tin (Nb-3 Sn) will never allow for a super-conducting magnet larger than 25 T. Yttrium barium copper oxide (YBCO) has good current-carrying capacity, allowing for a higher magnet strength, but the material is highly anisotropic, which introduces complications for magnet production. Isotropic round wire is easier to incorporate into a magnet design, is easier to wind, and makes it easier to achieve high levels of homogeneity. MagLab researchers recently discovered that round-wire bismuth strontium calcium copper oxide (BSCCO) can be processed in high-pressure oxygen, eliminating the formation of voids that plagued earlier round wire and allowing for the material to be used for magnet production with a high magnetic field strength.

Dr. Boebinger then discussed resistive pulsed magnets and continuous magnets. Once again, the materials constrain the magnets. He pointed out that the pressures inside the MagLab 100 T pulsed magnet are on the order of 200,000 psi (1.4 GPa), thus exceeding the strength of most steels. To ameliorate the huge explosive pressures inside the magnets, copper/niobium and copper/silver nano-composite materials are used in wire form for pulsed magnets and in sheet form for continuous magnets to increase the material strength.

Dr. Boebinger pointed out the uniqueness of magnetic fields, particularly when compared to techniques used at other facilities: Magnetic fields are a flexible thermodynamic parameter (as opposed to X-rays or neutrons, which are probes) and can be used in situ, rapidly, reversibly, and with infinite tunability. In this sense, magnetic field experiments are often more flexible than experiments that change other thermodynamic variables such as pressure or carrier densities. In addition, unlike temperature, pressure, and carrier concentration, magnetic fields are a vector, so an experiment can be designed to probe anisotropies or impose new anisotropies.

Dr. Han then described how high magnetic fields can be used to improve the properties of a material. By changing the phase transformation behavior (such as the solidification and the solid-phase transformations), the microstructure can be refined and improved. By altering the texture of a material, the anisotropy of the material can be tailored to suit a particular purpose. Examples of magnetic field processing include improving the mechanical properties of structural materials or the magnetic properties of magnetic materials. Dr. Han included several examples where magnetic fields were used to alter material properties.

The first example Dr. Han showed used a 33 T high magnetic field to change the mechanical properties of high-strength steels. The application of the 33 T field increased the martensitic transformation and pearlite transformation temperatures.

Dr. Han then showed a second example in which high-magnetic-field processing was used to align nanotubes in making buckypaper.² Alignment was created by filtering the nanotubes in a high magnetic field (up to 17 T), creating unique anisotropic properties in the material suitable for use as actuators. The strain magnitude increased by 15 percent, and the material acquired anisotropic properties suitable for an actuator. The asymmetry is a new feature generated by processing in a high magnetic field.

A third example was the influence of high-magnetic-field processing on the critical current density of $Bi_2Sr_2CaCu_2O_x/AgMg$ round wire. Dr. Han showed that heat treatment of superconducting wires can impact the critical current density in particular orientations when the treatment is conducted in the presence of a high (8 T) magnetic field.

A fourth example was improving rare earth magnets using high magnetic

 $^{^2\,}$ Buckypaper is a material made from carbon nanotubes that is 10 times lighter than steel and 250 times stronger than steel.

33

fields. The rare earth metal neodymium is critical today in the production of permanent magnets. However, the volatility of its price poses a challenge to magnet manufacturers. Neodymium cost \$10/kg in 2006, \$450/kg in 2011, and \$140/kg in the summer of 2012. There exists approximately 250 g of permanent magnets in a standard automobile and 1 kg of permanent magnets in a Toyota Prius, so its price is a significant concern in industry. The goal of the project Dr. Han described is to reduce the use of rare earth metals for magnets, replacing them with anisotropic nanocomposite magnets. To date, the theoretical maximum energy product for isotropic material is between 50 and 120 megagauss oersted (MGOe) for anisotropic nanocomposites. (The energy product measures the performance of the permanent magnet.) However, the highest experimental result to date is approximately 24 MGOe for isotropic, nonuniform nanostructures, which is well below the theoretical result. To reduce rare earth content, researchers have investigated using exchange-coupled hard and soft phase nanocomposite magnets.

Dr. Han provided a final example, one of high-magnetic-field annealing related to exchange-coupled nanocomposites. In this experiment, iron and palladium foils are annealed at a constant temperature for several hours in a high magnetic field (19 T) to change the material's magnetic properties. The high magnetic field introduces texture and affects the phase transition behavior. Different annealing temperatures provide different critical magnetic fields and energy products, and an optimal annealing temperature can be selected to give the largest increase in energy product.

Dr. Han summarized by saying that processing in a high magnetic field can improve material properties by changing a material's texture and/or microstructure. The improvement can occur through changes to the phase transformation temperatures. Alignment can occur in materials that are both ferromagnetic and nonferromagnetic. He pointed out that these improvements benefit structural materials (for instance, by improving strength) and functional materials (improving magnetic properties).

In response to a question about how experimenters determine processing field strength, Dr. Boebinger said that the peak field strength was chosen for the bore size that was needed; the larger the bore, the smaller the magnetic field. He said that field studies were also conducted to make certain that field strengths would be sufficient.

The presenters were asked how much consideration was given to microstructural alignment versus texture and how the two variables could be separated. Dr. Han responded that the MagLab measures texture. Understanding the detailed correlation between microstructural alignment and crystallographic texture remains for future work.

The presenters were also asked if the material property changes in the experiments were permanent. Dr. Han responded that at ambient temperatures, changes are permanent in the selected examples presented. However, the materials would reanneal at different temperatures, which could further change material properties. Another participant stated that high-temperature solution treatments tend to be stable, but it is important to understand what has changed and what has been manipulated in the microstructure.

FIELD-ASSISTED SINTERING TECHNOLOGY

Robert Dowding, Materials Engineer, U.S. Army Research Laboratory

Mr. Dowding began his talk by noting that his presentation was about electricfield-assisted sintering technology. This is not the first time the Army has been interested in this type of technology, he said. In one form or another, spark sintering apparatus has been in existence for quite a while. Approximately 20 years ago, the Army became interested in nanomaterials, and as a consequence became interested in rapid sintering technologies and developed a system called plasma pressure compaction. Plasma pressure compaction is one of many similar technologies, including electric-current-assisted sintering (ECAS), spark plasma sintering (SPS), field-assisted sintering technology (FAST), pulsed electric current sintering (PECS), plasma pressure compaction (PPC), and plasma-assisted sintering. Mr. Dowding said that although SPS is the most common name, it is not accurate because the technique has little to do with plasmas, sparks, or sintering. He suggested that FAST is the most accurate terminology of all the choices. For that reason, the FAST acronym will be used throughout the remainder of the presentation to describe the general category of electric-field-assisted sintering techniques.

Mr. Dowding stated that a rapid FAST system has several characteristics:

- One-step processing,
- Preservation and control of microstructure/nanostructure and metastable structures,
- High consolidated density (100 percent),
- Net and near-net shape processing,
- Potential cost savings,
- Potential energy savings (60-70 percent), and
- Novel joining of materials.

A FAST system uses conductive graphite tooling typically having a cylindrical shape. Metallic or ceramic powder goes in as loose powder or as a preconsolidated form, and energy is applied. The process is characterized by rapid heating and short dwell times. One problem associated with such a system is where to take

pyrometer or other temperature measurements; the temperature inside the powder bed is observed to be higher than anywhere else in the system. The process is not well scaled and as currently practiced is good for fairly simple components such as low-aspect-ratio shapes with rotational symmetry. It works well for sputter targets and thermal management applications. The production of body armor breastplates using a FAST system would push the process too close to its current limits.

FAST is similar to hot pressing in that both processes use indirect heating. FAST uses conduction heating at up to 10⁶ K/min, while hot pressing uses conduction/ convection heating at about 80 K/min. In a FAST system, the components are in physical contact, enabling joule heating if the powder being used is conductive. (If the powder is an insulator, the heating comes from around the powder bed, creating a miniature graphite furnace around the powder bed from the graphite tooling.) FAST techniques offer a number of distinct advantages compared to hot pressing, including shorter sintering times and lower temperatures, increased production rates, and lower energy costs. They also have shorter processing cycles and are easy to use. However, FAST techniques have a number of drawbacks. The physics involved are not well understood, and models describing the processes are lacking. Thermal gradients are a problem, causing gradients and variations in consolidation in certain materials. Typically, the overall specimen size is small: The thickness is most often smaller than the diameter, and the diameter is currently limited to around 8-12 in. Scaling up is also very uncertain.

Mr. Dowding explained that the mechanisms that describe FAST are not well understood but that it does appear clear that "there is no plasma generation, sparking, or arcing present during the SPS process and during neither the initial nor the final stage of sintering" (Hulbert et al., 2008). He described, and discounted, a number of explanations in the literature, including spark impact pressure, plasma cleaning of particle surfaces, joule rapid heating, local melting and evaporation, surface activation on the particles, electron wind force, field-assisted diffusion, and plastic deformation. Despite the poor understanding of the underlying physics, Mr. Dowding pointed out, the process is still a very useful one, and there is a growing interest in FAST technology; the number of publications and the number of pieces of equipment are both increasing.

Mr. Dowding then described the FAST devices made at the Army Research Laboratory. The first-generation devices, called PPC machines, were developed through an award from the Small Business Innovation Research (SBIR) program. They are "open air processing" machines. The second-generation devices were constructed in an atmosphere-controlled chamber. A graphite furnace was added to increase the overall temperature to avoid thermal gradients. These machines are used to process a variety of materials. The first example Mr. Dowding described was the processing of tungsten. Tungsten powder, which is sensitive to the amount of oxygen present, sinters better in the atmosphere-controlled environment. The

goal of the project was to process tungsten so that it would undergo a specific, required deformation transformation that can result in very fine grain sizes. The key measurement is adiabatic shear band susceptibility, which is related to strength and inversely related to the strain rate sensitivity, both of which vary with grain size. FAST-based processing of pure nanocrystalline tungsten resulted in either fine grain sizes or high consolidated densities, but it was not able to achieve both simultaneously.

Mr. Dowding then provided an example of processing ceramic powder. The goal was to create improved ceramic armor materials. In this case, the key performance indicator is the ductility parameter. The ductility parameter is inversely related to flaw size, which is again related to the size of the grain. When grain size is reduced, flaw size is also reduced and ductility increases. Using FAST techniques, processing times can be reduced to 10 percent of those used in commercial processing and temperatures are lowered by about 400°C to produce dense, fine grain sizes. Mr. Dowding also described how his laboratory is attempting to increase the toughness of boron carbide ceramic. In collaboration with Zhifeng Ren and his group at Boston College, Mr. Dowding and his group have modified carbon nanotubes with boron carbide and added them to boron carbide powder prior to FAST processing. To their surprise, the carbon nanotubes survived the sintering process but failed to provide enhanced reinforcement to the final processed ceramic.

Mr. Dowding then pointed out that there are no good models for FAST and FAST-like processing. He showed data for temperature contours for a punch-diecompact assembly of a rectangular compact. For a rectangular compact made of tungsten, the temperature contours showed significant thermal gradients across punch length, die height, and die diameter—gradients of 400-600°C. This is a significant problem that must be resolved before scaling up production rate and volume. Although a specimen can be processed in seconds, the chamber takes hours to cool down. Companies are investigating ways to speed up the throughput.

Mr. Dowding then described other materials under investigation. An aluminum nickel composition can be processed in different ways and yields very different structures. The results differ markedly when the aluminum is coated with nickel compared to when elemental powders are blended. He also presented an example of processing magnesium/nanodiamond. Because FAST processing allows for processing at lower temperatures, the nanodiamond structure is able to survive the processing.

Mr. Dowding was asked about manufacturers of FAST processing machines in this country. He replied that his machines were made under an SBIR contract in a partnership with Materials Modification Inc. of Fairfax, Virginia, and that they are commercial products. State-of-the-art machines are also made in Germany by FCT and in this country by Thermal Technologies of California.

In response to a question, Mr. Dowding said that diameter effects have been

noted during processing; homogeneity is more difficult to attain for larger pieces. He was also asked about microwave sintering, particularly for tungsten. He said that in that instance, owing to surface area/volume ratio considerations, the inverse is true: The bigger the piece processed, the more successful it is.

OPEN DISCUSSION: ELECTROMAGNETIC MANIPULATION OF PROPERTIES

Discussion Leaders: Rosario Gerhardt, Professor, School of Materials Science and Engineering, Georgia Institute of Technology, and George T. (Rusty) Gray III, Laboratory Fellow, Los Alamos National Laboratory

Dr. Gerhardt began by noting that the physics behind all these effects is not well understood. She also said that there had been many examples but not many details in the presentations of this session. She said that clearly the presenters were sold on the ability to change the material microstructure at will. She asked which research area(s) would have the highest priority if only one or two areas of research were possible. Dr. Ludtka said that while industry would not be interested in high-temperature superconductors, it would be most interested in changing the mechanical properties of materials. DOD would want to push the envelope for performance and therefore might be more interested in the high-temperature superconducting magnet technologies. Dr. Han noted that industry would be likely to look for where they could get the most value for the least investment. For instance, if manufacturers could achieve a 20-30 percent improvement in the key performance properties of a less-expensive low-performance material, they would be very pleased. For example, a 1 T magnet is inexpensive and can be large, and one could put an entire truck rail into it. That might be useful to industry.

Dr. Gerhardt also asked if once a magnetic field has been used to induce a particular change, the treated material would be in a metastable state. Would the material revert to its original state at different temperatures or change its properties in some way? Dr. Han responded that it depends on what material property has been changed. If the material's texture is changed and the material is in a solid state, the texture will not be lost. If the solubility is affected at a high temperature, that effect will not be lost. But if the material is processed at a certain temperature and then raised to a higher temperature, the effect that had been added could be lost.

Dr. Gray asked if the surface properties of a material could be impacted without affecting the bulk material. A participant responded that if a continuous magnetic field is used, it will permeate everywhere. If an induction coil is used, it is a function of frequency. A 400 kHz coil will provide shallow penetration, while a 10 kHz coil will provide deeper penetration. As far as the respondent knew, however, no one had shown this.

A participant asked about miniaturizing. The response was that if the superconducting material in a magnet is improved, the diameter of the magnet system can be smaller. The cost will increase, however. With respect to miniaturizing, one must also consider that the bore is an aluminum tube, which is a perfect microwave tube. If a large field is needed, however, either current or area must be increased, as field size equals current multiplied by area, with miniaturizing then becoming difficult. However, if a large force is needed, because force is related to the gradient, miniaturizing is not a problem.

A participant noted that aside from defense applications, there are applications in building and architecture where aligning crystals in a particular way would give a strong elastic modulus longitudinally, potentially enabling novel construction ideas.

Someone asked if there are any synergies between additive manufacturing and electromagnetic field manipulation. The general response was yes, particularly in high stress materials and in large-scale structures like bridges and beams. Electromagnetic manipulation after additive manufacturing may offer a way to provide a more homogeneous material and a lower temperature for annealing.

4 Design of Materials— Session Summary

MATERIALS GENOMICS PAST AND FUTURE FROM CALPHAD TO FLIGHT

Gregory B. Olson, Walter P. Murphy Professor of Materials Science and Engineering, Northwestern University; Chief Science Officer, QuesTek Innovations LLC

Dr. Olson began his presentation by restating the goals of President Obama's Materials Genome Initiative, which was announced in June 2011: to expand the system of fundamental materials databases and cut materials development cycles in half or more. He pointed to the study *Accelerating Technology Transition: Bridging the Valley of Death for Materials and Processes* (National Research Council, 2004), which used the Human Genome project as a model for recommending the construction of a fundamental database for materials, with the White House Office of Science and Technology Policy (OSTP) leading the effort. The purpose of a materials genome project would be to promote science-based engineering in materials instead of empirically based engineering, as is common today. While implementation of this recommendation has begun with the Materials Genome Initiative, Dr. Olson reiterated his support for the NRC's recommendation and said that he believes that focused support is necessary to make significant progress.

Dr. Olson then described what he believes to be the most significant milestone in materials genomics: the flight test of the QuesTek Ferrium S53 aircraft landing gear. Completed in December 2010, this was the first fully computationally designed and qualified material. The flight test provides a benchmark for the maturity level of the CALPHAD (calculation of phase diagrams) technology, which is described below.

Dr. Olson went on to discuss the materials genome timeline and the CALPHAD process, which has been under development for more than 50 years. The scope of CALPHAD has broadened beyond phase diagrams to include molar volumes, atomic mobilities, and elastic constants. Formerly an empirical science, CALPHAD is increasingly based on DFT calculations. The CALPHAD community brings together metals and ceramics. There are other communities in fields such as organics that use the same tools and techniques; the concept is to build a strategy to span all classes of materials. In the 1980s researchers successfully applied a CALPHAD-based process to predictively design a set of high-performance steels, which are now commercially available. Researchers then expanded into other metallic systems, followed by demonstration projects in polymers and ceramics. The successes in computational materials design helped the integrated computational materials engineering (ICME) process initiated by the DARPA-AIM program to gain acceptance, leading to a full optimization at the component level to predict design allowables and to put materials into use more rapidly. Full ICME has been demonstrated in metallics only, but Dr. Olson believes there is little question that the process will move to all materials, given the generic character of the CALPHADbased approach.

Dr. Olson then described how Cyrill Stanley Smith wrote extensively about the concept of multiscale interactive structural hierarchy of materials and how to apply a systems approach to materials. Morris Cohen described this as the reciprocity between the opposite philosophies of science and engineering, in which science, and its deductive cause-and-effect approach, flows in one direction, while engineering, and its inductive goals-means relations, flows in the opposite direction. This is shown schematically in Figure 4.1. The idea of reciprocity forms the backbone of a systems approach to the science-based engineering of materials. Each material design consists of performance metrics that map back to a set of quantitative property objectives that are connected to the structural hierarchy within the material. Process/structure/property relations can be identified and prioritized, and predictive models can be built. In particular, mechanistic models can be deliberately structured to extract maximum value from existing fundamental database systems.

Dr. Olson then explained a resulting hierarchy of design models, shown in Figure 4.2. He pointed out that at the most fundamental level, the maximum impact of the all-electron DFT calculations has been in the prediction of surface thermodynamic quantities, which are the most difficult to measure. The greatest accuracy and control have been in nanoscale precipitation behavior and associated strengthening behavior. Researchers have been able to integrate applied mechanics in simulating fracture and other failure modes. They have been able to include processability in the integration of all the solid state transformation models. Re-



FIGURE 4.1 Cohen's reciprocity, showing the reciprocity between science and engineering, in which science, and its deductive cause-and-effect approach, flows in one direction, while engineering, and its inductive goals-means relations, flows in the opposite direction. SOURCE: Gregory Olson, North-western University, presentation to the Standing Committee on Defense Materials, Manufacturing and Infrastructure on December 5, 2012, slide 7. From G.B. Olson, 1997, Computational design of hierarchically structured materials, *Science* 277(5330): 1237-1242.

searchers have also integrated solidification behavior both in terms of the accurate prediction of microsegregation as a function of process scale as well as with liquid buoyancy models, which can set constraints on macrosegregation phenomena. The model hierarchy integrates materials science, quantum mechanics, and applied mechanics. To get the maximum value out of the supporting database structure, the Thermo-Calc software is the central integrator of those systems. Parametric design (2D mappings) allows one to arrive at unique compositions and process temperatures with specified tolerances.

Dr. Olson then described the first four commercial cybersteels on the market, which include two types of aircraft landing gear steels and two types of case-hardened gear steels for automotive applications. All four of these alloys exploited an optimization of M_2C alloy carbides at a particle size of about 3 nm, providing a high level of strengthening efficiency with a 50 percent higher strength at a given carbon content compared to conventional steels.

Dr. Olson then discussed the Accelerated Insertion of Materials (AIM) program, an initiative sponsored by DARPA and conducted in collaboration with GE Aircraft Engines and Pratt & Whitney. The metals phase of the project involved a component-level process optimization for aeroturbine disc alloys, and research



FIGURE 4.2 Hierarchy of design models from the smallest length scales with quantum design all the way to solidification models needed in order to accurately predict the behavior of objects such as landing gears. SOURCE: Gregory Olson, Northwestern University, presentation to the Standing Committee on Defense Materials, Manufacturing and Infrastructure on December 5, 2012, slide 9. From G.B. Olson, 2000, Designing a new material world, *Science* 288(5468): 993-998.

was able to show there is enough accuracy to predict small spatial variation and micromechanical properties. The difficulty of this project was that the data sets were very small—large enough to determine the first and second moments of yield strength but not the shape of the distribution function. Researchers addressed this by using mechanistic Monte Carlo simulations to predict the shape of the distribution function of yield strength, and they integrated sparse data through linear transformation.

Dr. Olson then described the qualification process for S53 and M54, the two

landing gear steels developed by QuesTek. It took 8 years from material design to qualification for S53, and QuesTek is on track to get M54 qualified within 5 years. This computationally based qualification is much accelerated compared to the standard 10-20 year development cycle.

Closing the loop with the first workshop topic, additive manufacturing, Dr. Olson then described the DARPA Open Manufacturing project conducted collaboratively with Honeywell. In this project the laser-based additive manufacturing of a nickel-based 718+ alloy was being controlled. This will enable calibrated design tools to create new alloys optimized for the capabilities of the additive manufacturing process, particularly looking at alloys that can exploit faster solidification. He said that principles established in welding metal design can be adapted to additive manufacturing.

Addressing the second workshop topic, the electromagnetic manipulation of properties, Dr. Olson discussed magnetic field effects on steel. His research looked at high (12-17 T) magnetic field effects on the thermodynamics and kinetics of the martensitic transformations in steels. Dr. Olson and his team have recently exploited that knowledge to expand the performance envelope of secondary hardening gear steels. They would like to reduce the gear weight by half relative to current materials. While strengthening the steel with nanoscale carbides is possible, adding that much carbon (as well as nickel, which is needed for core toughness) results in a transformation temperature that is unacceptably low for conventional processing. However, the desired properties of the steel can be attained with combinations of cryogenic high-magnetic-field processing and multistep tempering.

Dr. Olson then turned to the third workshop topic, a vision for design and databases. One area of opportunity, he said, is in a large-scale public database system, which could reside at the National Institute of Standards and Technology (NIST). He suggested that this database should consist essentially of protodata that is, data below the assessed genome level: raw information on experimentally measured phase relations, thermochemical measurements, and DFT calculations. That data could be pooled and periodically assessed to generate usable databases with public and private development channels. There are also opportunities at the database level, he said, including the D3D project (which will be described below). There is a public website maintained by the Minerals, Metals, and Materials Society (see http://www.tms.org) that stores 3D microstructural information. The standard database for materials selection is the set of discrete properties of material searchable by the Ashby materials selection system. The opportunity exists to use the same architecture to search all databases at all levels, to select atoms and components the same way that higher-level systems are selected. Another opportunity is to hand off a material accompanied by its associated information system to adapt to future manufacturing/field experience; this opens up the possibility of moving beyond discrete properties into a system based on constituitive modeling with state variables for the microstructure of the material.

D3D was a QuesTek-led Office of Naval Research/DARPA-sponsored university consortium that brought together a suite of tomographic characterization and simulation tools for multiple scales. The properties of interest were strength, toughness, and fatigue resistance (particularly fatigue nucleation). At this point, while most structural component designs are strength-driven, some are fatigue-limited, but it takes too much data to quantify fatigue properties properly. The new frontier for this technology is to accurately predict minimum fatigue strength.

Dr. Olson was questioned about the types of models that should be used: datadriven or physics-based. He responded that the most successful projects use the physics-based model, with a mechanistic modeling-based approach rather than a data-driven one. A data-driven model might be good as an interim measure, he explained, but certain types of problems (such as fatigue) are too difficult to resolve with a data-driven model because they require too much empirical data and tend to provide superficial information. Modeling-based approaches can define new experiments and sometimes new discoveries.

Another questioner wanted to know about the use of the DFT as the basis for CALPHAD. The questioner pointed out that this was rather unsatisfying, as this type of modeling is of limited accuracy. Dr. Olson responded that these methods are still useful provided uncertainty is quantified. In surface thermodynamics, techniques are almost always DFT-based, and the accuracy has been sufficient to achieve substantial gains in grain boundary cohesion for enhanced stress corrosion resistance.

Another participant stated that in the last 15 years, six NRC reports have discussed the need for federal support for fundamental materials databases, but nothing is really taking place. Dr. Olson responded that the database project is happening, but not with enough force behind it; he would like to see more Human Genome-like energy behind it.

Referring to Cohen's reciprocity (Figure 4.1), a participant pointed out that it is easier to go from processing to performance than it is from performance to processing. Dr. Olson said that this is universally true: It is easier to move from the science to the engineering than from the engineering to the science. Materials science and engineering is no different from any other branch of technology; the dominance of science over engineering in the study of materials has been a limitation. He recommended "legalization" of engineering at our universities.

When asked how this dovetails with industry, Dr. Olson said it is essential that a material be designed for scale to make sure there will be no degradation in properties when moving up in size. Speaking specifically about costs and his own experience with QuesTek, he said that in the accelerated qualification of the stainless steel, QuesTek was able to share necessary inventory costs with the supplier because there was shared confidence in model accuracy.

SOME STEELS ON THE VERGE OF INDUSTRIALIZATION

John Speer, Professor, Department of Metallurgical and Materials Engineering, Colorado School of Mines

Dr. Speer began his presentation by describing partnerships at the Colorado School of Mines Advanced Steel Processing and Products Research Center (ASPPRC). The School of Mines partners primarily with industry, along with Los Alamos National Laboratory. The school is interested in conducting research that involves students, producers, and users of steel. In the 1990s sponsors were all based in North America; today, the partnerships are global and serve a diverse group of needs and perspectives. The school also performs some DOE- and NSF-sponsored programs.

Dr. Speer explained that he would not be giving a design talk, but rather would be discussing new steels of interest in the industrial realm that might have crossover application in defense. The steels under consideration include steels for automotive structures, pipeline steels, sheet products, plates, bars, heat treating, construction steels, and fire-resistant steels.

Dr. Speer provided an example in the steel manufacturing industry of a company (ArcelorMittal) that produced 172 billion lb of steel in 2011, at a profit of 1.3 ¢/lb. This figure underscores the scale of production and how cost is critical in the steel industry. It is a different paradigm compared to something like additive manufacturing in that steel manufacturing is a large-scale industry with severe cost constraints. Manufacturing issues often control the implementation of steel product research and development. These issues can include facilities, capital requirements, conversion costs, and end-user fabrication requirements (such as forming, joining, and painting).

Dr. Speer then described the role of automotive "lightweighting" as a research driver in steel. He discussed elongation versus tensile strength (Figure 4.3). The austenitic steels referenced in the upper right corner of the figure are usually not cost-competitive enough to be used on a massive scale, and researchers are seeking materials with better strength properties than the conventional steels included in the lower left of the figure. The gap in the middle is considered to be the materials design space, referred to as third-generation advanced high-strength steels (AHSS), where cost and performance requirements might be achieved. Dr. Speer explained that austenite is a crucial component of the microstructure in third-generation steels, which could be valuable to the defense industry as well as civilian industry,

46



FIGURE 4.3 Elongation versus tensile strength for a variety of steels, showing conventional steels in the lower left, high-cost austenitic steels in the upper right, and the area of opportunity in AHSS between them. SOURCE: John Speer, Colorado School of Mines, presentation to the Standing Committee on Defense Materials, Manufacturing and Infrastructure on December 5, 2012, slide 29, originally from the American Iron and Steel Institute.

where attention is currently focused. These steels can be processed in a variety of ways to create different microstructures and different strength/formability/ toughness properties.

Dr. Speer highlighted several types of advanced high-strength steels under consideration, including quenched and partitioned (Q&P) and medium-manganese (med-Mn) steels. He first described the Q&P process developed at the ASPPRC. First, the steel is heated into the austenitic phase field, and then it is quenched to form martensite. A unique aspect of the processing is that the quenching process is interrupted at a carefully selected, elevated temperature so that the material contains martensite along with untransformed austenite. There is a driving force for carbon atoms to migrate from the martensite back into the austenite; that carbon force stabilizes the austenite to room temperature more than if quenching had taken place at room temperature. Effectively, carbon is used as "cheap" austenite stabilizer. A Chinese company, Baosteel, is the first company to create commercially produced Q&P steels (with or without a corrosion-resistant coating); these steels have been in limited production and used in vehicles since January 2012.

The second concept Dr. Speer described was med-Mn steel. Manganese is an austenite stabilizer. The addition of manganese changes the microstructure of steel, and researchers at ASPPRC have stabilized 20-40 percent austenite through long-

term annealing and the addition of Mn. The microstructure is very interesting, with fine grains (approximately 1 μ m grain size). Research indicates that the annealing does not need to be done for weeks at a time; instead, the processing can be done in minutes to obtain Mn partitioning over short length scales.

Dr. Speer's final example was press-hardenable steels for hot stamping. The hot stamping concept has been around for more than 20 years and is growing in importance in the automotive industry. The concept is as follows: rather than heat treating a formed component to a high-strength martensitic microstructure, a flat piece of sheet material is heated to the austenitic field, then formed and die quenched. In this way, one can make high-strength products of complicated shape. Current research opportunities include increasing the sophistication of the heat treatments and exploring the use of zinc coatings.

In response to questions about cost, Dr. Speer pointed out that because steels are high-volume, production-lean alloy chemistries, small changes in chemical composition can change the cost of production. Thermomechanical processing does not add much to the cost if the capability is already in existence, though it can slow production rates in some applications (for instance, it takes time to cool during rolling, which can influence productivity). He also pointed out that while the automotive industry will always want more performance at a lower cost, the defense industry tends to be performance-driven, with cost constraints that are somewhat less severe.

Dr. Speer was asked about the increasingly complex contours in contemporary automobiles and if that has been made possible by alloy technology. He responded that shape technology has benefitted from improvements in forming and modeling technologies, thus enabling the use of stronger steels. There have been steady improvements in steel performance and corrosion resistance, but those are not the factors that would promote radical changes to body design.

During a discussion of the Q&P process, Dr. Speer clarified that, to date, Q&P has only been applied to sheets, not thick sections. For the Q&P process to be effective with thick section steel, the steel would have to be redesigned to enable a transformation response due to the cooling, and a method for controlling the quenching temperatures in the Q&P process in a thick section would be required.

A participant asked about global activity in steels research and production. Dr. Speer replied that steel production is stable in the United States and Europe. China has increased its steel production from about 100 million tons/year to 700 million tons/year over the past 15 years or so, while the rest of the world has remained stable at something over 600 million tons/year. Research activity is also increasing in the rest of Asia.

A participant pointed out that steel strengths are increasing and asked at what point steel could outperform aluminum. Dr. Speer said there is a continued pressure for all materials to achieve higher strengths. There will always be niche applications for different materials, he said. The competition between different materials has been dynamic for many years. For example, aluminum would be considered more competitive in automotive engine blocks and perhaps less so in body structures, but other participants noted that steel is superior in crashworthiness and recycling.

DATA-DRIVEN MATERIALS CODESIGN

Krishna Rajan, Wilkinson Professor of Interdisciplinary Engineering, Department of Materials Science and Engineering, Iowa State University

Dr. Rajan began his presentation by explaining his take-home messages. First, he said that just as biology has collected information about its many important molecules, formed it into massive databases, and appropriated *-omics* as a tag for some of its component disciplines, materials science should also look to informatics to enable "materials by design." Informatics involves a statistically based learning process—with physics, chemistry, and materials science all coupled together. Second, he said that his goal is to change materials databases from repositories where one can conduct search and retrieval exercises into laboratories where new and unexpected discoveries can be made. In his presentation, Dr. Rajan explained the co-design process, gave examples of co-design problems currently being addressed by DOD, and ended with a suggestion on how to integrate this information.

Dr. Rajan emphasized the importance of considering design manufacturing issues at the beginning of any materials development, as these issues are the main difference between discovering new materials and designing new materials. He said that a challenging goal in materials design is to discover the links that can help explain materials behavior across critical length scales. This was a focus of the AIM program of DOD over a decade ago; Dr. Rajan believes that AIM was one of the first major efforts to get the materials science and engineering design communities to establish a materials-mechanism-based design strategy for engineering systems. AIM highlighted the need to find ways to cooperatively and simultaneously design an engineering system from both the macro- and microscale. Enabling the inclusion of design manufacturing issues from the beginning of materials development is at the heart of this "co-design" process. Co-design is the cooperative design of materials taking into account, in parallel, the life cycle of materials: extraction, synthesis, processing, manufacturing, and recycling.

Dr. Rajan then went on to describe informatics. Informatics is a strategy to integrate information of all types (including experiments, modeling, data, and theory) in an environment where there is no preexisting model. Informatics in the context of materials design is the computational strategy of integrating

information associated with material structure, chemistry, and performance so as to extract patterns of multiscale behavior in materials. The requirements of statistical learning/machine learning guide the experiment. Dr. Rajan referred to this as "omics:" a whole set of length and timescale problems. He described multiscale modeling, which looks at different length scales and timescales, and where the interconnections and linkages between material structure, chemistry, and performance are not known. This becomes a network problem: Connections may be greater at higher length or timescales than at other places in the network, and a design process may be able to "leap" length scales or timescales because of how the information is networked together. Dr. Rajan pointed out that, currently, the primary ways to rapidly accelerate discovery and make unexpected jumps in materials design are (1) unexpected discovery or (2) failures. He pointed out that Nobel prizes that had a materials science component (such as superconducting ceramics, conductive polymers, quasicrystals, and Buckyballs) were outliers, or unexpected discoveries. Engineering failure analysis is another (unfortunate) way to discover material properties that cut across length scales in an accelerated manner. He wondered whether there are other ways to collect information that would lead to faster progress in materials design.

Dr. Rajan then described the genome equations: Each material can be described as a function of different state variables. The critical issue is then determining which variables are important in the engineering environment. (It may not be the materials science variables that guide the materials physics.) The next issue is to classify behavior among the variables. Borrowing a concept known as quantitative structure activity relationship (QSAR) from the biology community, Dr. Rajan suggested applying QSAR to assign a weighting parameter to individual variables, based on observed functionality or toxicity of each variable in question. The idea is not to assume a priori which variables are the most important, but to instead apply a systems biology approach to assess which variables are the most significant.

Dr. Rajan then introduced the "big data" framework. This paradigm is also from the health science and social science communities, where there are large volumes of data. He described four aspects of data, known as the four V's: volume, velocity, variety, and veracity. While one always tries to increase the volume of existing data, situations in which the volume is small, sparse, distributed, or skewed may require the use of predictions. In the case of the velocity variable, because data are received real time, inferential reasoning regarding their evolution and the in situ dynamics may be required. With the variety variable, data are in different forms: for instance, numbers, qualitative (such as good/bad), unstructured, or multimedia. The challenge is finding useful applications for the data. With the veracity variable, the question becomes one of quantifying uncertainty—that is, given the data on hand, and knowing the skew, sparseness, and uncertainties, can the model be justified?

Dr. Rajan then described how to "map" the materials genome: Determine the dominant features ("genes") that govern a material's characteristics and then reduce the dimensional space without losing the physics. In the reduced space, look for patterns, classifications, organizations, and clusters ("sequencing"). This provides a computational framework for the model.

Dr. Rajan then described examples of material co-design using big data. The first example he described was research on a drug delivery/vaccine system using co-design. This 5-year project was a Multidisciplinary University Research Initiative (MURI) with the Office of Naval Research on the vaccine and drug delivery for plague. The development bottleneck was that drug delivery material and vaccine are not typically developed in parallel, which adds delay and inefficiency. The goal of this project was to develop the drug delivery polymer, based on known characteristics of the vaccine, to couple the design of each. The research examined the polymer chemistry via a QSAR analysis. In parallel, vaccinated animals were given full body scans to track information at the cellular level. The data were quantified to a matrix, and image processing techniques were applied to develop descriptor ranking and outlier detection. This information was then put together to design a drug and delivery system that would warn the immune system to respond in a certain way when the drug was administered. The end result was that the materials science community developed connections based on the information gathered that the medical community would not have discovered. This is a good example of the co-design approach; the key was to link all the information together in the absence of valid models.

Dr. Rajan then described a second example of co-design based on the big data approach: high-temperature piezoelectric perovskites. In this case, the goal was to increase the Curie temperature while maintaining a material's ferroelectric properties. To develop this system, the options were (1) combinatorics: make lots of materials and see what happens or (2) computation: generate the lowest minimum energy solution (although this assumes the physics of the models is well understood). Dr. Rajan explained that when using the co-design with the big data method, the figure of merit is inherent to the process. There must be some scalar relationship(s) between the important properties of the material and some variable. In this case, Dr. Rajan explained that researchers developed a tolerance factor and then examined Curie temperature against the tolerance factor. This information was translated into a unified model to predict new chemistries.

Dr. Rajan then presented a plot demonstrating the contrast between materials development before and after informatics. The plot indicated that after informatics-based design, there are more materials with higher Curie temperatures.

Informatics informs experimentalists to tell them what to develop (validation), as well as informs the computational community, to tell them how to refine their models and theories. The point is that accelerated design occurs even with limited information.

Dr. Rajan then briefly mentioned a new program using co-design techniques to develop high-temperature superalloys. The idea is to avoid using rare earth elements and other critical elements. He also touched on a project applying principles of co-design to expand design limits for Ashby maps.

In conclusion, Dr. Rajan briefly described the materials bar code idea, in which a digital bar code is embedded in the material itself to encode information about the material's properties, modeling, evolution of the material properties, qualification, service, and manufacturing. The bar code can bridge the gap between basic materials science and manufacturing and may provide a framework for integrating materials discovery and manufacturing.

OPEN DISCUSSION: DESIGN OF MATERIALS

Discussion Leader: Haydn Wadley, University Professor and Edgar Starke Professor of Materials Science and Engineering, University of Virginia

Dr. Wadley opened the discussion by asking workshop participants what is important in the materials science field that is currently impossible to do. One participant reframed this question slightly by asking for challenge problems that would further the analytical capabilities in the design of materials. The responses focused on two areas. The first was how to match experimentation to models. One participant pointed out that we have heard about successes only, not failures, but that there are instances where fabrication does not match up with predictive approaches. It was suggested that perhaps there should be some statistics on failures so that any database built would be backed with the most meaningful data possible. Another participant noted that when the Human Genome Initiative started, it generated new experimental protocols to create new data; with the Materials Genome Project, the same type of new experimental protocols may be generated, causing a rapid expansion of fundamental databases. This could be the greatest impact of the project. The second area was related to how one could integrate models so they interact over different length scales and how to do that in a single system. However, other participants pointed out that we do currently have the knowledge needed to decouple the system and process in stages to make the system integration problem tractable.

Dr. Wadley then pointed out that a DFT calculation provides resolution on the order of 0.1 eV. Ambient temperature is on the order of 0.05 eV; he asked if that

resolution was good enough. Is the materials science community happy with that as state of the art? Others defended the use of DFT calculations, saying that although improvements could always be made to the fidelity of the DFT calculations, in practice most are measured, not calculated. In general, the use of DFT does not appear to be a showstopper in the design process. There is significant knowledge of the relative uncertainties involved.

Dr. Wadley then posed a question to the group, putting forth a scenario in which Team A is asked to design a material without any experimentation (only modeling), and Team B is asked to design a material without any modeling (only experimentation). He then asked which of these teams would win 30 years ago, today, and 30 years from now. This question generated a lot of discussion among the participants. One respondent pointed out that for a material to be accepted for use, experiments are necessary. Where experiments are weak is in the quantification of uncertainty from one step to the next; that is where computational tools are necessary. Dr. Olson's response was that 30 years ago, materials development was purely empirical. Today it is a mixture of experiments necessary to confirm them. It will be a theory-driven approach, which will change the nature of the experiments. Another participant pointed out that for a material to be accepted and qualified for use, experiments will always be necessary. However, experiments do not quantify uncertainty well; for that, computational tools are necessary.

Another participant noted that finite element modeling tools in the mechanical engineering community would be a good benchmark for the materials science community. Current success should not be considered sufficient, and the inclusion of additional functionality, such as the addition of informatics, should be a critical element.

A questioner said that presenters at the workshop described the possibility of using magnetic fields as a state variable, which would require vector thermodynamics, and asked if there have been developments in this area. Dr. Olson replied that a parametric design approach uses vector and matrix representations, extracting out scalar parameters to use as design parameters. The individual pointed out that that approach does not provide any information about grain boundary composition. Dr. Olson responded that other principles would apply if one was trying to design grain boundaries. When designing grain boundaries, one tends to design a "typical" boundary rather than the full distribution function.

Another question focused on process control. Dr. Wadley explained that before the (DARPA) AIM program, a program existed at DARPA called Virtual Integrated Processing (VIP), which developed models and controls concepts for materials processing, and that before that (20 years ago), another Intelligent Processing of Materials program developed sensors. The combination of these sensors and predictive models now allows some control of material state trajectory during processing (but probably not of the defects that motivate the need for much experimentation and materials certification). Dr. Olson added that alloys have been developed for the current processing technology, so the opportunity exists to develop more robust materials.

Dr. Wadley left the group with a final thought: With so many opportunities in the design of materials, how do we set priorities for what to pursue?

5 Workshop Wrap-up

Dr. Schafrik began the wrap-up session by noting that the morning session on the design of materials could have lasted all day. He mentioned that in his line of work he uses composites, which were not mentioned in the day's discussions. He noted the importance of starting materials design with models to guide the process. In the future, it may be helpful to have an entire session or workshop devoted to expanding the discussion of the design of materials even further.

Dr. Schafrik then asked for feedback from members of the Reliance team. Respondents said that the DMMI approach was an experiment, a means of establishing an interaction with the NRC to give an opportunity to step back to discuss broad problems, emerging technologies, gap analysis, etc. Overall, this series of workshops has been very successful. This particular workshop on emerging manufacturing and processing approaches has been equally successful. One person stated that it was the most compact, succinctly focused discussion of additive manufacturing, looking at the issue holistically and amplifying some of the issues that have been identified before. The discussion on magnetic properties was thought provoking. Field-assisted manipulation was examined in other places as well. Someone pointed out that Dr. Wadley had closed the session with a wonderful thought question when he asked how best to make investment decisions. This is particularly pertinent for those who have to make the investment decisions and other big decisions.

Another participant noted the importance of the discussion on electromagnetic interaction with matter. There are potential applications for the Department of the Army in this area, and it was valuable to learn of the numerous properties and how much the properties can be varied. The materials-by-design approach is accepted by the U.S. Army, and the Army wants to understand how best to adopt it, so the workshop was helpful for considering those questions. The discussion of additive manufacturing was also considered important because it could become important in moving forward with projects in spare parts.

Another participant pointed out that more questions than answers had come up at the workshop, which is the hallmark of a good workshop. Someone pointed out that the Air Force Research Laboratory does not have a large effort in magneticor electric-field-assisted processing, so the descriptions of that work were new to some of the participants. It was also noted that the challenges of certification will be enormous in additive manufacturing because a small sample size will not allow for statistical analysis. It will be important to connect with experts in certification. The discussion on informatics was also singled out as particularly important. In conclusion, it was noted that the aim of the workshop was to serve the needs of the Reliance group, and the workshop fulfilled that purpose. With that, Dr. Schafrik adjourned the workshop.

References

- Bourell, D., M.C. Leu, and D.W. Rosen. 2009. *Roadmap for Additive Manufacturing: Identifying the Future of Freeform Processing*, Workshop Report, Austin, Tex.
- Brady, M.P., Y. Yamamoto, M.L. Santella, P.J. Maziasz, B.A. Pint, C.T. Liu, Z.P. Lu, and H. Bei. 2008. The development of alumina-forming austenitic stainless steels for high-temperature structural use, JOM 60(7):12-18.
- Granroth, G., C. Broholm, F. Klose, G. Srajer, Z. Islan, Y. Lee, and J. Lang. 2005. Report from Probing Matter at High Magnetic Fields with X-Rays and Neutrons. Available at http://neutrons.ornl.gov/ workshops/Final_report_2005_Probing%20Matter.pdf. Accessed January 11, 2013.
- Hulbert, D.M., A. Anders, D. Dudina, D. Jiang, C. Unuvar, U. Anselmi-Tamburini, E. Lavarnia, and A. Mukherjee. 2008. The absence of plasma in "spark plasma sintering." *Journal of Applied Physics* 104: 033305.
- National Research Council. 2004. Accelerating Technology Transition: Bridging the Valley of Death for Materials and Processes. The National Academies Press, Washington, D.C.
- Wohlers Associates. 2012. Additive Manufacturing and 3D Printing State of the Industry: Annual Worldwide Progress Report. Fort Collins, Colo.

Appendixes

Copyright National Academy of Sciences. All rights reserved.

Novel Processes for Advanced Manufacturing: Summary of a Workshop

A

Workshop Statement of Task

An ad hoc committee will convene a 2-day public workshop to discuss future advances in materials processing and properties, including, but not limited to topics such as (1) additive manufacturing; (2) electromagnetic field manipulation of properties; (3) materials by design; and (4) the current state of materials processing capabilities in the U.S. The workshop will also consider additional topics close to and in line with the four mentioned above. The workshop will use a mix of individual presentations, panels, breakout discussions, and question-and-answer sessions to develop an understanding of the relevant issues. Key stakeholders would be identified and invited to participate. Approximately 8-10 speakers will make presentations. An individually-authored Workshop Summary document will be prepared by a designated rapporteur. This workshop is one of two workshops held every year on defense related issues in materials, manufacturing and infrastructure.
B

Workshop Participants

DMMI STANDING COMMITTEE MEMBERS

Robert H. Latiff, *Chair* U.S. Air Force Major General, retired President, R. Latiff Associates

Robert E. Schafrik, *Vice Chair* General Manager, Materials and Process Engineering Department GE Aviation

Valerie Browning ValTech Solutions, LLC

Jesus M. de la Garza Virginia Tech

George T. Gray III Los Alamos National Laboratory Michael F. McGrath Analytic Services, Inc.

E. Sarah Slaughter Built Environment Coalition

Denise F. Swink Private Consultant

A. Galip Ulsoy Professor of Manufacturing Director, Ground Robotics Research Consortium University of Michigan

Haydn N.G. Wadley University of Virginia

Steven G. Wax Private Consultant APPENDIX B

WORKSHOP SPEAKERS

Gregory Boebinger Director National High Magnetic Field Laboratory

David Bourell Temple Foundation Professor Mechanical Engineering and Materials Science and Engineering Departments University of Texas at Austin

Robert Dowding Materials Engineer U.S. Army Research Laboratory

Ke Han Scholar/Scientist National High Magnetic Field Laboratory

Gerard Ludtka Distinguished Research Staff Materials Processing and Manufacturing Group Materials Science and Technology Division Oak Ridge National Laboratory

Rich Martukanitz Assistant Director Applied Research Laboratory Penn State University

Gregory Olson Walter P. Murphy Professor of Materials Science and Engineering Northwestern University Krishna Rajan Wilkinson Professor of Interdisciplinary Engineering Department of Materials Science and Engineering Iowa State University

Prabhjot Singh Manager Additive Manufacturing Laboratory GE Global Research

John Speer Professor Department of Metallurgical and Materials Engineering Colorado School of Mines

WORKSHOP PLANNING GROUP (OTHER THAN DMMI STANDING COMMITTEE OR SPEAKERS)

Rosario A. Gerhardt Georgia Institute of Technology

OTHER PARTICIPANTS

Amit Bagchi Naval Research Laboratory

Beverly Brown U.S. Air Force

Ernest Chin Army Research Laboratory

Julie Christodoulou Navy Principal, Reliance 21 Materials and Processes Community of Interest Office of Naval Research Novel Processes for Advanced Manufacturing M_{A}

William Coblenz Defense Advanced Research Projects Agency

Khershed Cooper Naval Research Laboratory

Paul Deal Office of Naval Intelligence

Jeff DePriest Defense Threat Reduction Agency

Michael Dulevy U.S. Air Force Acquisitions

Rich Everett Naval Research Laboratory

Barry Farmer Air Force Research Laboratory

John Gloystein Air Force Research Laboratory

Natalie Gluck Institute for Defense Analyses (Support Contractor to Reliance 21 Materials and Processes Community of Interest)

Joycelyn Harrison Air Force Office of Scientific Research

Ashraf Imam Naval Research Laboratory Warren Johnson Universal Technology Corporation (Support Contractor to Reliance 21 Materials and Processes Community of Interest)

Murray Kent Office of Naval Intelligence

Wayne King Lawrence Livermore National Laboratory

Mick Maher Defense Advanced Research Projects Agency

Suveen Mathaudhu Army Research Office

Heidi Maupin Army Research Laboratory

Heather Meeks Defense Threat Reduction Agency

William Mullins Office of Naval Research

Bob Rapson Air Force Research Laboratory

Michael Rigdon IDA Support, Reliance 21 Materials and Processes Community of Interest Institute for Defense Analyses

62

APPENDIX B

Lewis Sloter OSD Principal, Reliance 21 Materials and Processes Community of Interest Office of the Assistant Secretary of Defense (Research and Engineering)/Weapons Systems

David Stepp Army Research Office

Katherine A. Stevens Director, Materials and Manufacturing Directorate Air Force Research Laboratory Wright-Patterson Air Force Base

Matt Trexler Materials and Manufacturing Technologies Branch Materials Division U.S. Army Research Laboratory

Jennifer Wolk Office of Naval Research Jeff Zabinski Army Principal and Chair, Reliance 21 Materials and Processes Community of Interest U.S. Army Research Laboratory

WORKSHOP STAFF

Dennis Chamot Acting Director National Materials and Manufacturing Board National Research Council

Erik Svedberg Senior Program Officer National Materials and Manufacturing Board National Research Council

Ann Larrow Program Associate National Materials and Manufacturing Board National Research Council

Maureen Mellody Rapporteur National Research Council

C

Workshop Agenda

WEDNESDAY, DECEMBER 5, 2012

8:30 a.m. Welcome, What Is DMMI?, Meeting Objectives Robert Schafrik, Chair, Workshop

Additive Manufacturing Session

9:00	Freeform Fabrication Speaker: David Bourell, Temple Foundation Professor, Mechanical Engineering and Materials Science and Engineering Departments, University of Texas at Austin
9:20	Q&A
9:40	Additive Manufacturing at GE Speaker: Prabhjot Singh, Manager, Additive Manufacturing Laboratory, GE Global Research
10:00	Q&A
10:20	Break

APPENDIX C

10:40	The Center for Innovative Materials Processing through Direct Digital Deposition (CIMP-3D) Speaker: Richard Martukanitz, Assistant Director, Applied Research Laboratory, Pennsylvania State University
11:00	Q&A
11:20	Open Discussion Related to Additive Manufacturing Discussion Leaders: Denise Swink, Private Consultant, and Robert Latiff, Chair, DMMI Standing Committee
Noon	Lunch
El	ectromagnetic Field Manipulation of Properties Session
1:00 p.m.	 High-Magnetic-Field Processing and Synthesis to Develop the Next Generation of Structural and Functional Materials Speaker: Gerard M. Ludtka, Distinguished Research Staff, Materials Processing and Manufacturing Group, Materials Science and Technology Division, Oak Ridge National Laboratory
1:20	Q&A
1:40	Materials Processing at the National High Magnetic Field Laboratory Speakers: Gregory Boebinger, Director, National High Magnetic Field Laboratory, and Ke Han, Scholar/Scientist, National High Magnetic Field Laboratory
2:00	Q&A
2:20	Field-Assisted Sintering Speaker: Robert Dowding, Materials Engineer, U.S. Army Research Laboratory
2:40	Q&A
3:00	Break

~	
ь	ь
υ	v

3:20	Open Discussion Related to Electromagnetic Field Manipulation of Properties		
	Discussion Leaders: Rosario Gerhardt, Professor, School of Materials Science and Engineering, Georgia Institute of Technology, and George T. (Rusty) Gray III, Laboratory Fellow, Los Alamos National Laboratory		
4:00	Adjourn for the day		
	THURSDAY, DECEMBER 6, 2012		
8:30 a.m.	Welcome, What We Heard Yesterday Robert Schafrik, Chair, Workshop		
Design of Materials			
9:00	Materials by Design Speaker: Gregory B. Olson, Walter P. Murphy Professor of Materials Science and Engineering, Northwestern University; Chief Science Officer, QuesTek Innovations, LLC		
9:20	Q&A		
9:40	Steels on the Verge of Industrialization Speaker: John Speer, Professor, Department of Metallurgical and Materials Engineering, Colorado School of Mines		
10:00	Q&A		
10:20	Break		
10:40	Design of Materials Speaker: Krishna Rajan, Wilkinson Professor of Interdisciplinary Engineering, Department of Materials Science and Engineering, Iowa State University		
11:00	Q&A		

APPENDIX C

11:20	Open Discussion Related to Design of Materials Discussion Leader: Haydn Wadley, University Professor and Edgar Starke Professor of Materials Science and Engineering, University of Virginia
Noon	Lunch
1:00 p.m.	Wrap-up Robert Schafrik, Chair, Workshop
2:00	Adjourn Workshop

D Acronyms

2D	two-dimensional
3D	three-dimensional
AHSS	advanced high-strength steel
AIM	Accelerated Insertion of Materials
ARL	Army Research Laboratory
ASPPRC	Advanced Steel Processing and Products Research Center
CALPHAD	calculation of phase diagrams
CIMP-3D	Center for Innovative Materials Processing through Direct Digital Deposition
DARPA	Defense Advanced Research Projects Agency
DFT	density functional theory
DMLM	direct metal laser melting
DMMI	Standing Committee on Defense Materials, Manufacturing and Infrastructure
DOD	Department of Defense
EBM	electron beam melting
ECAS	electric-current-assisted sintering
EMAT	electromagnetic acoustic transducer

APPENDIX D

FAST	field-assisted sintering technology
H&TMP	high and thermomagnetic processing
ICME	integrated computational materials engineering
ISO	International Organization for Standardization
MagLab	National High Magnetic Field Laboratory
MURI	Multidisciplinary University Research Initiative
NAMII	National Additive Manufacturing Innovation Institute
NIST	National Institute of Standards and Technology
NMMB	National Materials and Manufacturing Board
NRC	National Research Council
NSF	National Science Foundation
ORNL	Oak Ridge National Laboratory
OSTP	Office of Science and Technology Policy (White House)
PECS	pulsed electric current sintering
PPC	plasma pressure compaction
Q&P	quenched and partitioned
QSAR	quantitative structure activity relationship
S&T	science and technology
SBIR	Small Business Innovation Research (program)
SPS	spark plasma sintering
VIP	Virtual Integrated Processing (DARPA program)

Novel Processes for Advanced Manufacturing: Summary of a Workshop