Basic Research Needs for Transformative Manufacturing
March 9-11, 2020

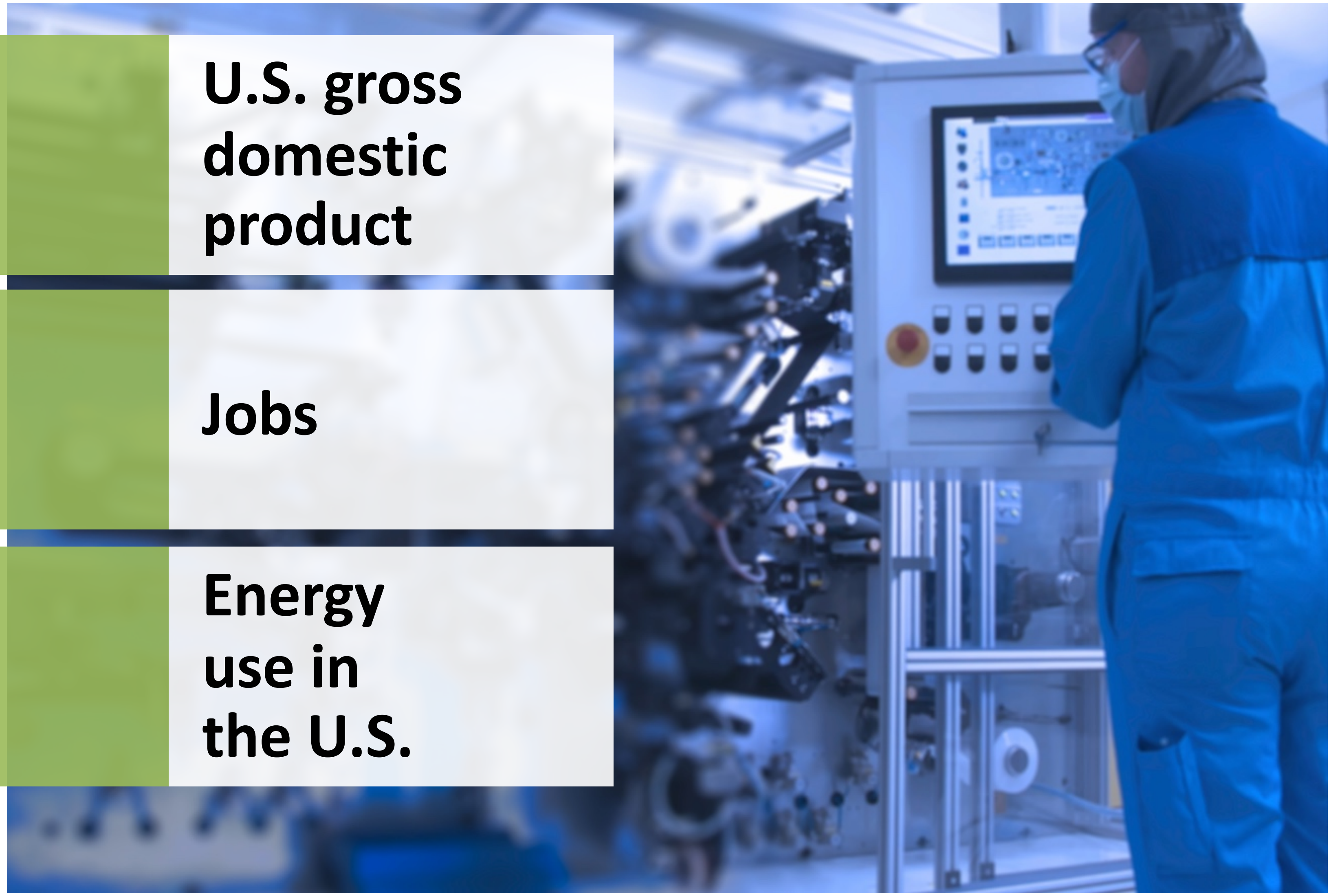
Chair: Cynthia Jenks, Argonne National Laboratory
Co-Chair: Ho Nyung Lee, Oak Ridge National Laboratory
Co-Chair: Jennifer Lewis, Harvard University



Briefing to the Basic Energy Sciences Advisory Committee

Cynthia Jenks
July 30, 2020

Why Manufacturing?



12%	**U.S. gross domestic product**
13M	**Jobs**
25%	**Energy use in the U.S.**

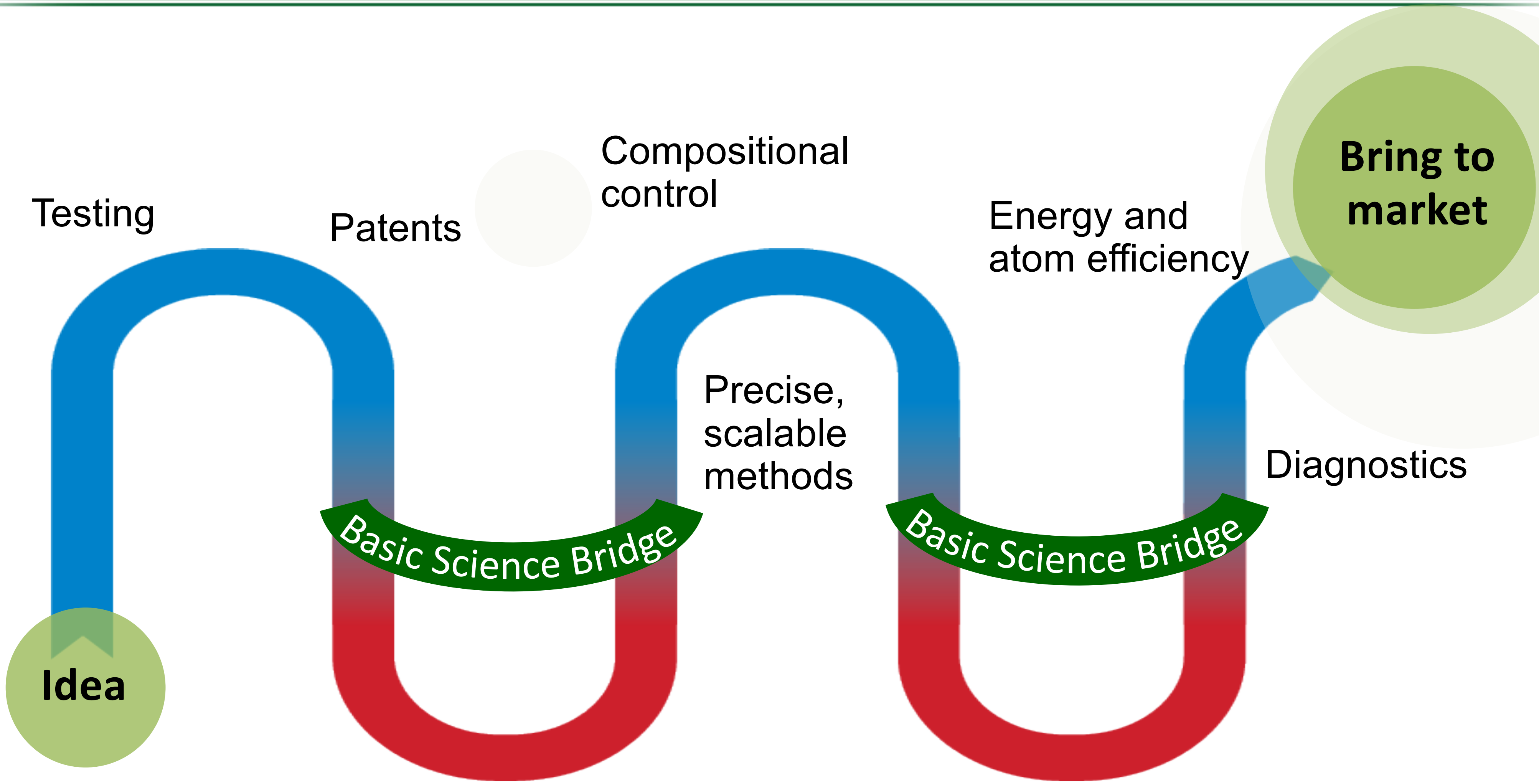
BRN Workshop Charge

Identify the basic science research priorities that would accelerate innovation & transform future manufacturing

Recommendations from prior reports relevant to this workshop include:

- Develop and transition new manufacturing technologies
- Allow for flexibility in operation, e.g., distributed manufacturing, to improve energy efficiency
- Address data issues in manufacturing
- Develop physics-based models across scales
- Consider manufacturing in a global environment
- Address root S&T causes that prevent basic science innovations from moving to market

Opportunities for Basic Science to Overcome Key Challenges



VALLEY OF DEATH #1
issues include scalability and mass production

VALLEY OF DEATH #2
issues include supply chains and energy consumption

Workshop Panels

1. Precision Synthesis Science

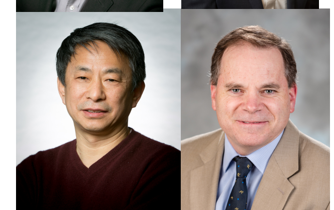
   Leads: Paul Nealey (UChicago/ANL) and Cherie Kagan (UPenn)

2. Processing and Scale-up Science

   Leads: Paul Braun (UIUC) and John Holladay (PNNL)

3. System Integration Science

   Leads: Yan Gao (GE) and David Sholl (GeorgiaTech)



4. Sustainable Manufacturing

   Leads: Brett Helms (LBNL) and John Sutherland (Purdue)

5. Digital Manufacturing

   Leads: Julia Greer (CalTech) and Chris Spadaccini (LLNL)

   Onsite: Ho Nyung Lee (ORNL)

6. Crosscutting Topics

   Leads: Elizabeth Holm (CMU), Anthony Rollett (CMU), and Cathy Tway (Johnson Matthey)

Orange = Virtual; Green = Onsite

Plenary Discussion Panel

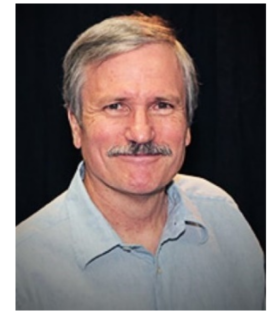
Valri Lightner
Acting Director
Advanced Manufacturing Office

Panel Moderator

Leo Christodoulou
Chief Technologist
Boeing

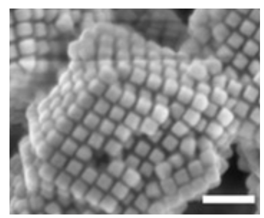
Oleg Gang
Professor
Columbia U.

William Grieco
CEO
RAPID Institute

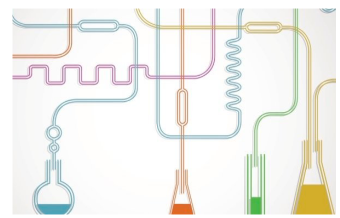


John Randall
President
Zyvek Labs

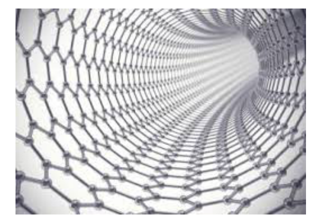
Digital & Sustainable



Precision Synthesis



Process Intensification



Digital Fabrication

Plenary Talks

Transformative Manufacturing and the DOE-BES User Facilities: An Opportunity for Progress

Simon Bare

SLAC National Accelerator Laboratory

Manufacturing with Micron-scale Devices: Scale-up in the Real World

David A. Weitz

Harvard University

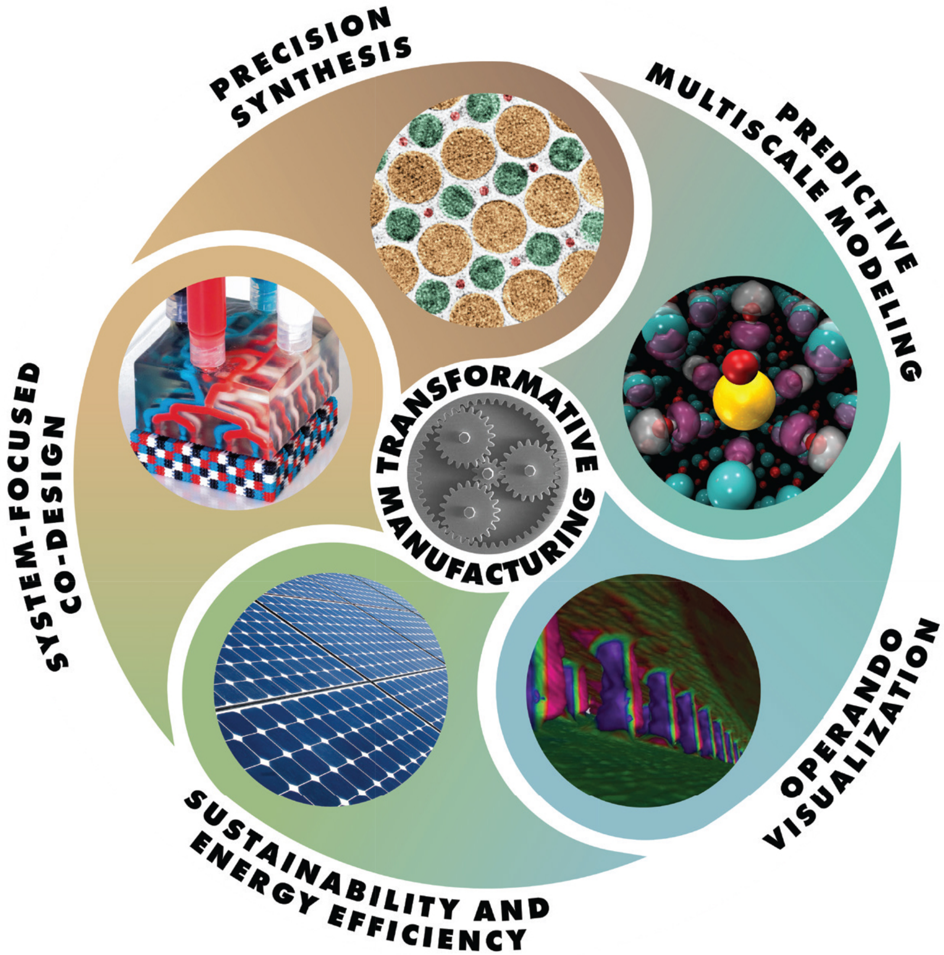
Every Atom in the Right Place: Towards Mastery of Processing Structure in Metals

Chris Schuh

MIT

Priority Research Directions

Priority Research Directions are the panelists' views of the high-priority research directions that have high potential for ultimately transforming manufacturing as we know it today through hypothesis-driven, fundamental research.



Priority Research Direction #1

Achieve precise, scalable synthesis and processing of atomic-scale building blocks for components and systems

Key Questions:

- What are the mechanisms needed for manufacturing multiscale, atomically and molecularly precise materials?
- How can basic research uncover structure-function relationships across multiple scales in components and systems?
- How can chemical processes readily be scaled from laboratory results?

Draft Thrust Areas:

- Thrust 1. Design of scalable atom-, electron-, and energy-efficient and precise synthetic routes
- Thrust 2. Detailed knowledge of structure-function relationships across multiple scales, in complex organizations and at interfaces
- Thrust 3. Achieving spatial and compositional control down to atomic scales in 0D, 1D, 2D, and 3D at manufacturing relevant scales

Priority Research Direction #2

Integrate multiscale models and tools to enable adaptive control of manufacturing processes

Key Questions:

- What are the frameworks required to model, monitor, and ultimately control manufacturing processes that tightly couple physics and chemistry across scales?
- How can complex multiscale models be translated to fast surrogate models for process control?

Draft Thrust Areas:

- Thrust 1. Validated multiscale, multi-physics models
- Thrust 2. Develop high speed, *in situ* diagnostics and characterization tools
- Thrust 3. Advances in data processing and fusion of heterogeneous data
- Thrust 4. Design of fast, predictive models
- Thrust 5. Develop new adaptive control and decision-making methods

Priority Research Direction #3

Unravel the fundamentals of manufacturing processes through innovations in operando characterization

Key Questions:

- How can manufacturing processes and products be “visualized” at the atomic level, in real time, and under operating conditions to reveal the intricate details of underlying physical or chemical events?
- How can these insights be used in control schemes that inform decision making?

Draft Thrust Areas:

- Thrust 1. Development of *operando* characterization for manufacturing processes and understanding of devices during operation
- Thrust 2. Design of *in situ* characterization methods for real-world conditions
- Thrust 3. Advances in data analytics, artificial intelligence and machine learning for manufacturing processes and device development

Priority Research Direction #4

Direct atom and energy flow to realize sustainable manufacturing

Key Questions:

- What are the methodologies to achieve atom and energy efficiency for sustainable manufacturing?
- How can science enable adaptive and resilient manufacturing across scales to exploit renewable or recycled feedstocks?

Draft Thrust Areas:

- Thrust 1. Harnessing diverse forms of energy for atom and energy efficient manufacturing
- Thrust 2. Understanding how to minimize entropic losses in circular manufacturing systems
- Thrust 3. Development of adaptive methods to enable manufacturing with recycled and renewable feedstocks

Priority Research Direction #5

Co-design materials, processes, and products to revolutionize manufacturing

Key Questions:

- How can bottom-up scientific discovery be combined with top-down system-focused design to identify new and efficient manufacturing modalities?
- What new approaches will allow the control of matter in the presence of impurities and/or nonequilibrium states?
- How can science enable multiple performance objectives to be achieved simultaneously for complex, multicomponent processes?

Draft Thrust Areas:

- Thrust 1. Discovery of structure-performance-process relationships across length and time scales to expand options for co-design
- Thrust 2. Development of multiscale co-design approaches
- Thrust 3. Elucidation of formation pathways of matter in equilibrium and nonequilibrium states
- Thrust 4. Understanding of uncertainty associated with interacting components in multi-material, multi-functional assemblies and processes

Current Status

- Brochure that provides a summary of the workshop is available on the BES website
- Workshop report is in preparation
  - Executive Summary and Introduction
  - Priority Research Directions
    - Scientific Challenges
    - Research Thrusts
    - Technology Impact
  - Panel Reports
- Factual document in final draft

https://science.osti.gov/bes/Community-Resources/Reports

A special thank you!

- Linda Horton
- Bruce Garrett
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- BES Program Managers (especially Bonnie Gersten, Mike Markowitz, and Viviane Schwartz)
- Panel Leads and co-Chairs
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- ORAU (Tammy Click and Tia Moua)
- Advanced Manufacturing Office (especially Valri Lightner and Joe Cresko)
- Panos Datskos
- Brenda Wyatt

Questions