LINKING TRANSFORMATIONAL MATERIALS and PROCESSING for an ENERGY EFFICIENT and LOW-CARBON ECONOMY:

Creating the Vision and Accelerating Realization

Innovation Impact Report

TMS ENERGY

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ABOUT THIS REPORT

Linking Transformational Materials and Processing for an Energy-Efficient and Low-Carbon Economy—Innovation Impact Report draws on the contributions of 50 technical experts from industry, academia, and government. These experts worked in five teams led by Brajendra Mishra (Functional Surface Technologies), Diana Lados (Materials Integration in Clean Energy Systems), John Lewandowski (Higher-Performance Materials), Ray Peterson (New Paradigm Materials Manufacturing Processes), and George Spanos (Materials and Process Development Acceleration Tools). The dedication and active involvement of all of the experts has been an integral part of this effort; the information enclosed in this *Innovation Impact Report* is the compilation of their contributions. References that serve as the basis of their interpretations have been provided wherever they are available.

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Executive Summary

Materials are fundamental to the generation, storage, delivery, and use of energy. As concerns regarding slow economic growth and global climate change require today's energy systems to become more efficient and productive, materials frequently determine the limits of system performance. Likewise, materials breakthroughs are often the key advances that improve the efficiency or reduce the cost of clean energy systems.

Materials advances have the potential to be the foundation for the clean energy age, making materials science and engineering (MSE) a critical national priority. While the United States is full of highly innovative, dynamic companies that are world leaders in the energy sector, they are often slow to incorporate new materials into energy systems at scale due to the massive investments and risks often associated with new technology. As a result, new materials discoveries typically require 10–20 years to become fully developed and integrated into commercial products.[1] Identifying and investing in MSE opportunities with the greatest potential for impact is extremely important to providing the clean, abundant, and secure energy that the United States and the world will increasingly require.

This *Innovation Impact Report*, the third phase of the *Linking Transformational Materials and Processing for an Energy Efficient and Low-Carbon Economy: Creating the Vision and Accelerating Realization* study, focuses on identifying the most significant opportunities for materials innovation that can deliver substantial energy savings, environmental gains, and economic advantage to the United States in the next 2–10 years. Focused research and development efforts in the MSE topics outlined in this report can deliver large energy, environmental, and economic impacts.

PROJECT BACKGROUND: CREATING THE VISION AND ACCELERATING REALIZATION

Linking Transformational Materials and Processing for an Energy Efficient and Low-Carbon Economy, a three-part study carried out by The Minerals, Metals, & Materials Society (TMS), aims to articulate a vision for the role that MSE can play in addressing national energy, carbon reduction, and economic development needs.

In the first phase of this work, subtitled *Vision Report of the Energy Materials Blue Ribbon Panel*,[2] the Energy Materials Blue Ribbon Panel identified the high-level areas of the U.S. energy sector where MSE could potentially make the most significant contributions. In their Vision Report, the Panel determined which parts of the energy sector could be most affected by MSE breakthroughs, identifying near-term and long-term priorities for MSE innovation. The Blue Ribbon Panel also identified foundational areas of MSE research (e.g., higher-performance materials for extreme environments) and crosscutting topics (e.g., computational modeling) that could be key enablers for many energy efficiency and carbon reduction solutions.

Building from this initial Vision, a second phase of the study, subtitled *Opportunity Analysis for Materials Science and Engineering*,[3] identified product and process innovations that, if successfully developed and deployed, would create significant economic impact, energy savings, and carbon emission reductions in the priority areas identified by the Energy Materials Blue Ribbon Panel in the first phase of work. The innovations identified in this phase are organized into two classes: performance breakthroughs (e.g., breakthrough thermoelectric materials) and radical cost reduction opportunities (e.g., new paradigm manufacturing processes of metallic and non-metallic materials and their composites).

In this third phase of the study, innovation impact teams (IITs) consisting of experts from industry, academia, and government (see the Appendix for contributors) identified a subset of specific materials and processing breakthrough opportunities and quantified the magnitude of the potential impacts of each breakthrough opportunity in key energy sectors. In this process, the IITs analyzed historical rates of progress and projected future advances in material properties and systems performance. The IITs also defined the research and development (R&D) priorities necessary to move these innovations toward commercial-scale implementation.

PHASE III: IDENTIFYING OPPORTUNITIES AND ASSESSING POTENTIAL IMPACT

The Phase III work was organized into five innovation impact areas that have significant potential to benefit U.S. energy sectors. These areas were originally identified by the Energy Materials Blue Ribbon Panel in Phase I and reaffirmed in Phase II of this work. The five innovation impact areas include the following:

- **Functional Surface Technologies**—Tomorrow's energy systems will require material surfaces that can effectively interact with service environments and withstand demanding operating conditions. Materials that can serve specific functions, such as speeding reaction times, capturing photons, and separating gases, can increase system efficiency.

- **Materials Integration in Clean Energy Systems**—Current and emerging energy systems are composed of different classes of materials that must work together to achieve desired system structure and functionality. Materials science and engineering advances have the potential to enable the integration of new materials and the effective interfacing of materials combinations as systems become more complex and service environments become more demanding.
- **Higher-Performance Materials**—For many energy systems, the path to realizing greater energy efficiency brings extreme conditions that today's materials cannot withstand, such as higher temperatures, more intense radiation, greater wear, or more corrosive environments. Higher-performance materials that can maintain their chemical and physical properties while increasing component and system life under extreme conditions can effectively enhance the efficiency of energy systems.
- **New Paradigm Materials Manufacturing Processes**—Materials manufacturing is fundamentally energy-intensive and often wasteful of resources. Process innovations and novel synthesis methods that minimize energy and material losses can improve manufacturing process efficiency and cost-effectiveness, ultimately enabling greater competitiveness in the U.S. manufacturing sector.
- **Materials and Process Development Acceleration Tools**—Materials and process development tools, including computational modeling and data visualization, are critical to understanding the nature of materials, preventing detrimental defects and faults, and simulating system performance. Ultimately, developing and using these tools will help reduce the cost and time necessary to facilitate materials discovery and development.

Using the methodology outlined in section II of this report, the IITs identified R&D pathways within the innovation impact areas and 54 specific breakthrough opportunities (shown in Figure 1) within the R&D pathways. These MSE breakthrough opportunities have significant potential to help address the nation's energy, environmental, and economic needs. Figure 1 shows a map of the breakthrough opportunities within each of the R&D pathways and broader innovation impact areas.

While each material or processing breakthrough opportunity has the potential to individually benefit the United States, the true impact will occur when these innovations come together and are applied to energy sectors at scale. The Phase III IITs agree that advancing the following energy sectors through materials and processing innovation has the greatest potential to help achieve U.S. clean energy and efficiency needs:[4]

- Energy Generation, including solar, wind, biomass, nuclear, and fossil (oil and gas as well as coal) energy
- Energy Storage, including batteries and fuel cells
- Energy Use, in both industrial and transportation sectors

Figure 1. Map of Breakthrough Opportunities for Delivering Significant Energy, Environmental, and Economic Impacts

INNOVATION IMPACT AREA	**R&D Pathway** • Breakthrough Opportunity			
FUNCTIONAL SURFACE TECHNOLOGIES	**Catalysts**	**Solar Materials**	**Gas-Separating Membranes**	**Coatings**
	• Catalysts with High Selectivity and Conversion Efficiency • Catalysts for Alternate Feedstocks	• Generation 1 and 2 Photovoltaics • Generation 3 and 4 Photovoltaics • Solar Thermal/ Concentrated Solar Power Technologies	• Ceramic Membranes • Metallic Membranes • Polymeric Membranes • Composite Membranes	• Wear/Tribology • High-Temperature and Thermal Barrier Coatings
MATERIALS INTEGRATION IN CLEAN ENERGY SYSTEMS	**Next-Generation Batteries and Fuel Cells**	**Joining Processes for Multi-Material Structures**	**Composites with Structural Capabilities**	
	• Short-Duration Stationary Storage and Conversion • Long-Duration Stationary Storage and Conversion • Transportation	• Adhesive Bonding • Solid-State Bonding • Design Data and Testing	• Metal-Matrix Composites and Nanocomposites • Polymer Composites and Nanocomposites • Layered, Sandwich, and Infiltrated Materials	
HIGHER-PERFORMANCE MATERIALS	**Thermoelectric Materials**	**Phase-Stable Metallic Materials**	**Surface Treatments**	**Lightweight High-Strength Materials**
	• Improved Manufacturing • Higher Figure of Merit (ZT) • Sealants • Substitute Materials	• Next-Generation Steels • Next-Generation Nickel-Cobalt • Irradiation-Resistant Materials • Next-Generation Zirconium Cladding	• Part Restoration • Surface Processing	• Processing and Synthesis • Hybrid Materials
NEW PARADIGM MATERIALS MANUFACTURING PROCESSES	**Net-Shape Processing**	**Additive Manufacturing**	**Low-Cost Composites Manufacturing**	**Energy-Efficient Metals Production**
	• Solid-State Forming • Powder Metallurgy • Casting	• Metals Manufacturing • Polymer Manufacturing • Direct Writing • Multifunctional Manufacturing	• Fibers Manufacturing • Composite Matrix Manufacturing	• Steel Production • Aluminum Production • Recycling • Titanium Processing
MATERIALS AND PROCESS DEVELOPMENT ACCELERATION TOOLS	**Collaborative Databases**	**Predictive Modeling of Material Performance**	**Process Modeling Codes**	**Integrated Computational Materials Engineering (ICME)**
	• Structural Materials Databases • Functional Materials Databases	• Deformation and Texture • Fracture and Fatigue • Materials Degradation	• Microstructural Evolution and Materials Performance • Materials/Compound Discovery • Process Manufacturing and Component Performance	• ICME Platforms

Figure 2. Impact of R&D Pathways on Energy Sectors

The IITs identified the energy sectors that could benefit from advancing the selected breakthrough opportunities. Figure 2 summarizes the market potential of the breakthrough opportunities at the R&D pathway level,[5] illustrating both the breadth of impact of each R&D pathway across the energy sectors (horizontal) and the potential for materials and processing innovation in individual sectors (vertical).

One of the important aspects of this phase of the study is the additional impact that Materials and Process Development Acceleration Tools can have on facilitating materials development and reducing their time to commercial readiness. Because the impact of these tools is on the MSE R&D process rather than energy applications, the IITs identified the breakthrough opportunities with the greatest potential to benefit the other innovation impact areas. Figure 3 includes the identified Materials and Process Development breakthrough opportunities and the R&D pathways they have the potential to benefit.

RESEARCH PRIORITIES

To realize the impacts that materials and processing innovations have the potential to deliver, the MSE community in the United States, including funding agencies, needs to make a significant, sustained commitment to R&D. Phase III identified R&D activities that can advance materials and processing innovations to commercial readiness in a 2–10 year time frame. Figures 4 through 8 summarize the top-priority R&D activities identified by the IITs in each of the five innovation impact areas. These activities are categorized as near term (0–2 years), mid term (2–5 years), and long term (5–10 years). This comprehensive list shows that many significant, yet focused, R&D efforts are needed to realize the 2–10 year commercial readiness target.

NOTES

1 National Science and Technology Council, *Materials Genome Initiative for Global Competitiveness* (Washington, DC: Office of the White House, June 2011) http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf.

2 The Minerals, Metals, & Materials Society (TMS) in support of the U.S. Department of Energy Industrial Technologies Program, *Linking Transformational Materials and Processing for an Energy-Efficient and Low-Carbon Economy: Creating the Vision and Accelerating Realization. Vision Report of the Energy Materials Blue Ribbon Panel* (Washington, DC: TMS, 2010).

3 The Minerals, Metals, & Materials Society (TMS) in support of the U.S. Department of Energy Industrial Technologies Program, *Linking Transformational Materials and Processing for an Energy-Efficient and Low-Carbon Economy: Creating the Vision and Accelerating Realization. Opportunity Analysis for Materials Science and Engineering*, (Washington, DC: TMS, 2010).

4 The energy sectors addressed in this report are based on the Blue Ribbon Panel's assessment of the components of the energy sector that will make the largest contributions toward addressing U.S. clean energy and efficiency needs. While other sectors, including energy transmission and energy use in buildings are important to the whole energy industry, the Blue Ribbon Panel did not identify them as sectors in which MSE has the greatest potential to reduce energy and carbon emissions and improve the U.S. economy.

5 The Materials and Process Development Acceleration Tools innovation impact area is discussed separately (see Figure 3) because it affects Functional Surface Technology, Materials Integration in Clean Energy Systems, Higher-Performance Materials, and New Paradigm Materials Manufacturing Processes.

Figure 3. Materials and Process Development Acceleration Tools with High Impact on Materials and Process Innovation

		COLLABORATIVE DATABASES		PREDICTIVE MODELING OF MATERIAL PERFORMANCE			PROCESS MODELING CODES			INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING
		Structural Materials Databases	Functional Materials Databases	Deformation and Texture	Fracture and Fatigue	Materials Degradation	Microstructural Evolution and Materials Performance	Materials/Compound Discovery	Process Manufacturing and Component Performance	ICME Platforms
FUNCTIONAL SURFACE TECHNOLOGIES	Catalysts		●			●		●		●
	Solar Materials		●			●			●	
	Gas-Separating Membranes		●		●					
	Coatings	●				●	●			●
MATERIALS INTEGRATION IN CLEAN ENERGY SYSTEMS	Next-Generation Batteries and Fuel Cells		●			●		●	●	●
	Joining Processes for Multi-Material Structures	●		●	●	●	●		●	●
	Composites with Structural Capabilities	●		●	●	●	●		●	●
HIGHER-PERFORMANCE MATERIALS	Thermoelectric Materials		●				●	●	●	
	Phase-Stable Metallic Materials	●		●	●	●	●	●	●	●
	Surface Treatments	●		●	●	●	●		●	●
	Lightweight High-Strength Materials	●		●	●	●	●		●	●
NEW PARADIGM MATERIALS MANUFACTURING PROCESSES	Net-Shape Processing	●		●			●		●	●
	Additive Manufacturing	●	●		●		●	●	●	●
	Low-Cost Composites Manufacturing						●		●	
	Energy-Efficient Metals Production	●		●			●		●	●

Figure 4. Functional Surface Technologies R&D Priority Activities

FUNCTIONAL SURFACE TECHNOLOGIES	Near Term (0–2 Years)	Mid Term (2–5 Years)	Long Term (5–10 Years)
CATALYSTS	• Integrate catalysis in membranes at the laboratory scale (e.g., via infiltration processes and membrane reactors).	• Integrate catalysis in membranes at larger scale than near-term efforts (e.g., via infiltration process and membrane reactors). • Conduct predictive modeling and testing of existing catalysts.	• Identify catalysts for alternate feedstocks (more advanced and on a larger scale than near-term work).
SOLAR MATERIALS	• Increase efficiency of generation 4 systems via materials substitution.	• Identify replacement materials for indium tin oxide to develop a new thermal conducting oxide with better electrical conductivity and optical transparency. • Improve the balance of solar systems (e.g., glass, protective coatings, self-cleaning surfaces, and dust/ water resistance).	• Bring generation 4 solar applications to market (e.g., solar onboard vehicle paint, recharging stations, and smart-grid interaction). • Scale existing manufacturing technologies to reduce cost.
GAS-SEPARATING MEMBRANES	• Develop a fundamental understanding of the trade-off of flux and stability in membrane systems. • Identify how materials react under real-world conditions (e.g., degradation mechanisms).	• Increase the flux of dense ceramic membranes. • Identify selectivity issues in polymers to decrease the system thickness.	
COATINGS	• Leverage materials substitution to create multifunctional coatings that are able to withstand high-wear environments. • Advance research in sensing/health monitoring to detect defects in coatings and prognostic tools.	• Develop a non-vacuum coating application process. • Identify key materials for coatings with high temperature stability, high electrical conductivity, and oxidation resistance.	

Figure 5. Materials Integration in Clean Energy Systems R&D Priority Activities

MATERIALS INTEGRATION IN CLEAN ENERGY SYSTEMS	Near Term (0–2 Years)	Mid Term (2–5 Years)	Long Term (5–10 Years)
NEXT-GENERATION BATTERIES AND FUEL CELLS	• Advance high-speed stacking for lithium-ion batteries so that prismatic cells consisting of layers of electrodes can be manufactured more quickly. • Develop roll-to-roll vacuum drying and advance water management for lithium-ion cell assembly. • Develop low-cost fabrication of redox flow battery systems. • Develop low-cost, mass fabrication of oxide membranes for sodium-sulfur batteries. • Improve cell formation and grading for lithium-ion cells to decrease the footprint and capital expenditures associated with the need to charge batteries after they are assembled. • Develop high-speed, 100% inspection, nondestructive evaluation techniques for battery joints (e.g., aluminum and copper), packs, and modules.	• Reduce or eliminate the use of organic solvents (e.g., lithium-ion electrode fabrication). • Develop new metal or ceramic surfaces with controlled porosity for direct bonding of polymers or elastomers to improve adhesion. • Reduce the use of inactive materials, expanding beyond thick electrodes. • Identify processes for functionalizing surfaces for polymer chemical bonding.	

MATERIALS INTEGRATION IN CLEAN ENERGY SYSTEMS	**Near Term (0–2 Years)**	**Mid Term (2–5 Years)**	**Long Term (5–10 Years)**
JOINING PROCESSES FOR MULTI-MATERIAL STRUCTURES	• Develop low-cost, flexible, mass-production joining processes for multi-material automotive sheet and tubular structures (e.g., aluminum to steel) and develop design data and fatigue data for each joining process. • Develop joining processes for high-temperature, oxide-dispersion-strengthened materials in extreme environments.	• Fabricate new metal or ceramic surfaces with controlled porosity for direct bonding of polymers or elastomers to improve adhesion of materials. • Develop processes for producing functional surfaces that can improve the integrity of polymer chemical bonding. • Develop low-cost (50% cost reduction) surface adhesives (e.g., prepolymers, epoxies, ultraviolet cure, thermal cure, and laser cure) that are not sensitive to substrate contamination. • Measure and analyze post-weld heat treatment properties and residual stresses in solid-state friction stir welding in real time and after processing. • Develop an integrated computational materials engineering process model for solid-solid joining that incorporates residual stress, diffusion, microstructure evolution, and mechanical properties and interlayers. • Develop high-speed and reliable nondestructive evaluation techniques to evaluate bond quality in similar and dissimilar materials. • Develop low-cost, mass-production joining processes for multi-material automotive sheet and tubular structures (e.g., steel with composites, aluminum, or magnesium).	

MATERIALS INTEGRATION IN CLEAN ENERGY SYSTEMS	**Near Term (0–2 Years)**	**Mid Term (2–5 Years)**	**Long Term (5–10 Years)**
COMPOSITES WITH STRUCTURAL CAPABILITIES	• Identify and deploy joining and oxidation-protection approaches that could be used to integrate refractory metal plates, foils, or sheets as the outer face of sandwich structures.	• Develop low-cost, in-situ fabrication of metal-matrix nanocomposites, including casting and powder metallurgy techniques. • Establish manufacturing processes and design criteria to enable low-cost, high-volume continuous fiber polymer composites for transportation lightweighting. • Discover high-performance polymers or polymer composites with higher thermal gradient and/or lower creep at elevated temperatures to substitute for metals. • Identify out-of-autoclave curing technologies (e.g., selective heating by microwave or radio frequency, cold processing by electron beam curing) to reduce curing times. • Conduct high-temperature evaluation of metal-matrix composites, metal-matrix nanocomposites, and layered materials.	

Figure 6. Higher-Performance Materials R&D Priority Activities

HIGHER-PERFORMANCE MATERIALS	Near Term (0–2 Years)	Mid Term (2–5 Years)	Long Term (5–10 Years)
THERMOELECTRIC MATERIALS	• Develop a range of thermoelectric polymers to enable wide-scale application of weight-optimized components for use in defense, automotive, and commercial applications.	• Develop highly conductive thermoelectric materials compatible with additive manufacturing systems to enable corrosion-resistant, highly functional polymer designs for multifunctional components with structurally integrated power and communication circuits.	• Develop capacitance materials compatible with additive manufacturing methods to enable structurally integrated electrical energy storage systems. • Develop an oxidation barrier coating for thermoelectric materials operating at 1,000°C.
PHASE-STABLE METALLIC MATERIALS	• Create high-strength, low-alloy steel for ultra-deep-well drilling. • Develop corrosion-resistant zirconium alloys with reduced hydrogen pickup.	• Develop stress-corrosion-cracking-resistant stainless steel variants (e.g., AISI 304 and 316 steels) for reactor applications. • Develop 1,200°F steels for use in power plant steam turbines. • Develop irradiation-resistant pressure vessel steels (e.g., A508 and A533 steels). • Create physics-based models to predict component lifetime in power plants.	• Identify alternate fuel cladding materials (e.g., silicon carbide metal-matrix composites). • Develop oxidation- and corrosion-resistant refractory alloys for next-generation gas turbines. • Develop a materials database to enable more accurate computational design. • Use new phase diagrams to create more accurate thermomechanical processing and heat treating of steels.
SURFACE TREATMENTS	• Create a user test facility for remanufactured parts testing. • Develop lower-cost coating materials that are validated for use and have appropriate cost-performance specifications, rather than overdesigning coatings as happens today.	• Develop low-cost laser hybrid processing that can metallurgically bond surface layers. • Conduct highly accurate non-planar or larger-scale surface treating without damaging substrates (e.g., laser, high-density infrared, high-precision hybrid deposition).	• Develop ceramics for gas turbine parts (e.g., air foils). • Develop ultra-high-temperature (~1,600°F) thermal barrier coatings for oxy-combustion turbines.

HIGHER-PERFORMANCE MATERIALS	Near Term (0–2 Years)	Mid Term (2–5 Years)	Long Term (5–10 Years)
LIGHTWEIGHT HIGH-STRENGTH MATERIALS	• Develop low-cost, improved processing methods of aluminum-, magnesium-, and metal-based composites for casting. • Improve wear resistance via a gradient-type approach or surface treatment of aluminum, magnesium, and other lightweight, high-strength materials. • Identify top transportation opportunities for custom optimized hybrid/gradient metallic systems.	• Develop new alloy designs with higher alloy retention for better recyclability. • Improve damage detection techniques for defects and mechanical reliability of all types of material systems. • Increase corrosion resistance of aluminum or magnesium via surface treatment and/or alloying approaches.	

Figure 7. New Paradigm Manufacturing Processes R&D Priority Activities

NEW PARADIGM MANUFACTURING PROCESSES	Near Term (0–2 Years)	Mid Term (2–5 Years)	Long Term (5–10 Years)
NET-SHAPE PROCESSING	• Use innovative joining methods to improve dimensional control and enable forged and formed components to replace machined components and assemblies (fits all time ranges because this is an ongoing effort).	• Increase closed-loop spring-back control and strain-distribution control for high-strength sheet metal components. • Improve room-temperature formability of magnesium, titanium, and aluminum sheet metals by controlling crystallographic texture. • Develop new nanomaterials (e.g., tooling and bearings) using spark plasma sintering techniques. • Develop a process for direct consolidation of titanium powder into tubular and structural shapes. • Develop and commercialize a process for high-property, thin-walled, complex light metal castings. • Develop a metal casting technique that uses a high magnetic field to achieve wrought properties and improved yield. • Develop multi-material processing techniques. • Use innovative joining methods to improve dimensional control and enable forged and formed components to replace machined components and assemblies (fits all time ranges because this is an ongoing effort).	• Develop processes that simultaneously improve both shape and material properties (e.g., variations of hot stamping, peen forming, and temperature-controlled stamping). • Use innovative joining methods to improve dimensional control and enable forged and formed components to replace machined components and assemblies (fits all time ranges because this is an ongoing effort).

NEW PARADIGM MANUFACTURING PROCESSES	Near Term (0–2 Years)	Mid Term (2–5 Years)	Long Term (5–10 Years)
ADDITIVE MANUFACTURING	• Develop and advance automated spark plasma sintering techniques for the production of metal-matrix composites (e.g., silicon carbide, silicon nitride, tungsten carbide). • Develop closed-loop hardware/software to provide Ti-6Al-4V (titanium-aluminum-vanadium) material/part traceability for quality standards, thus improving yield numbers. • Develop families of polymer compounds with nano-fillers that are compatible with additive manufacturing processes to create a wide spectrum of material properties. • Develop new inks and slurries for direct writing systems (fits all time ranges because this is an ongoing effort). • Set up additive manufacturing stations or areas for regional economic zones to lower shipping costs.	• Develop a continuous process for titanium metal production, preferably in powder form. • Develop methods to increase throughput of additive manufacturing systems while increasing accuracy and in-situ process monitoring. • Develop new inks and slurries for direct writing systems (e.g., silver and copper inks) (fits all time ranges because this is an ongoing effort). • Create an alternative file format to ".stl" to enable multi-material fabrication in a monolithic piece; less energy-intensive materials may be used functionally in place of a single energy-intensive material. • Develop larger chambers or multi-heads for direct metal deposition processes. • Develop a system for sensing and controlling surface quality and residual stresses.	• Develop large-scale printed energy storage batteries and capacitors (e.g., ones that may be used for wind farms). • Develop new inks and slurries for direct writing systems (fits all time ranges because this is an ongoing effort). • Create a residual stress analytical modeling system for non-vacuum-based additive manufactured systems; this will help predict residual stress or distortion of direct parts to increase yield numbers and increase part robustness. • Develop additive system techniques to integrate additive manufacturing systems seamlessly.
LOW-COST COMPOSITES MANUFACTURING	• Develop new autoclave-free continuous processes (e.g., automation of fiber lay-up in resin transfer molding and vacuum-assisted resin transfer molding) that ensure accurate shape and orientation of polymer-matrix composites. • Develop automated panel lay-up forming to achieve a high production rate.	• Create fiber manufacturing processes that require less energy to create the final product. • Develop a high-volume production technology to reduce production cycle times.	• Develop low-cost fiber feedstocks (e.g., by reducing energy input in fiber production or developing alternate precursors to pitch and polyacrylonitrile for carbon fibers).

NEW PARADIGM MANUFACTURING PROCESSES	**Near Term (0–2 Years)**	**Mid Term (2–5 Years)**	**Long Term (5–10 Years)**
ENERGY-EFFICIENT METALS PRODUCTION	• Improve instrumentation for aluminum reduction cells, leading to better process control.	• Develop new electrode materials for aluminum reduction cells. • Develop a continuous process for titanium metal production, preferably in powder form. • Develop a titanium molten metal delivery system (i.e., closed-coupled gas atomization) to lower the cost of production via a high-performance continuous process.	• Develop a process for the direct reduction of iron ore using an electrolytic hydrogen or other non-carbon-reduction process. • Develop novel electrochemistry processes for the production of aluminum and/or magnesium (e.g., lower-temperature ionic liquids). • Develop a continuous casting process for high-end alloys (e.g., titanium and nickel). • Advance scaling of melt facilities to increase product yield. • Develop a low-cost, high-property magnesium system for high-volume casting or sheet production. • Optimize the yield, use, and scale of vacuum-arc remelting and electroslag melting of high-end metals (e.g., iron, nickel, titanium); high-end alloys usually need multiple melting cycles.

Figure 8. Materials and Process Development Acceleration Tools R&D Priority Activities

MATERIALS AND PROCESS DEVELOPMENT AND ACCELERATION TOOLS	**Near Term (0–2 Years)**	**Mid Term (2–5 Years)**	**Long Term (5–10 Years)**
COLLABORATIVE DATABASES	• Establish fundamental databases for epoxy resin design and other polymers and for advanced metallics and composites systems. • Add topology/structure to databases and include a search function. • Establish a database for nanoparticle synthesis that may be used for catalysis-based work.	• Establish basic databases/infrastructure for photovoltaics, thermoelectrics, and fuel cells. • Enhance coatings and substrates databases intended for descriptive and predictive modeling.	
PREDICTIVE MODELING OF MATERIAL PERFORMANCE	• Create a statistical representation of microstructural evolution in codes for the prediction of material performance.	• Develop a coatings “degradation predictor” for energy technologies. • Develop practical and computationally efficient approaches in coupling multiphysics and multi-scale modeling of materials performance. • Establish probabilistic strategies for extending part life that account for microstructural variances.	• Improve the coupling of CALPHAD-type (CALculation of PHAse Diagrams) databases into corrosion models and irradiation-damage models.

MATERIALS AND PROCESS DEVELOPMENT AND ACCELERATION TOOLS	Near Term (0–2 Years)	Mid Term (2–5 Years)	Long Term (5–10 Years)
PROCESS MODELING CODES		• Develop physics-based material constitutive models with integrated experimentation and data generation for multi-axial straining (over a broad range of strain rates, temperatures, etc.) for metals and polymers. In addition, combine such models with interfacial constitutive models when deformation involves contact (e.g., tool/workpiece interface). • Develop the ability to model compounds of polymers and metals with nano-fillers. • Integrate models and databases for welding and joining issues of dissimilar materials.	• Create multi-scale codes that link density functional theory and kinetic Monte Carlo codes for microstructural evolution. • Develop methods to analyze finite element predictive performance for unique additive manufacturing internal structures. • Introduce composition-dependent models and data into higher-level process modeling codes for casting, deformation, etc.
INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING	• Develop a high-profile ICME example to show its applicability to energy problems (e.g., fuel cells, batteries, heat exchangers, or wind turbines).	• Advance and accelerate the qualification of high-temperature alloys. • Introduce materials design for novel joinability (e.g., automobile industry spot welding). • Advance materials design for additive manufacturing of magnesium and transformation-induced plasticity steels. • Integrate models and databases for welding and joining issues of dissimilar materials. • Develop inverse methodologies for materials design.	• Develop concurrent design of a material and its applicable component within an energy sector.

I. PROCESS OVERVIEW

To prepare this report, The Minerals, Metals, & Materials Society (TMS) convened five innovation impact teams (IITs) consisting of materials experts from academia, industry, and government in five innovation impact areas identified in earlier phases of this project. Each IIT met several times via phone and conducted independent analyses to identify the materials science and engineering breakthrough opportunities that hold the greatest promise for delivering significant energy, environmental, and economic impacts in the 2–10 year time frame. A significant part of this work required IIT members to investigate and document historical material systems improvements. This historical data provided a basis for later discussions on the projected improvements in materials performance.

Following the initial teleconferences and independent research, each team met for a one-and-a-half day working meeting at TMS headquarters to share information, discuss, debate, and ultimately come to consensus regarding the possible breakthrough opportunities, the energy sectors that would benefit from these advances, and the research and development (R&D) priority activities needed to realize these gains. After each workshop, the IIT members continued to share information and refine their work, culminating in this report.

Another important aspect of the process used to create this report was analysis conducted by Energetics Incorporated to quantify the energy savings and emissions reductions that could be realized via the successful commercialization of new material systems. These market opportunity analyses examined specific energy sectors likely to be impacted by the breakthrough opportunities, such as transportation or solar power, and estimated the magnitude of energy consumed and carbon dioxide (CO_2) emissions produced, thereby framing the potential market impact of each breakthrough opportunity. Because these market opportunity analyses required quantifiable information, the highlighted market opportunities for each R&D pathway may not be the opportunities with the greatest potential, but rather the opportunities with available market data. Each market opportunity analysis quantifies some portion of the potential impact of each R&D pathway, providing justification for pursuing the breakthrough opportunities in the respective pathways. The analysis intentionally stops short of predicting the energy savings and emissions reductions for individual breakthrough opportunities because of the high degree of uncertainty in such predictions.

BREAKTHROUGH OPPORTUNITIES: A CLOSER LOOK

The work of the IITs culminated in detailed discussions of each breakthrough opportunity, which compose the majority of this report. Each breakthrough opportunity is represented by one dedicated page that includes the background, gaps and limitations, potential energy market impact areas, historical trends, and expected advances of each breakthrough opportunity. The template used to provide this information is explained in Figure 9.

Figure 9. Template for Breakthrough Opportunities

R&D Pathway

Breakthrough Opportunity

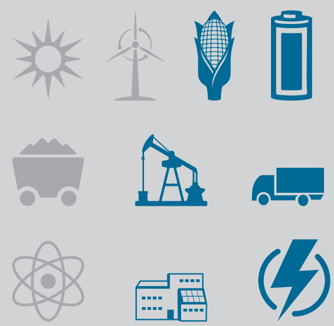
DESCRIPTION

Breakthrough opportunities are areas in which there is great potential for innovative progress toward a cleaner, more energy-efficient future. A breakthrough opportunity includes technologies that share common characteristics, limitations, trends, and market ties. In this section, each breakthrough opportunity is defined to reflect its importance within the R&D pathway and provide context for describing historical trends and future opportunities.

GAPS AND LIMITATIONS TO OVERCOME

Certain processes, operations, and technologies have limitations or restrictions that may inhibit a breakthrough opportunity's market potential. Some of these technological gaps can be surmounted, while others are limited by the laws of physics, requiring new approaches in order to advance the opportunity. Recognizing these boundaries helps define the path forward for realizing a breakthrough opportunity, resulting in new or improved technologies with increased efficiency, decreased carbon emissions, and economic savings.

Market Impact



Each breakthrough opportunity has an influence on certain energy generation, storage, and use sectors. The highlighted icons demonstrate the sectors that will benefit as advances are made in each breakthrough opportunity. The measurable impact on some of these sectors is provided in the market opportunities analyses included in each R&D pathway.

Historical Trends and Future Opportunities

Studying the recent history and current progress of a breakthrough opportunity helps to visualize technological progress and define a path toward realizing its potential impact on energy sectors.

This section provides a visual, where applicable, to illustrate the consensus of the IITs on the historical trends and expected advances in each breakthrough opportunity. The historical trends typically summarize the advances achieved over the past 10–20 years, unless the IITs thought a different time range better represented the advances. The projected advances are usually for the next 5–10 years, coinciding with the near-term potential (2–10 years) for commercial readiness.

Generally, the projected percent improvements assume a level R&D funding environment. The IITs approached this question from the basis of technical possibility, rather than scenarios for how the percent improvements would change given an increase or decrease in funding.

This sidebar provides a textual overview of the historical trends and future potential of a breakthrough opportunity, describing the visual portrayal to the left.

III. FUNCTIONAL SURFACE TECHNOLOGIES

New and emerging energy systems require material surfaces that can effectively interact with service environments and withstand demanding operating conditions. As U.S. demand increases for energy-efficient, cost-effective energy systems with reduced carbon dioxide (CO_2) emissions, the materials within these systems must serve functions that extend beyond the structure of the system. Materials that can serve specific functions, such as facilitating chemical reactions, capturing photons, and separating gases, can optimize the contributions of each material to the system.

Functional surface technologies that harvest energy and produce higher product yields can increase the efficiency and lower the cost of energy systems. These process innovations can ultimately reduce the environmental impact, cost, and energy requirements of energy generation, storage, and use across U.S. energy sectors, particularly in industrial processes, transportation technologies, and oil and coal energy systems.

The following pathways provide a guide for research and development (R&D) in the area of functional surface technologies:

- Catalysts
- Solar Materials
- Gas-Separating Membranes
- Coatings

CATALYSTS

Catalysts are important enabling technologies for many energy systems and an integral part of the production of more than 90% of all industrial chemicals,[1] including ammonia and methanol. Catalysts use functional surfaces to speed up or enable chemical reactions and therefore lower the amount of energy required. Increasing the selectivity and conversion efficiency of catalysts can improve industrial processes and manufacturing by effectively boosting the yield of chemical production. As a result, materials science and engineering (MSE) advances in this area can increase the cost-effectiveness and reduce the environmental impact and energy requirements of energy generation, storage, and use. Opportunities in industrial processes and oil and gas sectors provide a quantifiable justification for pursuing R&D of catalysts.

Market Opportunity: Industrial Processes

The chemicals industry consumes more than 3,000 trillion British thermal units (TBtu) of onsite energy per year,[2] of which 104 TBtu of energy is estimated to be lost from catalyst non-selectivity in 42 high-volume production petrochemical processes.[3] Advanced high-volume catalysts with increased selectivity can reduce these losses by requiring less process heating fuel for catalysis, which will increase energy efficiency and reduce CO_2 emissions and fuel costs. For example, reducing catalyst selectivity losses by 25% would save 26 TBtu of energy,[4] 2 million metric tons (MMT) of CO_2,[5] and $331 million in fuel costs each year.[6]

Market Opportunity: Oil and Gas

Natural gas can be converted to a liquid fuel through gas-to-liquids processes involving either direct conversion or the production of an intermediate synthesis gas followed by Fischer-Tropsch (FT) synthesis. Catalytic reactions synthesize the liquefied fuel from the intermediate synthesis gas (carbon monoxide and hydrogen) produced during the FT stage of the gas-to-liquids conversion process.[7] Because this process is currently energy-intensive and costly, natural gas flaring is often used to dispose of unwanted gas that cannot be transported because of limited natural gas transport mechanisms. An economically viable gas-to-liquids process enabled by the development and manufacturing of advanced catalyst materials can eliminate some of the 2.1 billion cubic meters (bcm) of natural gas that is flared and vented in the United States each year,[8] resulting in energy savings and reduced CO_2 emissions and fuel costs. For example, eliminating 10% of natural gas flaring (0.21 bcm) through the increased use of gas-to-liquids processing would save 8 TBtu of energy,[9] 0.4 MMT of CO_2 emissions,[10] and $15 million in fuel costs each year.[11]

Breakthrough Opportunities

The MSE community can advance catalysts by developing and improving catalysts with high selectivity and conversion efficiency and catalysts for alternate feedstocks. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow catalysts to make significant contributions toward addressing energy, environmental, and economic needs.

Catalysts

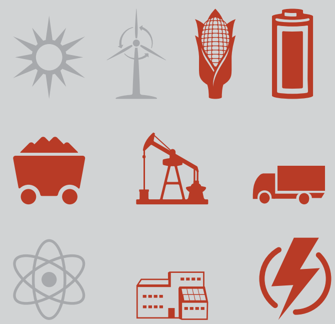
Catalysts with High Selectivity and Conversion Efficiency

The production of almost all industrially important chemicals, such as ammonia, involves catalysts. Catalytic processes yield products at a relatively constant rate over the life of a catalyst. However, as the catalyst ages, its reaction temperature increases, resulting in an increase in activity but a decrease in selectivity and conversion efficiency. The catalyst will remain in use until the selectivity is unacceptably low, which may occur after a couple of years. Advanced catalysts with higher initial selectivity and conversion efficiency will enable more efficient surface catalysis reactions and more cost-effective manufacturing by increasing product yield over a catalyst's usable life.

GAPS AND LIMITATIONS TO OVERCOME

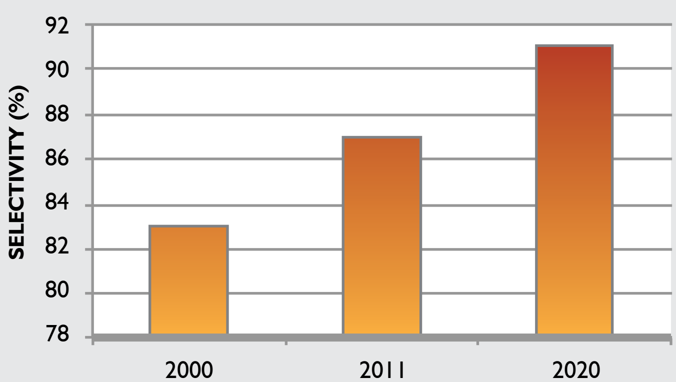
- Many advanced catalysts have inadequate mechanical stability and/or resistance to contamination, which limits their efficiency, lifetime, and range of application.
- Certain catalysts (e.g., catalysts for ammonia synthesis) have insufficient low-temperature reactivity.
- Materials scientists lack adequate understanding and capabilities for predicting the reactive properties of new catalysts, and therefore require a trial-and-error approach to identifying new catalysts.
- Microscopic analysis capabilities are inadequate, preventing materials scientists from fully characterizing catalyst surfaces and defects and distinguishing the relative reactivity of various geometric regions of the catalyst structure (e.g., crystal surfaces in comparison to terraces).

Market Impact



Historical Trends and Future Opportunities

SELECTIVITY OF ETHYLENE OXIDE CATALYSTS



Ethylene oxide is representative of high-selectivity catalysts. Selectivity of ethylene oxide has increased from 83% to 87% in the past 10 years. With advances in unique nanotechnology catalyst structures, the selectivity and yield of this catalyst is expected to continue to improve at an average of 4% per decade, increasing to 91% in the next 10 years.[12]

Selectivity

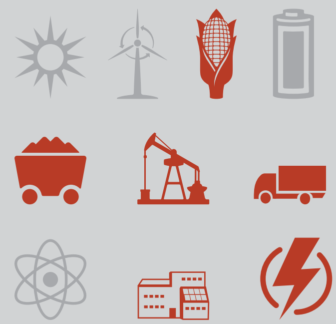
- 2000: 83%
- 2011: 87%
- 2020: 91%

Catalysts

Catalysts for Alternate Feedstocks

Advanced catalysts that convert alternate feedstocks can create fuels that have the potential to compete with natural gas and petroleum for the production of commodity chemicals. Coal and biomass are two alternate feedstocks that require biocatalysis—the selective formation of products using enzymes—to become more attractive fuel options. The successful development and implementation of a novel biocatalytic process requires a suitable biocatalyst, methods for enzyme stabilization to ease its application and reuse, process engineering to select an appropriate reaction system (e.g., aqueous or solvent system, batch or continuous, packed-bed or membrane reactor), and upstream and downstream processing.[13]

Market Impact

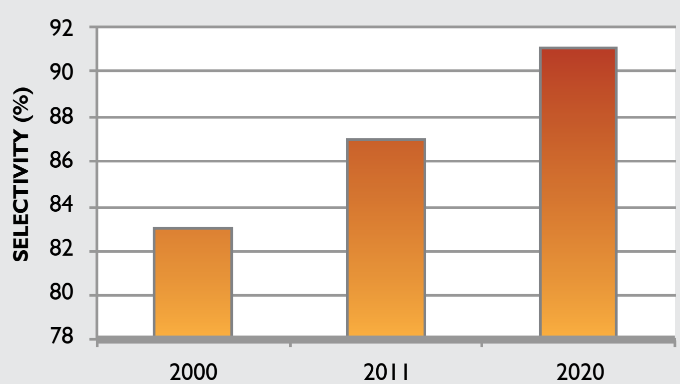


GAPS AND LIMITATIONS TO OVERCOME

- It is cost-intensive to advance catalysts for alternate feedstocks with acceptable selectivity and resistance to denaturing.
- Catalysts that operate on alternate feedstocks are subject to accelerated aging with frequent switching between feedstocks.
- Alternate feedstocks typically contain contaminants that can severely accelerate the aging of relevant catalysts. Mineral pretreatments need major advances to reduce these contaminants.

Historical Trends and Future Opportunities

SELECTIVITY OF CATALYSTS FOR PRODUCTION OF ALTERNATE FEEDSTOCKS



Catalysts with increased selectivity can decrease the consumption of water, materials, and energy during alternate feedstock conversion, as well as the dispersion of toxins and pollutants. Historically, selectivity of catalysts for alternate feedstocks has increased by about 4% per decade, the same rate as ethylene oxide catalysts. This rate of selectivity improvement is expected to continue for the next 10 years.[14]

Selectivity

- 2000: 83%
- 2011: 87%
- 2020: 91%

R&D Priority Activities: Catalysts

To overcome the gaps and limitations within the catalyst breakthrough opportunities, the MSE community must focus their efforts on identifying catalysts for use with alternate feedstocks, integrating catalytsts into membranes, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Catalysts for Alternate Feedstocks** • Identify promising concepts for alternate feedstock catalysts (e.g., biofuels, alkenes, and olefins) at the laboratory scale. **Crosscutting** • **Integrate catalysis in membranes at the laboratory scale (e.g., via infiltration processes and membrane reactors).** • Conduct active site modeling of existing catalysts (e.g., nanoparticle thermo-stability, catalyst regeneration, and oxygen production/replacement via redox reactions).
MID TERM (2–5 YEARS)	**Crosscutting** • **Integrate catalysis in membranes at larger scale than near-term efforts (e.g., via infiltration process and membrane reactors).** • **Conduct predictive modeling and testing of existing catalysts.** • Develop multifunctional/multi-site catalysts or systems with multiple catalysts.
LONG TERM (5–10 YEARS)	**Catalysts for Alternate Feedstocks** • **Identify catalysts for alternate feedstocks (more advanced and on a larger scale than near-term work).** **Crosscutting** • Develop infiltration process for membrane with stacks (large-scale work). • Develop a membrane reactor for propane dehydrogenation at low operating temperatures (500°C–600°C).

*The experts identified the **bolded activities** as high priority.

SOLAR MATERIALS

Solar materials—such as photovoltaics (PVs) (e.g., silicon, cadmium telluride, copper indium gallium selenide), encapsulants, and conductive oxides—work together to absorb photons and convert them to electrical energy. However, current solar materials are only able to absorb a narrow range of solar energies from the broad solar spectrum (low-energy infrared to high-energy and ultraviolet), leaving photons of lower ranges unabsorbed while photons of higher ranges are absorbed and mostly lost as heat. Increasing the absorption range and conversion efficiency of solar materials can reduce the cost of these materials and expand the contributions of renewable solar energy to U.S. electricity generation.

Market Opportunity: Electricity Generation

Solar energy is a renewable energy source that can decrease U.S. reliance on imported fossil fuels for electricity generation while also lowering CO_2 emissions. In 2010, of the nearly 40,000 TBtu of energy consumed by the electric power sector, about two-thirds of this energy (27,028 TBtu) was derived from fossil fuels.[15] By displacing a portion of fossil fuel consumption, solar energy can also reduce CO_2 emissions and fuel costs. If solar energy gained a 1% market share of U.S. electric power sector electricity production (compared to current U.S. net electricity production from solar of 0.1% from all sectors, a generation capacity of 2.6 gigawatts),[16] it could displace 396 TBtu of conventional electricity generation,[17] decrease CO_2 emissions by 23 MMT,[18] and reduce fuel costs to investor-owned utilities (which represent only a portion of U.S. power producers) by $402 million per year.[19]

Breakthrough Opportunities

The MSE community can advance solar materials by focusing on generation 1 and 2 PVs, generation 3 and 4 PVs, and thermal/concentrated solar power technologies. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow solar materials to make significant contributions toward addressing energy, environmental, and economic needs.

Solar Materials

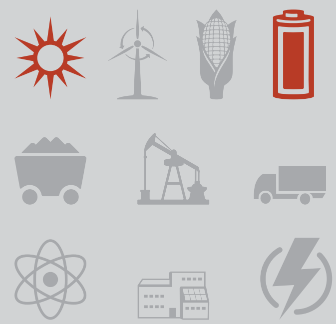
Generation 1 and 2 Photovoltaics

Photovoltaics are based on a principle known as the photoelectric effect, which involves the conversion of solar radiation into electricity using semiconductors. Generation 1 PVs are single-junction amorphous silicon cells, and generation 2 PVs refer to thin-film cadmium telluride (CdTe) or copper indium gallium selenide (CIGS) cells. Photovoltaic systems continue to increase in efficiency through laboratory-scale testing and advances in processing techniques, which can also lower the cost of production and make these PVs cost-competitive.

GAPS AND LIMITATIONS TO OVERCOME

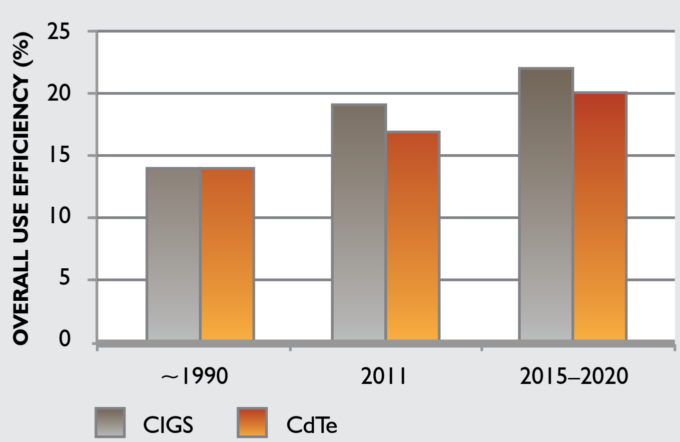
- There is a lack of knowledge about and an inability to manipulate the interface between the PV dye molecule and the PV surface to minimize energy loss.
- Solar PV surfaces lack self-cleaning or contaminant-resistant layers, which are necessary to increase system efficiency.
- The high costs of solar PV production and installation reduce the business case for building owners and limit wide-scale PV distribution.
- PV production defects lower the efficiency of PV systems, necessitating improvements in the production process.

Market Impact



Historical Trends and Future Opportunities

EFFICIENCY OF GENERATION 2 PV MATERIALS



Over the past 20 years, first- and second-generation PVs have undergone processing and manufacturing changes, and new and alternative materials have been integrated into PV systems. As a result, the efficiency—the ratio of electricity generated to sunlight captured—of CIGS cells has increased by about 5% and the efficiency of CdTe cells has increased by 3%, making today's commercial CIGS cells about 19% efficient and CdTe cells about 17% efficient. With further advancements, efficiency is expected to increase by 3% in the next 5–10 years for each technology.[20]

Use Efficiency

- ~1990: 14% for both cells
- 2011: 19% for CIGs, 17% for CdTe
- 2015–2020: 22% for CIGs, 20% for CdTe

Solar Materials

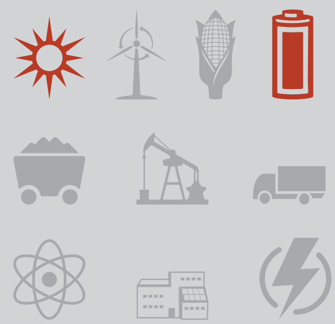
Generation 3 and 4 Photovoltaics

Photovoltaics are based on a principle known as the photoelectric effect, which involves the conversion of solar radiation into electricity using semiconductors. Generation 3 and 4 PVs have stacked, thin single-junction cells, also known as tandem or multijunction cells, with several band gaps to capture more wavelengths of light and increase efficiency. These PVs are still undergoing laboratory testing but have the potential to offer significantly higher efficiencies than Generation 1 and 2 PVs.

GAPS AND LIMITATIONS TO OVERCOME

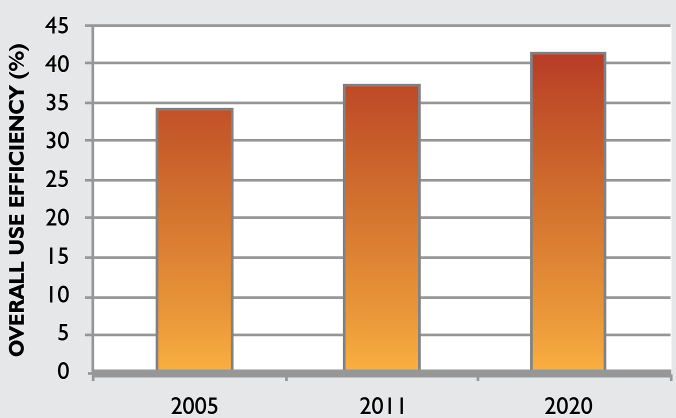
- Materials scientists have little control of the band gap of PV materials, particularly oxide semiconductors, to optimize capture of the solar spectrum.
- Materials scientists have not yet been able to optimize PV power output, which increases as visible light bandwidth increases. Most light escapes because low-energy photons do not have enough energy to excite PV electron-hole pairs across the energy gap. High-energy photons excite PV electron pairs with energy above the gap, resulting in lost heat energy rather than usable electrical energy.
- There is a lack of knowledge about and an inability to manipulate the interface between the PV dye molecule and the PV surface to minimize energy loss.
- Solar PV surfaces lack self-cleaning or contaminant-resistant layers, which are necessary to increase system efficiency.
- The high costs of solar PV production and installation reduce the technology confidence of building owners and limit widespread PV distribution.
- PV production defects lower the efficiency of PV systems, necessitating improvements in the production process.

Market Impact



Historical Trends and Future Opportunities

EFFICIENCY OF GENERATION 3 AND 4 PV MATERIALS



While generation 3 and 4 PVs are still under laboratory development, their efficiency—the ratio of electricity generated to sunlight captured—has already increased from 34% to 37% since 2005. In the next 10 years, advances in manufacturing methods and materials properties are expected to yield a 4% increase in the efficiency of generation 3 and 4 PVs. The most advanced solar cell efficiencies are already approaching 40% in laboratories.[21]

Use Efficiency

- 2005: 34%
- 2011: 37%
- 2020: 41%

Solar Materials

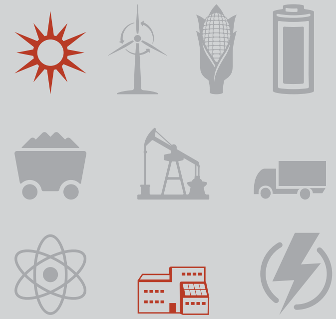
Solar Thermal / Concentrated Solar Power Technologies

Concentrated solar power (CSP) technologies use mirrors to redirect sunlight for use as a heat source in power plants or to provide industrial process heating or cooling. The four types of CSP systems are parabolic trough, parabolic dish/engine, power tower, and linear Fresnel receivers. Parabolic troughs use circular-arc mirrors to focus sunlight inward on a long tube containing a moving fluid that captures heat. Parabolic dishes/engines focus light onto a closed cylinder with a piston that moves as gas is expanded by high temperatures. Power towers are central receiver systems raised high above the ground that contain a moving fluid that is heated by sunlight reflected by multiple surrounding mirrors. Linear Fresnels use special lenses to focus sunlight onto a fixed absorber at common focal points.

GAPS AND LIMITATIONS TO OVERCOME

- CSP mirror surfaces lack self-cleaning or contaminant-resistant layers, which lowers system efficiency from contaminant exposure.
- CSP systems have a poor ability to store excess thermal and electrical energy.

Market Impact



Historical Trends and Future Opportunities

OVERVIEW OF CSP TECHNOLOGY EFFICIENCIES, LAND OCCUPANCY, AND FUTURE OUTLOOK

Technology	Annual Solar-to-Electric Efficiency	Land Occupancy	Outlook for Improvements
Parabolic Troughs	15%	Large	Limited
Parabolic Dishes	25%–30%	Small	Through Mass Production
Towers (central receiver systems)	20%–35%	Medium	Very Significant
Linear Fresnel Receivers	8%–10%	Medium	Significant

The current state and expected advances of the four types of CSP systems are described to the left. Technology advances are under development that will enable CSP to boost electricity production and reduce costs, notably by achieving higher temperatures that bring greater efficiency.

Other technologies now under development will enable the production of liquid or gaseous fuels by concentrating solar energy. With concerted effort, these milestones can be achieved in the next 2–5 years.[22]

R&D Priority Activities: Solar Materials

To overcome the gaps and limitations within the solar materials breakthrough opportunities, the MSE community must focus their efforts on increasing the efficiency of solar materials, lowering their cost, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Generation 3 and 4 Photovoltaics** • **Increase efficiency of generation 4 systems via materials substitution.** **All Photovoltaics** • Develop alternative processing techniques to lower production costs of CIGS and CdTe. • Advance encapsulant characteristics (e.g., stability, performance degradation, life extension, durability, and temperature fluctuations).
MID TERM (2–5 YEARS)	**Generation 1 and 2 Photovoltaics** • Identify new materials for CIGS/CdTe to reduce cost and increase efficiency (e.g., toxicity assessment, multijunction devices). **Generation 3 and 4 Photovoltaics** • **Identify replacement materials for indium tin oxide to develop a new thermal conducting oxide with better electrical conductivity and optical transparency.** **All Photovoltaics** • Advance research in PVs for building integration. **Solar Thermal / Concentrated Solar Power Technologies** • Identify materials needs for general electrical collection and storage (e.g., increasing the thermal conductivity and fluid heat capacity and increasing the heat transfer coefficient of collecting tube fluid). **Crosscutting** • **Improve the balance of solar systems (e.g., glass, protective coatings, self-cleaning surfaces, and dust/water resistance).**
LONG TERM (5–10 YEARS)	**Generation 3 and 4 Photovoltaics** • **Bring generation 4 solar applications to market (e.g., solar onboard vehicle paint, recharging stations, and smart-grid interaction).** **All Photovoltaics** • **Scale existing manufacturing technologies to reduce cost.**

*The experts identified the **bolded activities** as high priority.

GAS-SEPARATING MEMBRANES

Gas-separating membranes[23] can be significantly more energy efficient than other gas-separation methods, including absorption/adsorption, distillation, and cryogenics. Unlike these traditional processes, membranes often do not require energy-intensive phase changes of the gas being separated. Improving membrane processing, reducing maintenance requirements, optimizing selectivity and membrane surface-to-volume ratio, and increasing the ability to retrofit membranes in existing systems could increase energy efficiency and reduce costs in energy sectors. Opportunities for carbon capture in electricity generation and industrial processes in the chemicals, petrochemicals, and forest products industries provide a quantifiable justification for pursuing R&D of gas-separating membranes.

Market Opportunity: Electricity Generation

In 2010, the total U.S. energy consumption for electricity generation by the electric power sector was 39,579 TBtu;[24] of this consumption, 19,133 TBtu was from coal.[25] Advanced membranes with increased flux can have a significant role in carbon capture, addressing intrinsic challenges such as efficiently separating CO_2 from nitrogen given their similar molecule sizes (0.33 nanometers [nm] and 0.36 nm, respectively) and the tendency for CO_2 molecules to move through membranes relatively slowly.[26] For example, if advanced membrane-enabled carbon capture technology reduced CO_2 emissions from coal-fired power plants by 10%, it could decrease CO_2 emissions by more than 180 MMT.[27] In addition to their use for carbon capture, advanced membranes can enable more efficient separation of oxygen and hydrogen, which can lower energy penalties in new power plants and coal plant retrofits while also reducing energy use, CO_2 emissions, and fuel costs.

Market Opportunity: Industrial Processes

Gas separation in industrial processes, including the production of oxygen, nitrogen, hydrogen, and carbon monoxide, is energy-intensive. Gas-separating membranes can help reduce some portion of the total 4,519 TBtu of energy consumed by the chemicals sector and the resulting 275 MMT of CO_2 emissions.[28] Specifically, the chemicals and allied products industry consumes about 2,600 TBtu each year for separation processes.[29] According to a study by Lawrence Berkeley National Laboratory, the use of membrane technologies instead of existing separation processes requires 30% less energy.[30] The integration of gas-separating membranes in the chemicals and allied products industry has the potential to significantly reduce energy use and emissions.

Breakthrough Opportunities

The MSE community can advance gas-separating membranes by developing and improving ceramic, metallic, polymeric, and composite membranes. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow gas-separating membranes to make significant contributions toward addressing energy, environmental, and economic needs.

Gas-Separating Membranes

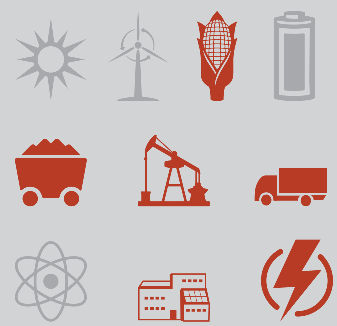
Ceramic Membranes

Ceramic membranes are made from inorganic materials such as alumina, titania, silica, or zirconia and can be used for the separation of hydrogen and oxygen from gas mixtures in industrial processes. They have superior intrinsic properties, including stability at high temperatures, rigid porous structures, long lifetimes, the greatest number of chemical compatibilities, and the widest range of filtration sizes. There are currently two types of ceramic membranes: dense systems with high selectivity and low flux, and porous systems with low selectivity and high flux. The challenge is to maximize both selectivity and flux.

GAPS AND LIMITATIONS TO OVERCOME

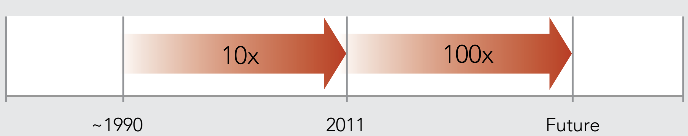
- Microporous ceramic membranes for water-gas shift reaction applications have been difficult to manufacture at large scales and have low hydrothermal resistance.
- Ceramic membranes with high selectivity experience catastrophic cracking when exposed to large temperature gradients.
- It is difficult to simultaneously increase selectivity and flux.

Market Impact

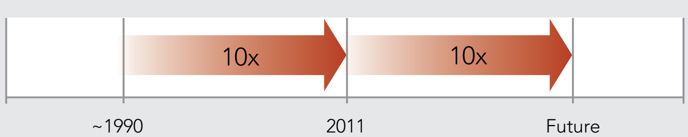


Historical Trends and Future Opportunities

IMPROVEMENT IN CERAMIC MEMBRANE SCALE



IMPROVEMENT IN CERAMIC MEMBRANE FLUX



Ceramic membrane improvements are measured by increases in scale and rates of flux, which result from processing, composition, and materials property improvements. The scale, or size, of ceramic membranes has increased by one order of magnitude (10x) over the past 20 years and is expected to increase again by two orders of magnitude (100x) in the future. The rate of flux in dense ceramic membranes has increased by one order of magnitude (10x) over the past 20 years and has the potential to improve by up to one order of magnitude (10x) in the future.

Scale

- ~1990–2011: 10x improvement
- 2011–Future: 100x improvement

Flux

- ~1990–2011: 10x improvement
- 2011–Future: 10x improvement

Gas-Separating Membranes

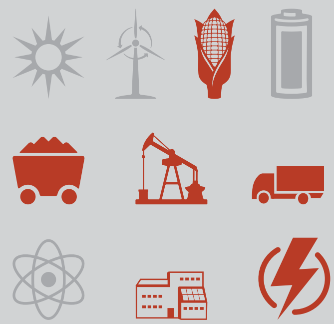
Metallic Membranes

Metallic membranes used for gas separation can be made of various metals, metal alloys, or layered systems (e.g., palladium, tantalum, vanadium, and niobium). Membrane composition and density dictate the size of gases and elements that can pass through a membrane and also determine which gases a membrane can separate. Unlike other membrane materials, dense metallic membranes, such as palladium-based membranes, generally have infinite selectivity for hydrogen, the ability to be manufactured in a variety of configurations, and high thermal and mechanical stability.

GAPS AND LIMITATIONS TO OVERCOME

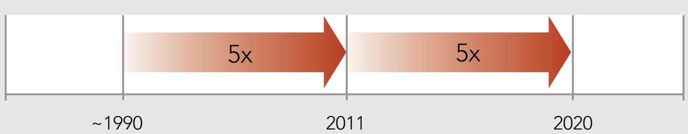
- Metallic membranes, especially palladium-based membranes, are extremely susceptible to contaminants such as sulfur, CO_2, and heavy metals. As materials scientists make thinner metallic membranes to achieve higher levels of flux, these surface-poisoning effects are more detrimental.
- Metallic membranes generally have lower flux compared to polymers and porous ceramics and often encounter chemical degradation in applied environments.

Market Impact

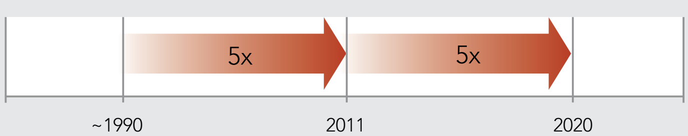


Historical Trends and Future Opportunities

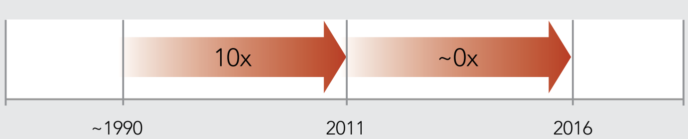
IMPROVEMENT IN METALLIC MEMBRANE THERMAL STABILITY



IMPROVEMENT IN METALLIC MEMBRANE CHEMICAL STABILITY



IMPROVEMENT IN METALLIC MEMBRANE FLUX



Metallic membrane improvements are measured by increases in service life (thermal stability and chemical stability) and performance (rate of flux), which result from processing, composition, and materials property improvements. The thermal and chemical stability of metallic membranes has improved by 5x in the past 20 years from the development of thinner, more stable membranes. Thermal and chemical stability is expected to improve again by up to 5x in the next 10 years. In the past 20 years, flux has improved by one order of magnitude (10x); minimal improvements are expected over the next 5 years.

Thermal/Chemical Stability

- ~1990–2011: 5x improvement
- 2011–2020: 5x improvement

Flux

- ~1990–2011: 10x improvement
- 2011–2016: Minimal improvement

Gas-Separating Membranes

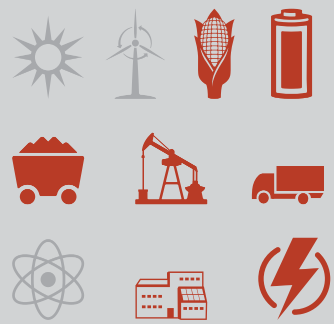
Polymeric Membranes

Polymeric membranes cost less than other materials and are used at lower operating temperatures. Different polymers produce a variety of membrane compositions that range from rubbery to glassy. Rubbery polymeric membranes (e.g., poly dimethyl siloxane) have high permeability and low selectivity while glassy polymeric membranes (e.g., thermoplastic polyimide) have low permeability and high selectivity.

GAPS AND LIMITATIONS TO OVERCOME

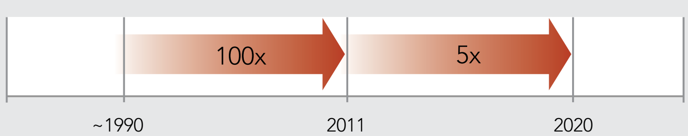
- Polymeric membranes are not suitable for high-temperature applications and are limited to effective operating temperatures of about 120°C.
- An inverse relationship exists between permeability and selectivity in polymeric membranes, which makes it difficult to simultaneously recover and purify gas.

Market Impact

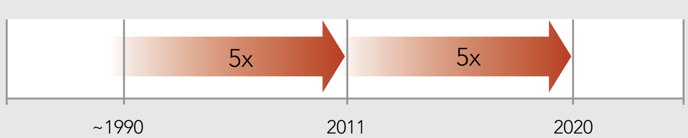


Historical Trends and Future Opportunities

IMPROVEMENT IN POLYMERIC MEMBRANE THERMAL STABILITY



IMPROVEMENT IN POLYMERIC MEMBRANE SELECTIVITY



The thermal stability of polymeric membranes has increased by two orders of magnitude (100x) over the past 10–20 years, making current polymeric membranes stable at about 120°C. Thermal stability is expected to improve by 5x over the next 10 years, adding a few more degrees of stability. Selectivity has improved by 5x over the past 20 years and is expected to improve another 5x over the next 10 years.

Thermal Stability

- ~1990–2011: 100x improvement
- 2011–2020: 5x improvement

Selectivity

- ~1990–2011: 5x improvement
- 2011–2020: 5x improvement

Gas-Separating Membranes

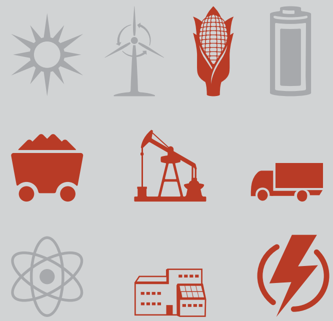
Composite Membranes

Composite membranes cover a wide range of types, all consisting of different ceramics, metals, and polymers either layered on top of each other or integrated into a composite matrix. Different materials can produce different properties depending on the application need. Dense composite membranes made of palladium supported on porous stainless steel substrates are currently in development for high-temperature operations with the goal of providing pure hydrogen. Integrated ceramics and metals for membranes (cermets) are primarily focused on separating hydrogen and oxygen. Polymer membranes with an inorganic phase (mixed-matrix membranes) are focused on light gas separation. Scientists expect composite membranes to play an important role in fuel cells due to their potential for low water retention, high thermal stability, and high mechanical stability.

GAPS AND LIMITATIONS TO OVERCOME

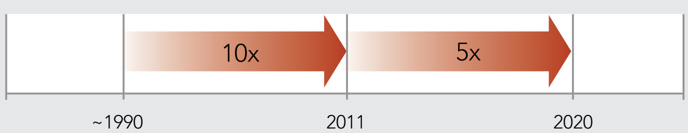
- Metal-particle-reinforced polymer membranes exhibit poor high-temperature stability.
- Ceramic membranes with metal substrates experience corrosion problems due to salt in the membrane capillaries.
- Two-phase materials can experience failure from thermal expansion at high temperatures.

Market Impact

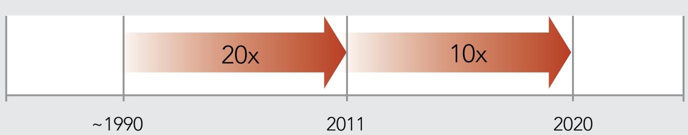


Historical Trends and Future Opportunities

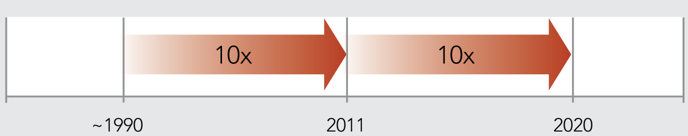
IMPROVEMENT IN COMPOSITE MEMBRANE THERMAL STABILITY



IMPROVEMENT IN COMPOSITE MEMBRANE SELECTIVITY



IMPROVEMENT IN COMPOSITE MEMBRANE FLUX



Advances in manufacturing methods and materials composition have led to improvements in the thermal stability, selectivity, and flux rates of composite membranes. Thermal stability of composite membranes has improved by 10x over the past 20 years and is expected to improve by 5x over the next 10 years. Selectivity has improved by 20x over the past 20 years, and is expected to improve by 10x over the next 10 years. Flux rates have progressed at a rate of 10x over the past 20 years, and will improve at the same rate over the next 10 years.

Thermal Stability

- ~1990–2011: 10x improvement
- 2011–2020: 5x improvement

Selectivity

- ~1990–2011: 20x improvement
- 2011–2020: 10x improvement

Flux

- ~1990–2011: 10x improvement
- 2011–2020: 10x improvement

R&D Priority Activities: Gas-Separating Membranes

To overcome the gaps and limitations within the gas-separating membranes breakthrough opportunities, the MSE community must focus their efforts on increasing understanding of membrane activity, integrating catalysts into membranes, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Crosscutting** • **Develop a fundamental understanding of the trade-off of flux and stability in membrane systems.** • **Identify how materials react under real-world conditions (e.g., degradation mechanisms).** • Conduct a techno-economic assessment of membrane-catalyst integration schemes and applications.
MID TERM (2–5 YEARS)	**Ceramic Membranes** • **Increase the flux of dense ceramic membranes.** **Polymeric Membranes** • **Identify selectivity issues in polymers to decrease the system thickness.** **Crosscutting** • Develop novel processing techniques/automation for low-cost membranes. • Conduct long-term testing of membranes.
LONG TERM (5–10 YEARS)	**Crosscutting** • Conduct predictive modeling of catalysis in membranes.

*The experts identified the **bolded activities** as high priority.

COATINGS

Coatings protect substrates from wear and corrosion in harsh environments (e.g., high-temperature and high-friction environments) to increase system performance and lifetime. Chemical, structural, and processing innovations in coatings can prevent parasitic energy loss in automobiles, reduce corrosion in biomass systems, and improve oxidation resistance in industrial processes. These advances have the potential to increase the energy efficiency of U.S. energy sectors by reducing the need to replace system components frequently. Opportunities in electricity generation and industrial processes provide a quantifiable justification for pursuing R&D of coatings.

Market Opportunity: Electricity Generation

In 2010, the total U.S. energy consumption for electricity generation by the electric power sector was 39,579 TBtu,[31] which was 40% of total U.S. energy consumption.[32] Approximately 88% of electricity was generated using steam turbine engines (61% of generating capacity) or gas turbine engines (27% of generating capacity).[33] Applying thermal coatings to steam and gas turbines and combustor engine components used in power generation plants can enable gas to enter turbines at higher temperatures, improving plant efficiency, decreasing emissions, and reducing fuel costs. For example, a 1% reduction in both coal and natural gas consumed for gas and steam turbine power generation would result in 348 TBtu in energy savings[34] and 22 MMT of reduced CO_2 emissions.[35] A 1% reduction in total fuel consumption by major U.S. investor-owned utilities (which represent only a portion of total U.S. power producers) would result in $400 million in fuel cost savings.

Market Opportunity: Industrial Processes

Corrosion and wear affect the metallic surfaces of industrial equipment and lead to progressive deterioration that can reduce plant efficiency and cause equipment failures and/or plant shutdowns. The annual cost of corrosion in various industrial processes totals $3.7 billion in the petroleum refining industry, $1.7 billion in the chemicals industry, and $5.9 billion in pulp and paper production and processing.[36] Wear-resistant coatings can prevent the damaging effects of corrosion and wear, increase operating efficiency, and prevent the premature replacement of equipment. A 10% reduction in corrosion costs in these three industries could save about $1.1 billion each year.[37]

Breakthrough Opportunities

The MSE community can advance coatings by focusing on wear and tribology and high-temperature/thermal barrier coatings. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow coatings to make significant contributions toward addressing energy, environmental, and economic needs.

Coatings

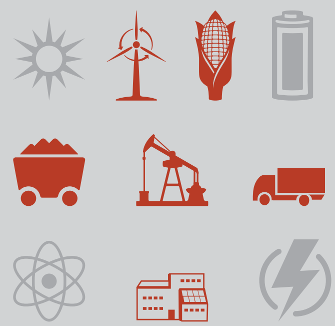
Wear/Tribology

Wear-resistant coatings are ideal for use with system components that operate in high-friction environments. These coatings can help extend component life, reduce the amount of material required for an application, and decrease the use of in-service materials, such as lubricants in machining operations. The use of wear and tribological coatings can save a significant amount of energy when used in metals and materials production. The use of coated tools and dies in these applications enhances productivity and directly helps to lower carbon emissions.[38] Current R&D in wear and tribological coatings is focusing on developing materials designs that enable coatings to be repaired, minimizing the need to refurbish the substrate.

GAPS AND LIMITATIONS TO OVERCOME

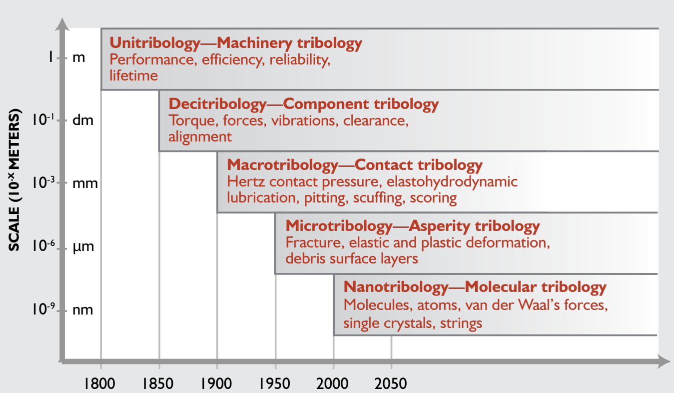
- High coefficient of thermal expansion can lead to separation between the coating and substrate.
- Multi-layer coatings experience major problems with delamination, often due to thermal expansion during tooling. These coatings can also experience interdiffusion, an undesirable mixing of layers that causes failure.

Market Impact



Historical Trends and Future Opportunities

LEVELS OF STRUCTURE OF TRIBOLOGICAL COATINGS



The figure presents a 250-year snapshot of tribological process development from the perspective of scale. These decreases in scale have facilitated the use of tribological coatings in applications with the greatest potential for materials performance improvements. The current focus on nano- or molecular tribology has the potential to increase coatings performance by one order of magnitude. If developed, these advanced coatings, primarily ceramic or ceramic-matrix composites, could improve wear performance, provide better oxidation and corrosion resistance, and achieve extremely low surface friction properties.[39]

Coatings

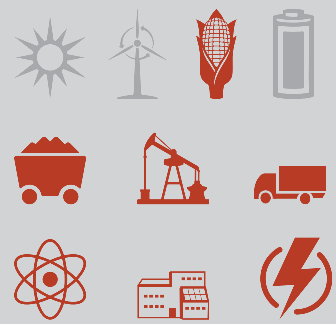
High-Temperature and Thermal Barrier Coatings

Applying a coating with low thermal conductivity to a part surface can drastically lower the temperature of that part during operation. In addition to reducing the occurrence of thermally induced failure mechanisms, thermal barrier coatings reduce the onset of oxidation in metals that typically have high oxidation rates at higher temperatures. This results in longer part life, increased efficiency, and lower costs.

GAPS AND LIMITATIONS TO OVERCOME

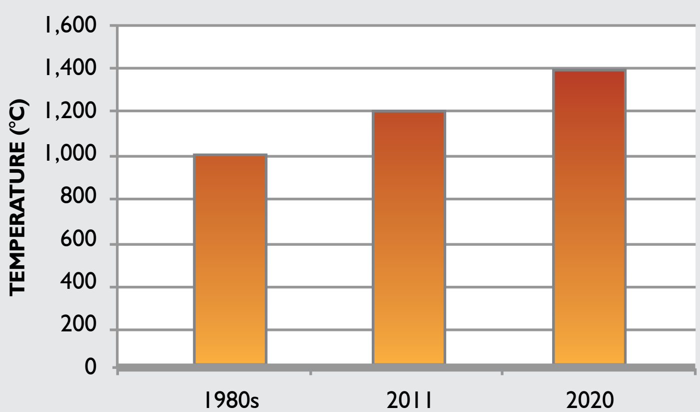
- Multifunctional coatings with high-temperature operating capabilities and corrosion resistance are currently unable to meet all of the industry's needs. Major improvements must be made to simultaneously improve thermal stability and corrosion resistance before multifunctional coatings can be more widely used.
- Thermal barrier coatings have adhesion problems and generally do not bond well to surfaces. Changes in the coating composition or the coating deposition process are necessary to better integrate coated parts into a system.

Market Impact



Historical Trends and Future Opportunities

MAXIMUM TEMPERATURE AT WHICH HIGH-TEMPERATURE COATINGS REMAIN STABLE



In the 1980s, gas turbines benefited greatly from the introduction of high-temperature coatings with thermal stability as high as 1,000°C. Currently, state-of-the-art high-temperature coatings are stable at temperatures up to 1,200°C. Thermal stability is expected to increase to allow temperatures of 1,400°C in the next 10 years.

Thermal Stability

- 1980s: 1,000°C
- 2011: 1,200°C
- 2020: 1,400°C

R&D Priority Activities: Coatings

To overcome the gaps and limitations within the coatings breakthrough opportunities, the MSE community must focus their efforts on developing coatings with higher tolerance to high-wear and corrosive environments, advancing technologies that can detect coating defects, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Wear/Tribology** • **Leverage materials substitution to create multifunctional coatings that are able to withstand high-wear environments.** **Crosscutting** • **Advance research in sensing/health monitoring to detect defects in coatings and prognostic tools.** • Improve understanding of microscale geometry on wetting angles. • Identify key materials for coatings in metal die-casting to withstand high temperatures, wear, etc. • Develop high-emissivity coatings for building/roof applications. • Develop high-speed, low-cost processes for applying coatings.
MID TERM (2–5 YEARS)	**Crosscutting** • **Develop a non-vacuum coating application process.** • **Identify key materials for coatings with high temperature stability, high electrical conductivity, and oxidation resistance.**
LONG TERM (5–10 YEARS)	**Wear/Tribology** • Develop self-lubricating coatings in high-wear applications. **Crosscutting** • Develop self-healing/repairable coatings that can extend component life. • Advance techniques to improve the speed of deposition of physical vapor deposition coatings by one order of magnitude.

*The experts identified the **bolded activities** as high priority.

NOTES

1 John Armor, "A History of Industrial Catalysts," *Catalysis Today* 163, no.1 (2011): 3–9.

2 Prepared by Energetics Incorporated for the U.S. Department of Energy Industrial Technologies Program, "Manufacturing Energy and Carbon Footprint: Chemicals Sector," last updated August 1, 2011, accessed August 29, 2011, http://www1.eere.energy.gov/industry/pdfs/chemicals_footprint.pdf. This energy consumption does not include feedstock energy and off-site electricity generation, transmission, and distribution losses.

3 Maarten Neelis et al., "Approximation of Theoretical Energy-Saving Potentials for the Petrochemical Industry Using Energy Balances for 68 Key Processes," *Energy* 32, no. 7 (2007): 1,104–1,123. 104 TBtu is calculated by assuming a U.S. share of 19% of global non-selectivity losses, totaling 550 TBtu for 42 petrochemical processes cited. The 19% share assumption is based on a 2010 American Chemistry Council estimate of U.S. chemicals production as a share of global chemicals production.

4 Ibid. Calculation: 25% of total selectivity energy losses = 25% * 104 TBtu = 26 TBtu.

5 Ibid. Calculation: 25% of total emissions associated with selectivity losses = 8 $MMTCO_2$ * 25% = 2 $MMTCO_2$.

6 U.S. Census Bureau, "2009 Annual Survey of Manufactures," December 3, 2010, accessed August 29, 2011, http://www.census.gov/manufacturing/asm/index.html. Calculation: $331 million = (26 TBtu/3,195 TBtu) * $40.7 billion.

7 P. Samuel, "GTL Technology—Challenges and opportunities in Catalysis," *Bulletin of the Catalysis Society of India* 2, no. 5, (2003): 82–99.

8 World Bank Global Gas Flaring Reduction Partnership, "Estimated Flared Volumes from Satellite Data, 2006–2010," last updated March 23, 2011, accessed August 29, 2011, http://web.worldbank.org/WBSITE/EXTERNAL/TOPICS/EXTOGMC/EXTGGFR/0contentMDK:22137498~pagePK:64168445~piPK:64168309~theSitePK:578069,00.html.

9 U.S. Energy Information Administration (EIA), *Monthly Energy Review, June 2011* (Washington, DC: EIA, 2011), Table 4.3. Calculation: 8 TBtu = (0.21 bcm/683 bcm) * 24,800 TBtu.

10 Ibid. Calculation: 0.4 $MMTCO_2$ = (0.21 bcm/683 bcm) * 1,285 $MMTCO_2$.

11 Michael Farina for GE Energy, *Flare Gas Reduction: Recent Global Trends and Policy Considerations*, (GE, 2010), 7. Assuming price of $2/MBtu of natural gas, 1 bcm of natural gas is equivalent to $72 million. Calculation: $15 million = (0.21 bcm/2.1 bcm) * $152 million.

12 Neelis et al., "Approximation of Theoretical Energy-Saving Potentials for the Petrochemical Industry," 1,104–1,123; "Ethylene Oxide Catalysts – Hybrid & High Performance Catalysts," CRI Catalysts, accessed June 13, 2011, http://www.cricatalyst.com/home/content/cri_catalyst/catalysts/ethylene_oxide/; Nexant Chem Systems, *PERP Report, Ethylene Oxide / Ethylene Glycol* (White Plains, NY: Nexant, Inc., 2006); Sven Panke, Martin Held, and Marcel Wubbolts, "Trends and Innovations in Industrial Biocatalysis for the Production of Fine Chemicals," *Current Opinion in Biotechnology* 15, no. 4 (2004): 272–279.

13 Uwe Bornscheuer, "Trends and Challenges in Enzyme Technology," in Advances in Biochemical Engineering/Biotechnology, 100 (Berlin: Springer, 2005) 181–203; Christian Wandrey, Andreas Liese, and David Kihumbu, "Industrial Biocatalysis: Past, Present, and Future," Organic Process Research & *Development* 4, no. 4 (2000): 286–290.

14 Neelis et al., "Approximation of Theoretical Energy-Saving Potentials for the Petrochemical Industry," 1,104–1,123; "Ethylene Oxide Catalysts – Hybrid & High Performance Catalysts," CRI Catalysts, accessed June 13, 2011, http://www.cricatalyst.com/home/content/cri_catalyst/catalysts/ethylene_oxide/; Nexant Chem Systems, *PERP Report, Ethylene Oxide / Ethylene Glycol* (White Plains, NY: Nexant, Inc., 2006); Sven Panke, Martin Held, and Marcel Wubbolts, "Trends and Innovations in Industrial Biocatalysis for the Production of Fine Chemicals," *Current Opinion in Biotechnology* 15, no. 4 (2004): 272–279; William H. Scouten and Gene Petersen, *New Biocatalysts: Essential Tools for a Sustainable 21st Century Chemical Industry* (Washington, DC: Council for Chemical Research, 2000).

15 U.S. Energy Information Administration (EIA), *Monthly Energy Review, May 2011* (Washington, DC: EIA, 2011), Table 2.6, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_13.pdf.

16 Solar Energy Industries Association and GTM Research, *U.S. Solar Market Insight™ 2010 Year in Review: Executive Summary*, (Washington, DC: SEIA/GTM Research, April 2011), www.seia.org/galleries/pdf/SMI-YIR-2010-ES.pdf.

17 Calculation: 396 TBtu = 1% * 39,579 TBtu.

18 U.S. Energy Information Administration (EIA), *Monthly Energy Review, May 2011* (Washington, DC: EIA, 2011), Table 12.6, http://www.eia.gov/totalenergy/data/monthly/pdf/sec12_9.pdf; Ibid, Table 2.6, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_13.pdf. Calculation: 23 MMT = 1% * (39,579 TBtu / (39,579 TBtu - 13 TBtu)) 2,271 MMT. (CO_2 emissions are for the electric power sector; solar technologies do not produce emissions when generating electricity.)

19 U.S. Energy Information Administration (EIA), *Electric Power Annual* (Washington, DC: EIA, April 2011), Table 8.1, http://www.eia.doe.gov/cneaf/electricity/epa/epat8p1.html; U.S. Energy Information Administration (EIA), Monthly Energy Review, May 2011 (Washington, DC: EIA, 2011), Table 2.6, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_13.pdf. Calculation: $402 million = 1% (39,579 TBtu / (39,579 TBtu - 13 TBtu)) * $40.2 billion in fuels purchased by major investor-owned utilities. (Based on average fuel costs for non-solar production; solar technologies do not incur fuel costs while generating electricity.)

20 National Renewable Energy Laboratory, "Best Research-Cell Efficiencies," revised June 2011, accessed June 13, 2011, www.nrel.gov/pv/thin_film/docs/kaz_best_research_cells.ppt.

21 Ibid.

22 International Energy Agency (IEA), *Technology Roadmap—Concentrating Solar Power* (Paris, France: OECD/IEA, 2010), http://www.iea.org/papers/2010/csp_roadmap.pdf.

23 Note: It was the consensus of the experts that MSE advances have a greater opportunity to improve gas-separating membranes than liquid-separating membranes. As a result, liquid-separating membranes have not been included in this report.

24 U.S. Energy Information Administration (EIA), *Monthly Energy Review, May 2011* (Washington, DC: EIA, 2011), Table 2.6, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_13.pdf.

25 Ibid.

26 The Minerals, Metals, & Materials Society (TMS) in support of the U.S. Department of Energy Industrial Technologies Program, *Linking Transformational Materials and Processing for an Energy-Efficient and Low-Carbon Economy: Creating the Vision and Accelerating Realization* (Washington, DC: TMS, 2010).

27 1,828 $MMTCO_2$ are released from coal-fired power plants. Calculation: 180 MMT = 10% * 1,828 $MMTCO_2$

28 Prepared by Energetics Incorporated for the U.S. Department of Energy, Industrial Technologies Program, "Manufacturing Energy and Carbon Footprint: Chemicals Sector," last updated August 1, 2011, accessed August 29, 2011, http://www1.eere.energy.gov/industry/pdfs/chemicals_footprint.pdf. Calculation: 275 $MMTCO_2$/4,519 TBtu = 0.061 $MMTCO_2$/TBtu.

29 Ernst Worrell, Lynn Price, and Christina Galitsky, *Emerging Energy-Efficient Technologies in Industry: Case Studies of Selected Technologies*, (Berkeley, CA: Lawrence Berkeley National Laboratory, 2004), http://ies.lbl.gov/iespubs/54828.pdf.

30 Ibid.

31 U.S. Energy Information Administration (EIA), *Monthly Energy Review, May 2011* (Washington, DC: EIA, 2011), Table 2.6, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_13.pdf.

32 Ibid. Table 2.1, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_3.pdf.

33 U.S. Energy Information Administration, Form EIA-860, "Annual Electric Generator Report," http://www.eia.gov/cneaf/electricity/page/capacity/existingunits2008.xls.

34 U.S. Energy Information Administration (EIA), *Monthly Energy Review,* May 2011 (Washington, DC: EIA, 2011), Table 2.1, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_3.pdf; EIA, Form EIA-860, "Annual Electric Generator Report," http://www.eia.gov/cneaf/electricity/page/capacity/existingunits2008.xls. Calculations: 348 TBtu = 39,579 TBtu * (88%) * 1% (calculation assumes equal capacity factors of various generation Technologies); 22 $MMTCO_2$ = 1% * (1,828 $MMTCO_2$ + 399 $MMTCO_2$).

35 U.S. Energy Information Administration (EIA), *Electric Power Annual* (Washington, DC: EIA, April 2011), Table 8.1, http://www.eia.doe.gov/cneaf/electricity/epa/epat8p1.html.

36 Gregory Ruschau and Mohammed A. Al-Anezi, for CC Technologies Laboratories, under a cooperative agreement with the Federal Highway Administration and NACE International, "Appendix S: Oil and Gas Exploration and Production," in *Corrosion Costs and Preventive Strategies in the United States*, (Dublin, OH: CC Technologies Laboratories, September 2001), Si–S14, http://www.corrosioncost.com/pdf/oilgas.pdf.

37 Calculation: $1.1 billion = ($3.7 billion + $1.7 billion + $5.9 billion) * 10%.

38 J. Lin, et al., "Design Methodology for Optimized Die Coatings: The Case for Aluminum Pressure Die-Casting: Invited paper B7-1-1, ICMCTF, presented Monday May 2nd, 2005, San Diego," *Surface and Coatings Technology* 201, no. 6 (2006): 2,930–2,941.

39 A. Matthews, S. Franklin, and K. Holmberg, "Tribological Coatings: Contact Mechanisms and Selection," *Journal of Physics D: Applied Physics* 40, no. 18 (2007): 5,463–5,475.

IV. MATERIALS INTEGRATION IN CLEAN ENERGY SYSTEMS

Current and emerging energy systems are composed of different classes of materials that must work together to achieve desired system structure and functionality. These components must be joined in a way that maintains the desired properties of each material and prevents defects (e.g., improper bonding and contamination from unclean parts) that can jeopardize system performance.

Materials science and engineering (MSE) advances have the potential to enable the integration of new materials and the effective interfacing of materials combinations as systems become more complex and service environments become more demanding. Ultimately, improvements in material properties and joining processes can reduce the cost, environmental impact, and energy requirements of energy generation, storage, and use across U.S. energy sectors, particularly in transportation technologies, electricity generation and storage, and the oil and gas industry.

The following pathways provide a guide for research and development (R&D) in the area of materials integration in clean energy systems:

- Next-Generation Batteries and Fuel Cells
- Joining Processes for Multi-Material Structures
- Composites with Structural Capabilities

NEXT-GENERATION BATTERIES AND FUEL CELLS

Energy storage technologies such as next-generation batteries and fuel cells are key enablers of electric grid modernization and integral to the successful commercialization and adoption of electric vehicles. Increasing the energy density, power capacity, efficiency, life, and safety of these technologies and reducing their cost and weight can lead to the development of more cost-effective, efficient, and environmentally friendly energy storage products. As a result, these improved products can enable the widespread integration of renewable energy, reduce widespread power outages, provide substitutes for transmission and distribution upgrades, and make it possible for electric and fuel cell vehicles to travel farther between recharging/refueling.

Market Opportunity: Transportation

In 2008, the tank-to-wheel energy consumption of light-duty vehicles totaled 16,436 trillion British thermal units (TBtu).[1] The U.S. transportation sector tank-to-wheel emissions totaled 1,790 million metric tons (MMT) of carbon dioxide (CO_2) in 2008, of which 1,113 MMT of CO_2 were emitted by light-duty vehicles.[2]

According to a study by the Massachusetts Institute of Technology (MIT), future battery-powered electric vehicles and fuel cell-powered hydrogen vehicles could decrease the energy consumed by light-duty vehicles because they can have lower well-to-wheel energy intensities than conventional vehicles. The study estimates that, in 2030, battery-powered vehicles could have well-to-wheel intensities of 2,715 Btu per mile[3] and fuel cell vehicles could have well-to-wheel intensities of 2,075 Btu per mile.[4] These numbers are 47% and 59% lower, respectively, than the well-to-wheel intensities of a 2006 Toyota Camry with a 2.5-liter engine, which served as the MIT study's baseline.[5]

The MIT study estimates that future battery-powered electric vehicles could have well-to-wheel emissions of 186 grams of CO_2 per mile in 2030,[6] a 54% reduction compared to the 2006 Toyota Camry, which emits 405 grams of CO_2 per mile.[7] Future fuel cell vehicles could have well-to-wheel emissions of 144 grams of CO_2 per mile[8]—a 64% reduction in CO_2 emissions per mile over the study's baseline.[9]

Market Opportunity: Electricity Generation

Total U.S. energy consumption for electricity generation by the electric power sector was 39,579 TBtu in 2010,[10] with about two-thirds of this energy (27,028 TBtu) generated from fossil fuels, mostly coal (19,133 TBtu).[11] Emphasis on cleaner energy and decreased reliance on fossil fuels and other nonrenewable sources has drawn greater attention to renewable sources for electricity generation. While beneficial from an environmental standpoint, the demand for renewables-generated power can present additional challenges for the electric grid. Energy storage technologies are well positioned to help offset the intermittent electricity generation from renewable sources and could play an integral role in their increased adoption. This would help displace some portion of the 27,028 TBtu of fossil fuels that are consumed by the electric power sector, as well as the 2,271 MMT of CO_2 associated with this energy use.[12]

Breakthrough Opportunities

The MSE community can advance batteries and fuel cells by developing and improving technologies for short-duration stationary storage and conversion, long-duration stationary storage and conversion, and transportation applications. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow next-generation batteries and fuel cells to make significant contributions toward addressing energy, environmental, and economic needs.

Next-Generation Batteries and Fuel Cells

Short-Duration Stationary Storage and Conversion

Stationary electrical energy storage technologies used for short-duration storage (milliseconds to two hours) and conversion applications have the potential to alleviate momentary electricity interruptions and facilitate the integration of significant amounts of renewable energy. Such advances will help to ensure the availability of reliable and affordable electricity.

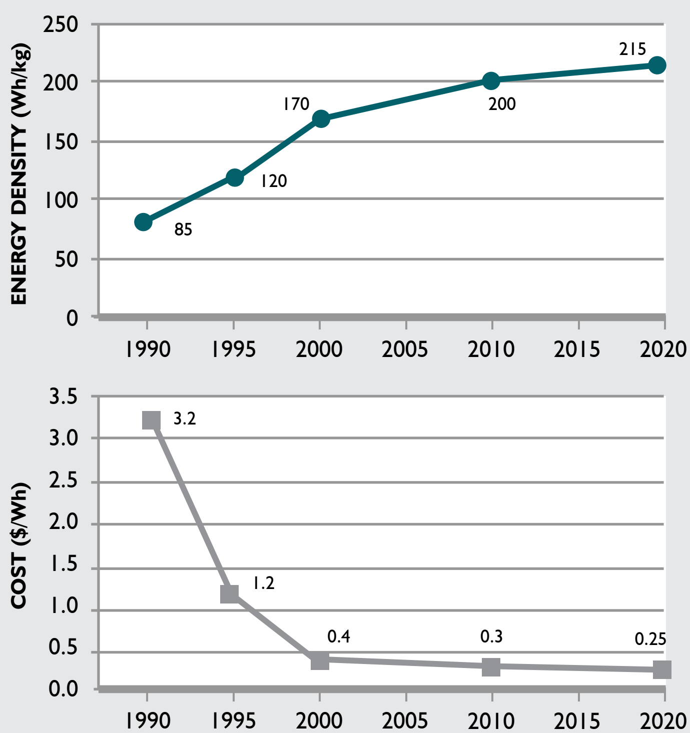
GAPS AND LIMITATIONS TO OVERCOME

- Materials scientists have an inadequate understanding of solid electrolyte interfaces, high ionic-conductivity electrolytes at room temperature, and low environmental impact materials.

Market Impact

Historical Trends and Future Opportunities

LITHIUM-ION BATTERY COST AND ENERGY DENSITY



The historical trends and future improvements in stationary storage technologies can be represented by advances in lithium-ion batteries in consumer electronics. Over the past 20 years, lithium-ion batteries in consumer electronic cells have drastically changed in cost and energy density. Energy density has increased from 85 watt-hours per kilogram (Wh/kg) to 200 Wh/kg, while cost has decreased from \$3.2/Wh to \$0.3/Wh. In the next 10 years, energy density is expected to increase to about 215 Wh/kg, and cost is expected to potentially decrease to \$0.25/Wh.[13]

Specific Energy

- 1991: 85 Wh/kg
- 2010: 200 Wh/kg
- 2020: 215 Wh/kg

Cost

- 1991: \$3.2/Wh
- 2010: \$0.3/Wh
- 2020: \$0.25/Wh

Next-Generation Batteries and Fuel Cells

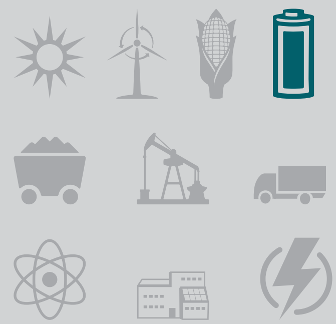
Long-Duration Stationary Storage and Conversion

Stationary electrical energy storage will help ensure reliable and affordable electricity. Several long-duration storage and conversion applications (longer than two hours) can help the electric grid meet peak electricity demand, postpone or avoid upgrades to grid infrastructure, and facilitate the integration of significant amounts of renewable energy.

GAPS AND LIMITATIONS TO OVERCOME

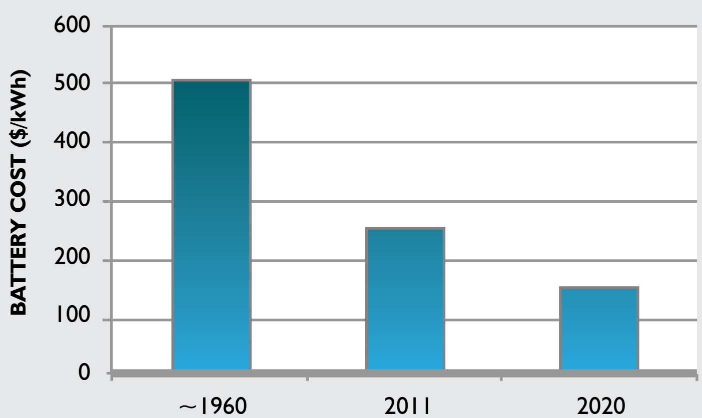
- Materials scientists have an inadequate understanding of solid electrolyte interfaces, high ionic-conductivity electrolytes at room temperature, and low environmental impact materials.
- Available battery materials, even those capable of moderate performance, are cost-prohibitive and not amenable to simple large-scale processing. In particular, low-cost materials for large-scale energy storage and processing are not available.

Market Impact



Historical Trends and Future Opportunities

BATTERY COST OF LONG-DURATION ENERGY STORAGE



Battery cost, which is largely driven by manufacturing scale-up, process development, and improved use of active materials, is a key metric for measuring the improvement of long-duration storage technologies. Over the past 50 years, the average cost of long-duration energy storage technologies has dropped from about $500 per kilowatt hour (kWh) to $250/kWh. The target cost for long-term energy storage in the next 10 years is $150/kWh.[14]

Battery Cost ($/kWh)

- ~1960: $500/kWh
- 2011: $250/kWh
- 2020: $150/kWh

Next-Generation Batteries and Fuel Cells

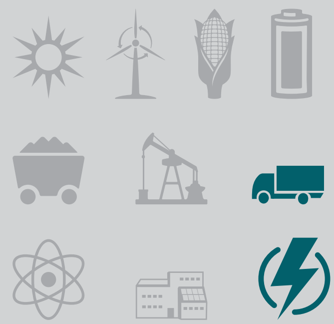
Transportation

Advanced energy storage and conversion systems such as batteries and fuel cells can help define the future of transportation. Current electric vehicles range from mild hybrids to all-electric vehicles, and fuel cell vehicles are powered by hydrogen. While batteries and fuel cells used for public and private transportation require major materials science advances to lower cost, improve safety, and increase energy output and storage capacity, these technologies are gaining market share at the expense of traditional gasoline- and diesel-powered vehicles due, in part, to significant cost reductions.

GAPS AND LIMITATIONS TO OVERCOME

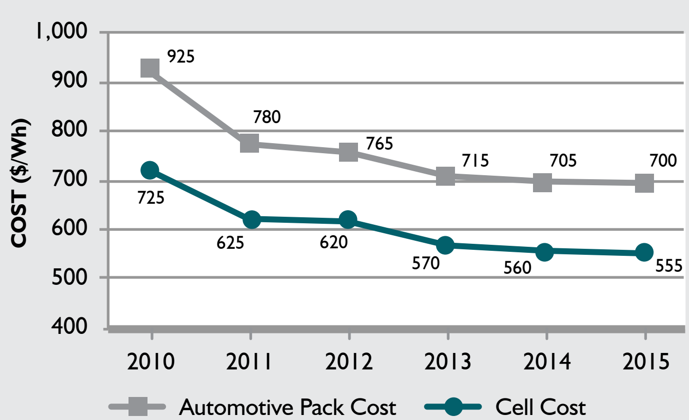
- Lead-acid batteries have low specific energy, poor cold-temperature performance, and short life cycles.
- Batteries such as lithium-polymer, nickel-metal hydride, and lithium-ion need to be more cost-effective to enable widespread adoption in the U.S. passenger vehicle sector at current petroleum prices.
- Nickel-metal hydrides have high self-discharge and heat generation at high temperatures, and suffer from hydrogen loss.
- Fuel cell vehicles require a new propulsion system and new infrastructure.
- The positive and negative electrodes on automotive lithium-ion batteries are currently cost-prohibitive and heavy.

Market Impact



Historical Trends and Future Opportunities

LARGE-FORMAT LITHIUM-ION COSTS



Lithium-ion systems are representative of electric vehicle batteries. Over the next 5 years, the costs of both the automotive pack and the battery cell of these large-format storage technologies are expected to decrease. Cell costs are expected to decrease from $725/Wh to $555/Wh and automotive pack costs are expected to decrease from $925/Wh to $700/Wh.[15]

Cell Cost ($/Wh)

- 2010: $725/Wh
- 2015: $555/Wh

Automotive Pack Cost ($/Wh)

- 2010: $925/Wh
- 2015: $700/Wh

R&D Priority Activities: Next-Generation Batteries and Fuel Cells

To overcome the gaps and limitations within next-generation batteries and fuel cells breakthrough opportunities, the MSE community must focus their efforts on advancing high-speed processing techniques, developing new battery component materials, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Short-Duration Storage and Conversion** • **Advance high-speed stacking for lithium-ion batteries so that prismatic cells consisting of layers of electrodes can be manufactured more quickly.** • **Develop roll-to-roll vacuum drying and advance water management for lithium-ion cell assembly.** **Long-Duration Storage and Conversion** • **Develop low-cost fabrication of redox flow battery systems.** **All Stationary Storage and Conversion (Short- and Long-Duration)** • **Develop low-cost, mass fabrication of oxide membranes for sodium-sulfur batteries.** • Develop effective, durable seals between dissimilar materials (e.g., steel alloys to ceramics) in high-temperature electrochemical devices. • Reduce the cost of the balance-of-system (i.e., incorporate low-cost and reliable housing, cooling mechanisms, controls, electronics, etc.). • Advance high-speed electrode quality assurance. **Transportation** • **Improve cell formation and grading for lithium-ion cells to decrease the footprint and capital expenditures associated with the need to charge batteries after they are assembled.** **Crosscutting** • **Develop high-speed, 100% inspection, nondestructive evaluation techniques for battery joints (e.g., aluminum and copper), packs, and modules.** • Develop thick electrodes (thicker than 100 micrometers) to increase the energy density of batteries. • Conduct nondestructive evaluation and closed-loop feedback during the coating process.
MID TERM (2–5 YEARS)	**Short-Duration Storage and Conversion** • **Reduce or eliminate the use of organic solvents (e.g., lithium-ion electrode fabrication).** • Develop low-cost, high-efficiency heat exchangers and insulators for solid oxide fuel cells and high-temperature sodium batteries. **Long-Duration Storage and Conversion** • Develop low-cost optimized membranes and separators for redox flow batteries. • Develop redox chemistries with higher concentrations and increased stability. **Transportation** • Identify materials (e.g., better dielectrics) for higher-voltage isolation in automotive applications to reduce the mass of current bus and electric motors and to reduce waste heat. **Crosscutting** • **Develop new metal or ceramic surfaces with controlled porosity for direct bonding of polymers or elastomers that can improve adhesion.** • **Reduce the use of inactive materials, expanding beyond thick electrodes.** • **Identify processes for functionalizing surfaces for polymer chemical bonding.** • Reduce heat treatment temperature of raw materials.

LONG TERM (5–10 YEARS)	**Short-Duration Storage and Conversion** • Develop bipolar cell sealing and filling, primarily for lithium-ion batteries. **All Stationary Storage and Conversion (Short- and Long-Duration)** • Identify next-generation manufacturing for flexible, all solid-state batteries. • Develop co-extruded electrode and electrolyte fabrication. **Crosscutting** • Fabricate load-bearing/structural batteries.

*The experts identified the **bolded activities** as high priority.

JOINING PROCESSES FOR MULTI-MATERIAL STRUCTURES

Joining processes, which use lasers, electron beams, adhesives, heat treatments, or chemical reactions to connect dissimilar materials, are a key enabler of the mass production and increased use of multi-material structures, particularly for use in extreme (e.g., high-temperature and corrosive) operating environments. Increasing the robustness, life, and strength of joining processes will preserve core materials properties and eliminate defects, improving the performance of multi-material systems and structures and potentially increasing the energy efficiency of U.S. energy sectors. Opportunities for these advances to enable reduced vehicle weight and more effective cladding for oil and gas extraction provide quantifiable justification for pursuing R&D of joining processes for multi-material structures.

Market Opportunity: Transportation

The U.S. transportation sector consumed 28,103 TBtu in 2008, which was 28% of total U.S. energy consumption.[16] Advanced joining processes could join vehicle structures (e.g., frames and bodies) more seamlessly and enable the integration of lighter-weight materials with more desired properties, such as the ability to withstand high temperatures near the vehicle engine. A study from MIT estimates that for every 10% reduction in vehicle weight, fuel economy could increase by 6% for cars and 8% for light-duty trucks.[17] Considering that the annual U.S. energy consumption of cars and light-duty trucks is above 16,000 TBtu,[18] if joining processes could enable a 10% reduction in the weight of cars and light-duty trucks, such advances could save 1,060 TBtu of energy,[19] 72 MMT of CO_2 emissions,[20] and over $34 billion in fuel costs each year (assuming an estimated cost of motor gasoline of $3.98 per gallon or $31.84 per million Btu [MBtu]).[21]

Market Opportunity: Oil and Gas

A 2001 study from CC Technologies Laboratories, Inc. estimated that the annual cost of corrosion in the U.S. oil and gas sector is $1,372 million.[22] Cladding, a joining process that bonds two or more material layers to form a composite,[23] can reduce these corrosion costs by covering materials that are susceptible to corrosion with materials that have a higher resistance to corrosion.[24] Using the 2001 estimated cost of corrosion for downhole tubing expenses ($463 million) as an example, a 10% reduction in downhole tubing corrosion costs would save $46.3 million each year.[25] In addition, the increased corrosion resistance of downhole tubing from this cladding process could reduce the need to manufacture new downhole tubes, which would yield energy savings and reduce emissions.

Breakthrough Opportunities

The MSE community can advance joining processes for multi-material structures by developing and improving adhesive bonding, solid-state bonding, and design data and testing. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow joining processes for multi-material structures to make significant contributions toward addressing energy, environmental, and economic needs.

Joining Processes for Multi-Material Structures

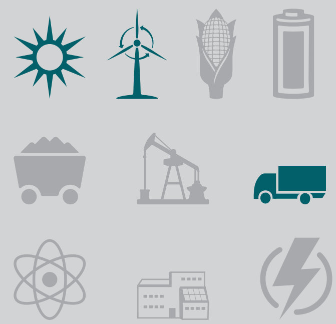
Adhesive Bonding

Adhesive bonding joins new materials, such as composites, and dissimilar materials in one assembly using an adhesive substance that is typically made of natural or synthetic polymer. This technique is quick and affordable, provides good strength and fatigue resistance, and saves weight compared to alternative joining techniques, such as bolting using heavy metal joiners. For example, adhesively bonding polymer matrix composites to metals and dissimilar polymers is a key enabling technology for vehicle lightweighting.

GAPS AND LIMITATIONS TO OVERCOME

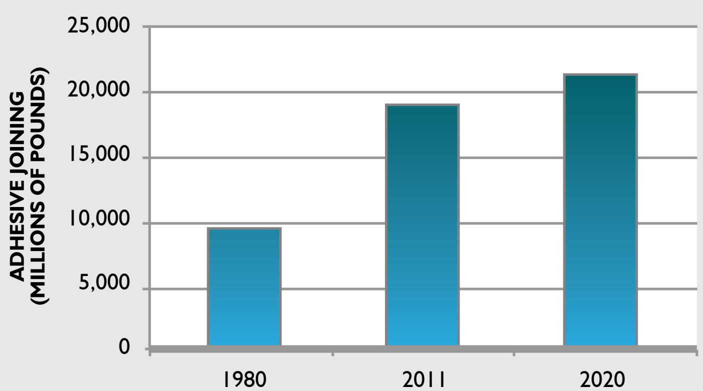
- There are no current methods to predict bond life, nor are there nondestructive evaluation methods to ensure a level of bond integrity. Current nondestructive evaluation methods can only detect the location of a bond line.
- Most polymer adhesives are unstable beyond 350°F.
- Surface insensitive adhesives cannot currently mitigate the need for expensive surface preparation of the materials being bonded.
- There is currently no industry-wide design database for adhesive joining that includes proper finite element modeling techniques.

Market Impact



Historical Trends and Future Opportunities

ADOPTION OF ADHESIVE JOINING IN THE AUTOMOTIVE SECTOR



Adoption rate demonstrates the increased reliance on adhesives as a joining mechanism. Adhesives were adopted at the rate of 9,000 million (MM) lbs in 1980, with 18,500MM lbs of adhesive joining in use today. This value is expected to increase to 20,700MM lbs over the next 10 years.[26]

Adoption Rate

- 1980: 9,000MM lbs
- 2011: 18,500MM lbs
- 2020: 20,700MM lbs

Joining Processes for Multi-Material Structures

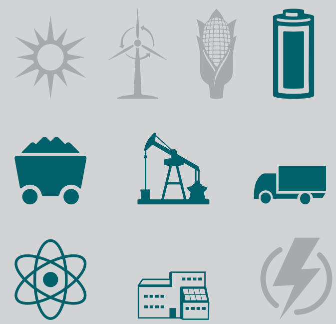
Solid-State Bonding

Solid-state bonding, including all variants of friction welding (e.g., direct drive, inertia, stir, and linear), resistance processing (e.g., upset, flash, and projection welding), thermo-compression welding, hot-press welding, diffusion bonding, and auto-vacuum welding, forms bonds between two nominally flat materials using material flow and elevated pressures and temperatures. The desired result is a strong, reliable interface without discontinuities or solidification-related microstructural changes. Solid-state bonding technologies can join a wide range of materials, including dissimilar materials combinations, at productivity levels that are appropriate for mass-produced structures.

GAPS AND LIMITATIONS TO OVERCOME

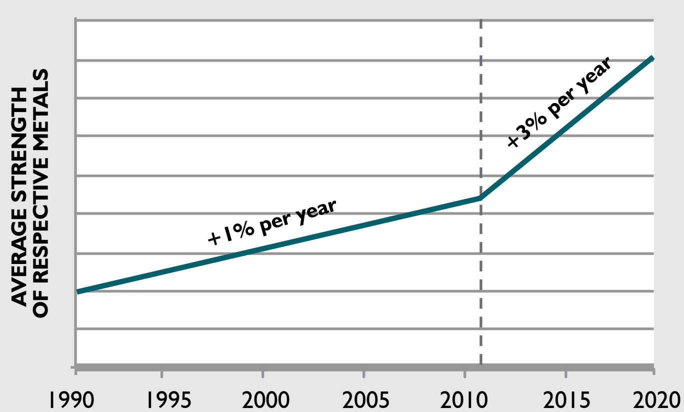
- Nondestructive evaluation of solid-state welds is the single biggest impediment to more broad-based applications of solid-state bonding.
- In-process monitoring has not yet been developed to allow quality assurance at high productivity levels.
- Capital equipment costs are currently high, requiring the development of new equipment configuration strategies.
- The formation of deleterious intermetallic phases limits joint performance.
- Materials scientists lack understanding of the specific processing features (e.g., joint design, upset, upset speed, and heating time) that are unique for each material system.
- Materials scientists have not addressed the role of secondary shielding to prevent contamination or oxidation.

Market Impact



Historical Trends and Future Opportunities

AVERAGE STRENGTH OF METALS



Over the past 10–20 years, the average strengths of aluminum, titanium, and stainless steels have increased by roughly 1% per year. The average strength of revolutionary compositions of amorphous and multi-phase metals is expected to increase by about 3% per year for the next 10 years. Solid-state bonding will need to continue to advance at a similar rate to take full advantage of these base metal improvements.[27]

Average Strength of Respective Metals

- 1990–2011: 1% per year
- 2011–2020: 3% per year

Joining Processes for Multi-Material Structures

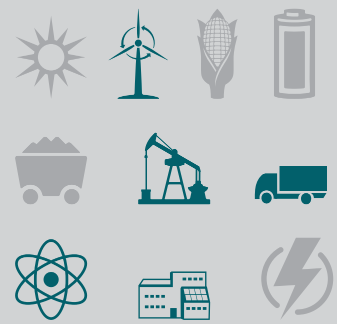
Design Data and Testing

Design data and testing is required for the statistical analysis of material properties. Designers use these analyses to develop fail-safe design approaches and to approximate failure risk. Databases on dissimilar material properties for specific joining process are also necessary for designing structures. Materials scientists use design data and testing to establish the statistical variation of a given set of best practices for integrating dissimilar materials into a system using joining processes.

GAPS AND LIMITATIONS TO OVERCOME

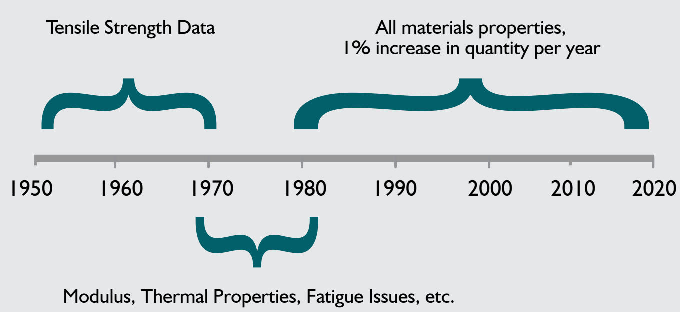
- Specific tests have not yet been defined that address both material combinations and specific joining approaches.
- Specific failure criteria that address static, fatigue, and crash modes have not been developed for multi-material systems.
- Methodologies for multi-material systems have not been defined to allow the integration of failure criteria into vehicle designs.
- Processing variations can potentially lead to wide variations in joint performance. Approaches must be defined that assess process robustness and use the data gathered to create statistically based design guidelines.
- The feasibility of joining dissimilar metallic materials and metal-matrix composites by friction stir welding (FSW) has been demonstrated, but the mechanical property evaluation is limited. No reported studies have progressed to the level of design allowables.
- Localized stress-corrosion in dissimilar alloys of the same system (e.g., 2024 and 7050 aluminum), galvanic corrosion in strongly dissimilar systems (e.g., 2024 aluminum and Ti-6Al-4V [titanium-aluminum-vanadium]), and mismatching of the coefficient of thermal expansion in strongly dissimilar systems are challenges in testing multi-material systems.

Market Impact



Historical Trends and Future Opportunities

TRENDS IN MATERIALS PROPERTY DATA COLLECTION



Prior to 1970, there was an emphasis on studying tensile strength data. Since 1970, this emphasis has decreased and materials scientists have begun to study other materials properties, such as modulus, thermal, and fatigue characteristics. Since the 1980s, all materials properties data has increased in quantity by roughly 1% per year and is expected to increase at this rate for the next 10 years.[28]

R&D Priority Activities: Joining Processes for Multi-Material Structures

To overcome the gaps and limitations within the joining processes for multi-material structures breakthrough opportunities, the MSE community must focus their efforts on improving joining processes, advancing testing and nondestructive evaluation approaches, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

<table>
<tr>
<td>NEAR TERM (0–2 YEARS)</td>
<td>
Adhesive Bonding

Develop a manufacturing process and design guidelines for hybrid bonding that may include combining adhesives with welding or mechanical fasteners, or using graded adhesives to combine mechanical properties more effectively.

Solid-State Bonding

Develop low-cost, flexible, mass-production joining processes for multi-material automotive sheet and tubular structures (e.g., aluminum to steel), and develop design data and fatigue data for each joining process.
Develop joining processes for high-temperature, oxide-dispersion-strengthened materials in extreme environments.
Develop process and equipment requirements for solid-state welding of similar and dissimilar material systems.
Develop FSW for the re-racking of composites (e.g., aluminum to boron carbide) used in nuclear fuel storage pools to extend plant life.
Develop automated finish machining of metal additive manufacturing.
Develop residual stress and distortion control for large-puddle metal additive manufacturing.
Automate nondestructive testing for friction joining and metal additive manufacturing processes (e.g., FSW and linear friction welding [LFW]).
Automate friction joining processes (e.g., FSW and LFW).

Design Data and Testing

Create specific testing protocols for dissimilar materials joints, based on material combinations and assembly processes.
Define a failure criterion strategy for dissimilar materials joints that can be integrated into vehicle structural analyses.

Crosscutting

Fabricate localized metal-matrix composites (MMCs) and reinforce ceramic matrix composites (e.g., aluminum castings with ceramics) to reduce vehicle weight by 5%–7%.

</td>
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MID TERM (2–5 YEARS)	

MID TERM (2–5 YEARS)

Adhesive Bonding

- **Fabricate new metal or ceramic surfaces with controlled porosity for direct bonding of polymers or elastomers to improve adhesion of materials.**
- **Develop processes for producing functional surfaces that can improve the integrity of polymer chemical bonding.**
- **Develop low-cost (50% cost reduction) surface adhesives (e.g., prepolymers, epoxies, ultraviolet cure, thermal cure, and laser cure) that are not sensitive to substrate contamination.**
- Create highly conductive adhesives for photovoltaic bus connections.
- Develop adhesives for the manufacture of heat exchangers.

Solid-State Bonding

- Develop nondestructive evaluation strategies, including process monitoring and secondary joint inspection, for solid-state joints.
- Develop portable variants of solid-state technologies to enable multi-materials vehicle construction.
- Develop FSW of aluminum-aluminum, aluminum-magnesium, and nonferrous-ferrous (e.g., nickel-steel) for use in nuclear applications.
- Create in-situ composites through FSW that contain particles (nano- and micro-scale particles) capable of controlling weld properties.
- Develop co-extrusion of dissimilar materials with significantly different flow stress at extrusion temperatures.
- Identify low-cost methods to incorporate titanium into heat exchangers, enabling increased system performance, especially in corrosive environments.

Design Data and Testing

- Develop guidelines and a database for performance mechanisms (e.g., damage, fatigue, failure, and repair of welds) and loading requirements of multi-material joints that are made by different joining methods and joint designs.
- Study process robustness to provide a statistical database for dissimilar joint performance.
- Create numerical interfaces to facilitate the integration of defined failure criteria into standardized structural performance models.

Crosscutting

- **Measure and analyze post-weld heat treatment properties and residual stresses in solid-state FSW in real time and after processing (Solid-State Bonding, Design Data and Testing).**
- **Develop an integrated computational materials engineering process model for solid-solid joining that incorporates residual stress, diffusion, microstructure evolution, and mechanical properties and interlayers (Solid-State Bonding, Design Data and Testing).**
- **Develop high-speed and reliable nondestructive evaluation techniques to evaluate bond quality in similar and dissimilar materials.**
- **Develop low-cost, mass-production joining processes for multi-material automotive sheet and tubular structures (e.g., steel with composites, aluminum, and magnesium) (Adhesive Bonding, Solid-State Bonding).**
- Join high-temperature materials to lower-temperature materials (e.g., ceramics to metals, metals to polymers, and refractories to metals) (Adhesive Bonding, Solid-State Bonding).
- Design a database for adhesive joining that includes proper finite element modeling techniques (Adhesive Bonding, Design Data and Testing).
- Develop processes, analysis methods, and fracture methodologies for friction-joined dissimilar materials.

LONG TERM (5–10 YEARS)	**Adhesive Bonding** • Develop de-bondable adhesives for the end-of-life recycling of hybrid structures to mitigate the loss of the embodied energy of component materials. **Solid-State Bonding** • Integrate ceramics in extreme environments (e.g., silicon carbide joining) for energy applications, including nuclear power and heat exchangers. • Identify metal-ceramic joining solutions (e.g., gradient interfaces) for forming robust bonds that minimize residual stress.

*The experts identified the **bolded activities** as high priority.

COMPOSITES WITH STRUCTURAL CAPABILITIES

Composites can achieve properties that are superior to those of any of their individual components. Their high-strength and lightweight characteristics make them a preferred alternative to metals in certain structural components, including load-bearing structures composed of two or more materials. Decreasing the cost and weight of composites and increasing their stiffness, strength, and resilience can boost their implementation and will increase the energy efficiency of U.S. energy sectors. Opportunities in heat exchanger applications and vehicle lightweighting provide quantifiable justification for pursuing R&D of composites with structural capabilities.

Market Opportunity: Industrial Processes (Heat Exchangers)

According to a 2008 report from the U.S. Department of Energy, unrecovered waste heat accounts for 1,478 TBtu of the 8,400 TBtu consumed by select manufacturing processes each year.[29] Composites integrated into heat exchangers could be used to reduce or recover this waste heat in the manufacturing sector, where heat is lost in streams of hot exhaust gases and liquids; through heat conduction, convection, and radiation from hot surfaces; and from heated product streams.[30] Recovering the waste heat from these processes would have a total work potential—the maximum work that can be obtained by using the identified unrecovered waste heat to drive an engine—of 589 TBtu/year,[31] which has the opportunity to reduce the emissions of the U.S. manufacturing sector by 34 MMT of CO_2[32] and save $56 billion each year.[33]

Market Opportunity: Transportation

In 2008, the U.S. transportation sector consumed 28,103 TBtu—28% of total U.S. energy consumption.[34] Compared to conventional materials, composite materials could reduce transportation energy use by decreasing vehicle weight. A study from MIT estimates that for every 10% reduction in vehicle weight, fuel economy could increase by 6% for cars and 8% for light-duty trucks.[35] Considering that the annual U.S. energy consumption of cars and trucks is above 16,000 TBtu,[36] if composites with structural capabilities could reduce the vehicle weight of cars and light-duty trucks by 10%, such advances could save 1,060 TBtu of energy,[37] 72 MMT of CO_2 emissions,[38] and $34 billion in fuel costs each year (assuming an estimated cost of motor gasoline of $3.98 per gallon or $31.84 per MBtu).[39]

Breakthrough Opportunities

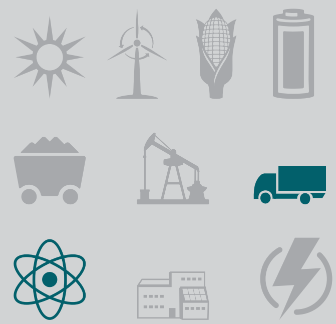
The MSE community can advance composites with structural capabilities by developing or improving metal-matrix composites and nanocomposites, polymer composites and nanocomposites, and layered, sandwich, and infiltrated materials. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow composites with structural capabilities to make significant contributions toward addressing energy, environmental, and economic needs.

Composites with Structural Capabilities

Metal-Matrix Composites and Nanocomposites

Materials scientists have been historically interested in discontinuous metal-matrix composites (DMMCs) for their scientific merits and promise of commercialization. DMMCs are commercially available and can provide significant value from an energy perspective in nuclear and internal combustion engine (ICE) applications. Aluminum-boron (Al-B) or aluminum-boron-carbide DMMCs can extend nuclear plant life in fuel storage applications through re-racking. ICE applications can use DMMCs to replace cast-iron cylinder liners with a wear-resistant cylinder wall surface and to provide selective reinforcement to highly thermally loaded, high-stress areas (e.g., engine bore bridges), ultimately decreasing engine size and weight.[40]

Market Impact

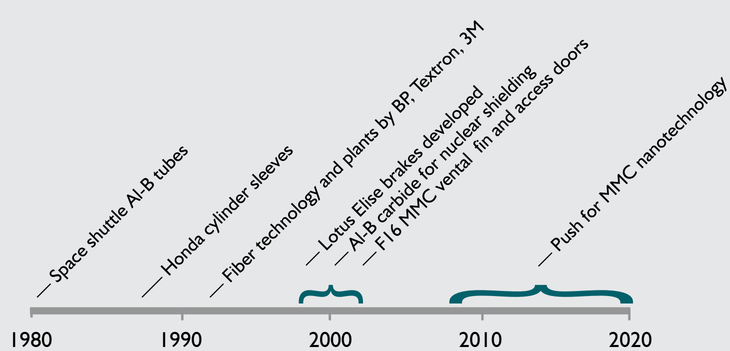


GAPS AND LIMITATIONS TO OVERCOME

- The current cost of DMMCs has prevented the widespread penetration of structural MMCs into the marketplace and limited the number of MMC producers.
- Reactions (e.g., corrosion) between ceramic reinforcements and the metal matrix (e.g., aluminum-silicon-carbide [Al-SiC] composites) during both manufacture and use cause property degradation and variation.
- The uniform distribution of reinforcements, particularly at the nano-scale level, is difficult to achieve.
- There is a lack of statistically based design data that can be easily utilized by existing component design tools (e.g., finite element modeling).

Historical Trends and Future Opportunities

TRENDS IN METAL-MATRIX COMPOSITES R&D AND COMMERCIALIZATION



In the 1970s and 1980s, MMC R&D focused on structural MMCs. In the 1990s, this work led to investments from large corporations in product development activities and large-scale production infrastructure. The majority of this effort was abandoned from 2000 to 2010 due to a shift to smaller, niche markets. In the next 10 years, commercial activity in MMCs will increase with the demand for and development of nanotechnology.

Composites with Structural Capabilities

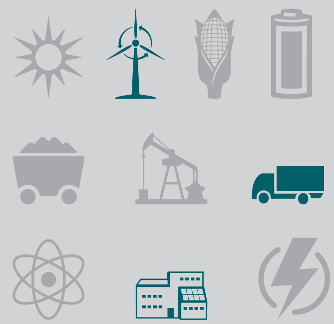
Polymer Composites and Nanocomposites

Polymer composites, which contain a polymer matrix and a reinforcement of a different material (e.g., fibers and particulates), offer a unique combination of properties that are not possible with individual constituents. The most common polymer matrix types are made of epoxy resins, a class of thermoset polymers that react with curatives or hardeners to produce a solid matrix. Epoxy resins offer high strength, low shrinkage, good adhesion to substrates, low toxicity, and chemical resistance. Carbon fiber is a common fiber used in structural polymer composites with an epoxy matrix.[41]

GAPS AND LIMITATIONS TO OVERCOME

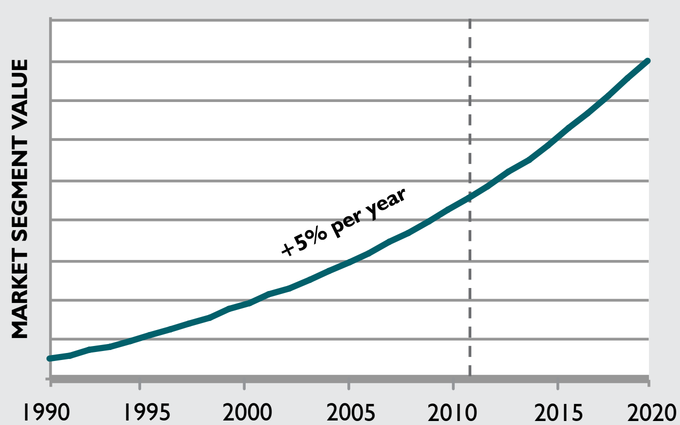
- Cured polymer composites are prone to irreversible damage, such as stress concentrations and delamination, when cut or bolted.
- There is no nondestructive evaluation method that can confirm a perfect bond between polymer composites and other joined materials.

Market Impact



Historical Trends and Future Opportunities

MARKET SEGMENT VALUE OF FIBER-REINFORCED POLYMER COMPOSITES



The market value of fiber-reinforced polymer composites has advanced at an average rate of 5% per year over the past 20 years. The value of polymer nanocomposite technologies is expected to increase at this rate for the next 10 years.

Market Segment Value

- 1990–2011: 5% per year
- 2011–2020: 5% per year

Composites with Structural Capabilities

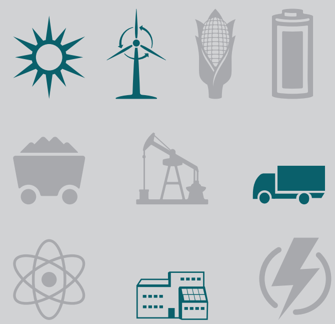
Layered, Sandwich, and Infiltrated Materials

Layered, sandwich, and infiltrated materials offer significant opportunities for improving the performance of engineered structures. Cored sandwich materials, which have a face sheet of one material and an internal core of another material, offer improved strength and modulus relative to density and can use high-temperature materials to improve process efficiency (e.g., incorporating high-temperature refractory metals to enable step changes in efficiency in solar thermal and industrial processes).

GAPS AND LIMITATIONS TO OVERCOME

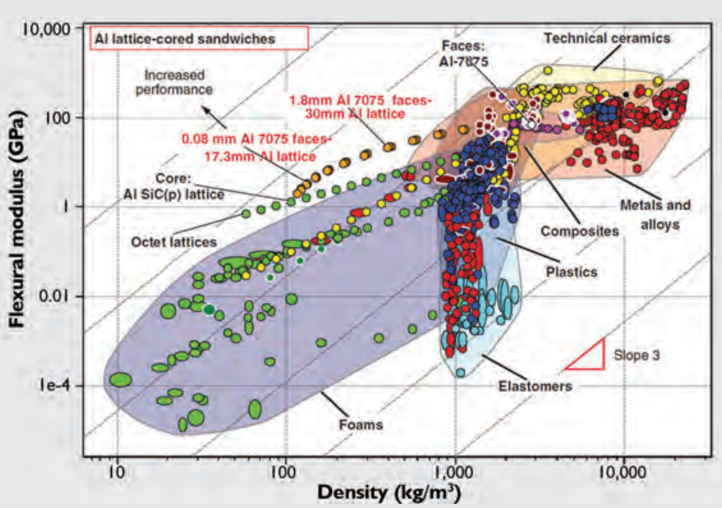
- As wind turbine efficiency increases with size, sandwich materials used in both the blades and tower experience increased stress. Sandwich materials require increased strength and more cost-effective integration to continue decreasing costs.[42]
- Due to the advantages of sandwich materials strength-to-density, these materials could contribute to vehicle lightweighting. However, manufacturing and joining techniques are not advanced enough to cost-effectively integrate into vehicle platforms.[43]

Market Impact



Historical Trends and Future Opportunities

MODULUS VS. DENSITY OF TRADITIONAL MONOLITHIC MATERIALS AND MODERN SANDWICH STRUCTURES



Plot of modulus vs. density of traditionally manufactured monolithic materials (shaded areas), and with modern aluminum lattice-cored sandwich structures showing improvement in modulus vs. density performance[44]

Many classes of monolithic materials have been developed for structural applications; however, their modulus-to-density ratio is clustered around similar values and follows similar trends. Over the next 10 years, advances in structure and composition of aluminum lattice-cored sandwich structures will allow this class of composites to make incremental increases in modulus-to-density ratios, resulting in stiffer, lighter sandwich structures.

R&D Priority Activities: Composites with Structural Capabilities

To overcome the gaps and limitations within the composites with structural capabilities breakthrough opportunities, the MSE community must focus their efforts on developing new manufacturing and fabrication processes, advancing nondestructive evaluation techniques, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Layered/Sandwich/Infiltrated Materials** • **Identify and deploy joining and oxidation-protection approaches that could be used to integrate refractory metal plates, foils, or sheets as the outer face of sandwich structures.** • Create modulus or plasticity gradients for robust, damage-tolerant, and wear-resistant materials. • Determine fundamental failure mechanisms, behavior at interfaces, testing methods, and finite element analysis modeling of composites and layered materials. **Crosscutting** • Conduct nondestructive evaluation of polymer composite or sandwich materials.
MID TERM (2–5 YEARS)	**Metal-Matrix Composites and Nanocomposites** • **Develop low-cost, in-situ fabrication of metal-matrix nanocomposites, including casting and powder metallurgy techniques.** • Identify new approaches to manufacture cost-effective metallic fillers for structured sandwich materials, and develop supporting engineering data. **Polymer Composites and Nanocomposites** • **Establish manufacturing processes and design criteria to enable low-cost, high-volume continuous fiber polymer composites for transportation lightweighting.** • **Discover high-performance polymers or polymer composites with higher thermal gradients and/or lower creep at elevated temperatures to substitute for metals.** • Identify low-cost and robust nondestructive evaluation methods for measuring the state of cure. • Develop ultra-low-wear polymers and composites for bushings and bearings that can replace metals, reduce or eliminate maintenance or downtime, and eliminate the need for lubricants. • Identify methods to incorporate sensors into polymers for damage detection. **Crosscutting** • **Identify out-of-autoclave curing technologies (e.g., selective heating by microwave or radio frequency, and cold processing by electron beam curing) to reduce curing times.** • **Conduct high-temperature evaluation of MMCs, metal-matrix nanocomposites, and layered materials.** • Develop processes for evaluating and recycling metal/polymer matrix composites that can be used for structural applications (Metal-Matrix Composites and Nanocomposites, Polymer Composites and Nanocomposites).
LONG TERM (5–10 YEARS)	**Layered/Sandwich/Infiltrated Materials** • Conduct modeling and experiments to identify foams with high strength-to-weight and modulus-to-weight ratios. **Crosscutting** • Develop bio-synthesis and bio-processing routes that mimic biological processes and can achieve equal or better properties with decreased energy and emissions, with the ultimate goal of replacing petroleum feedstocks.

*The experts identified the **bolded activities** as high priority.

NOTES

1 To properly compare the energy and emissions efficiency of different vehicles, it is important to consider their well-to-wheel efficiencies—the energy and emissions associated with fuel use over the vehicle lifetime. The well-to-wheel energy and emissions consist of two components: 1) The well-to-tank energy and emissions, which includes the energy and emissions associated with fuel production (such as refining) and the energy and emissions associated with transporting the fuel from its primary source to the vehicle tank, and 2) the tank-to-wheel energy and emissions associated with fuel use by the vehicles; Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls.

2 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008,* (Washington, DC: U.S. Department of Energy, July 2010), Table 11.7, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table11_07.xls.

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4 Ibid.

5 Ibid.

6 Kromer and Heywood, *Electric Powertrains: Opportunities and Challenges in the U.S. Light-Duty Vehicle Fleet*, 115, Table 50.

7 Calculation: Percentage change between 186 grams of greenhouse gas emissions per mile and 405 grams of greenhouse gas emissions per mile = 54%.

8 Kromer and Heywood, *Electric Powertrains: Opportunities and Challenges in the U.S. Light-Duty Vehicle Fleet*, 115, Table 50.

9 Note that the tank-to-wheel section of battery-powered and fuel cell vehicles does not result in CO_2 emissions. The MIT study made several assumptions to arrive at the 2030 estimates for batteries and fuel cells, including improvements in technology, fuel mix of electricity generation, and generation pathways for hydrogen. These assumptions have a direct impact on the estimated energy and CO_2 emissions of future battery and fuel cell vehicles.

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17 Lynette Cheah, John Heywood, and Randolph Kirchain, "The Energy Impact of U.S. Passenger Vehicle Fuel Economy Standards," (presentation, IEEE International Symposium on Sustainable Systems and Technology, Washington, DC, May 17–19, 2010), http://web.mit.edu/sloan-auto-lab/research/beforeh2/files/IEEE-ISSST-cheah.pdf. (Note that the study assumed that powertrains are resized to maintain same acceleration performance when vehicle weight is reduced. Fuel consumption [or economy] refers to adjusted figures, which are revised upward [or downward] to better reflect actual, on-road figures, rather than dynamometer test results obtained in the laboratory); Lynette Cheah et al., "Factor of Two: Halving the Fuel Consumption of New U.S. Automobiles by 2035," in *Reducing Climate Impacts in the Transportation Sector*, edited by Daniel Sperling and James S. Cannon (New York: Springer, 2008), web.mit.edu/sloan-auto-lab/research/beforeh2/files/cheah_factorTwo.pdf.

18 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls.

19 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008,* Table 2.6, (Washington, DC: U.S. Department of Energy, July 2010) http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls. In 2008, cars consumed 8,831 TBtu and light-duty trucks consumed 7,572 TBtu. A 6% increase in car fuel economy results in a 5.66% decrease in fuel consumption. An 8% increase in light-duty truck fuel economy results in a 7.41% decrease in fuel consumption. Calculation of energy savings for cars = 500 TBtu = 8,831 TBtu * 5.66%; Calculation of energy savings in light-duty trucks = 561 TBtu = 7,572 * 7.41%; 500 TBtu + 561 TBtu = 1,061 TBtu.

20 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 11.7, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table11_07.xls. Calculation, assuming car CO_2 emissions make up 54% of total car and truck emissions, based on the fraction of energy consumed by cars compared to light trucks: 54% = 8,831 TBtu/(8,831 TBtu + 7,572 TBtu). Then 34 $MMTCO_2$ = 1,113.3 $MMTCO_2$ * 5.66% * 54%; 38 $MMTCO_2$ = 1,113 * 7.41% * 46%; 34 $MMTCO_2$ + 38 $MMTCO_2$ = 72 $MMTCO_2$.

21 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008,* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls; U.S. Energy Information Administration (EIA), *Monthly Energy Review*, *June 2011* (Washington, DC: EIA, 2011), Table 9.4, http://www.eia.gov/totalenergy/data/monthly/pdf/sec9_6.pdf; EIA, *Annual Energy Review 2009*, (Washington,

DC: EIA, August 2010), Appendix A, Table A1, http://www.eia.gov/totalenergy/data/annual/pdf/sec13_1.pdf; EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics," last updated July 5, 2011, accessed July 13, 2011, http://www.eia.gov/energyexplained/index.cfm?page=oil_home#tab2. Note that the price of motor gasoline is used in this example for simplicity purposes. Using diesel in these examples would yield different results because of differences in prices and heat content. Cost of motor gasoline based on $3.98 per gallon or $31.84 per MBtu, including taxes, (data from EIA, *Monthly Energy Review, May 2011*), energy content for motor gasoline of 5.253 MBtu per barrel (EIA, *Annual Energy Review 2009*), barrel to gallon conversion for petroleum products of 42 gallons per barrel (EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics").

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31 BCS Incorporated for the U.S. Department of Energy (DOE) Industrial Technologies Program (ITP), *Waste Heat Recovery: Technology and Opportunities in U.S. Industry*, (Washington, DC: DOE ITP, 2008), 53, http://www1.eere.energy.gov/industry/intensiveprocesses/pdfs/waste_heat_recovery.pdf.

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33 U.S. Department of Energy, Energy Information Administration, *2006 Manufacturing Energy Consumption Survey* (Washington, DC: U.S. Department of Energy, June 2009), Table 724, http://www.eia.gov/emeu/mecs/mecs2006/2006tables.html. In 2006, the U.S Department of Energy's Energy Information Administration reported that average prices of purchased energy sources for the manufacturing sector were $9.49 per MBtu. Calculation: $9.49 per MBtu * 589 TBtu = $5.6 billion.

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38 Ibid, Table 11.7, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table11_07.xls; Assuming car CO_2 emissions make up 54% of total car and truck emissions, based on the fraction of energy consumed by cars compared to light trucks: 54% = 8,831 TBtu/(8,831 TBtu + 7,572 TBtu). Then 34 $MMTCO_2$ = 1,113.3 $MMTCO_2$ * 5.66% * 54%; 38 $MMTCO_2$ = 1,113 $MMTCO_2$ * 7.41% * 46%; 34 $MMTCO_2$ + 38 $MMTCO_2$ = 72 $MMTCO_2$.

39 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls; U.S. Energy Information Administration (EIA), *Monthly Energy Review*, *June 2011* (Washington, DC: EIA, 2011), Table 9.4, http://www.eia.gov/totalenergy/data/monthly/pdf/sec9_6.pdf; U.S. EIA, *Annual Energy Review 2009* (Washington, DC: EIA, August 2010), Appendix A, Table A1, http://www.eia.gov/totalenergy/data/annual/pdf/sec13_1.pdf; U.S. EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics," last updated July 5, 2001, accessed July 13, 2011, http://www.eia.gov/energyexplained/index.cfm?page=oil_home#tab2. Cost of motor gasoline based on $3.98 per gallon or $31.84 per MBtu, including taxes (EIA, *Monthly Energy Review, May 2011*), energy content for motor gasoline of 5.253 MBtu per barrel (EIA, *Annual Energy Review 2009*), and a barrel to gallon conversion for petroleum products of 42 gallons per barrel (EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics").

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V. HIGHER-PERFORMANCE MATERIALS

For many energy systems, the path to realizing greater energy efficiency brings extreme conditions that today's materials cannot withstand, such as higher temperatures, more intense radiation, greater wear, or more corrosive environments. Increasing the efficiency of industrial combustion and conversion systems, for example, requires higher temperatures and the use of aggressive chemicals that can degrade materials and cause them to fail. Advancing other energy-related processes and technologies, such as nuclear fission and fusion, solar technologies, fuel cells, and even transportation technologies, similarly push materials to their limits.

Higher-performance materials that can maintain their chemical and physical properties while increasing component and system life under extreme conditions can effectively enhance the efficiency of energy systems. Improvements in material properties and surface treatments are needed so that materials can support increases in the efficiency of systems used in industrial processes, transportation technologies, and electricity generation. Such higher-performance materials can also significantly extend the life of system components, reducing the need for replacement parts and eliminating the consumption of energy and materials required to make those parts. These innovations can ultimately reduce the cost, environmental impact, and energy requirements of energy generation, storage, and use across U.S. energy sectors.

The following pathways provide a guide for research and development (R&D) in the area of higher-performance materials:

- Thermoelectric Materials
- Phase-Stable Metallic Materials
- Surface Treatments
- Lightweight High-Strength Materials

THERMOELECTRIC MATERIALS

Thermoelectric materials are used in devices that convert waste heat into useful electricity. Developing low-cost, stable thermoelectric materials with low thermal conductivities and simultaneous high electric conductivities (i.e., high ZT [figures of merit] values) can offer an efficient alternative to processes such as mechanical generation and refrigeration and can improve the harvesting of waste heat. As a result, these advances can increase energy and fuel efficiency in energy sectors. Opportunities in industrial processes and transportation provide quantifiable justification for pursuing R&D of thermoelectric materials.

Market Opportunity: Industrial Processes

During manufacturing a significant amount of energy is lost as heat. According to a recent report from the U.S. Department of Energy, unrecovered waste heat for the industrial processes analyzed in the report totaled 1,478 trillion British thermal units (TBtu) per year.[1] Thus, low-cost, stable thermoelectric materials with high ZT values have the potential to benefit U.S. energy sectors significantly by aiding in the conversion of industrial waste heat into electricity—particularly low-temperature waste heat.

Developing thermoelectric materials with a ZT of 2 or greater may be able to provide thermal-to-electric efficiencies above 15%,[2] which could displace a portion of purchased electricity. For example, if thermoelectric materials operating at 15% thermal-to-electric efficiency are applied to 1,478 TBtu of unrecovered waste heat, 222 TBtu of grid-generated electricity will be displaced,[3] resulting in a reduction of approximately 42 million metric tons (MMT) of carbon dioxide (CO_2)[4] and a cost savings of approximately $3.6 billion[5] for the U.S. manufacturing sector.

Market Opportunity: Transportation

Approximately 40% of input energy to internal combustion vehicles is lost as waste heat in the exhaust gas.[6] Stable thermoelectric materials with high ZT values can recover and convert waste heat into electricity without releasing CO_2 emissions, improving vehicle fuel economy by reducing vehicle electrical power requirements placed on the engine (e.g., for lights, pumps, stability controls, navigation systems, stereo systems, electronic braking, and powertrain controllers and sensors). Advances in thermoelectric materials could help displace some portion of the 8,831 TBtu consumed by cars and 7,572 TBtu consumed by light-duty trucks each year.[7] If thermoelectric materials development improves the total U.S. car and light-duty truck fleet fuel economy by 5% (identified by the U.S. Department of Energy Vehicle Technologies Program as a thermoelectric generator project objective), the resulting energy savings would total 781 TBtu,[8] with a total CO_2 emissions reduction of 53 MMT[9] and a $25 billion reduction in vehicle fuel costs (assuming an estimated cost of motor gasoline of $3.98 per gallon or $31.84 per million Btu [MBtu]).[10]

Breakthrough Opportunities

The materials science and engineering (MSE) community can advance thermoelectric materials by improving manufacturing, developing materials with higher ZTs, improving sealants, and developing substitute materials. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow thermoelectric materials to make significant contributions toward addressing energy, environmental, and economic needs.

Thermoelectric Materials

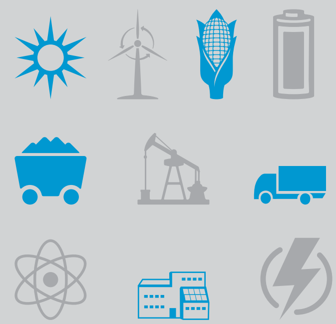
Improved Manufacturing

Today's manufacturing processes for the production of thermoelectric materials are labor intensive, which increases the cost of thermoelectric devices. These manufacturing methods include direct melt crystallization, pressed powder metallurgy, doping, and other complex processes. Advanced methods that can improve existing manufacturing processes and increase device efficiency are essential for the large-scale market penetration of thermoelectric materials.[11]

GAPS AND LIMITATIONS TO OVERCOME

- There are no low-cost manufacturing methods that produce net-shape thermoelectric materials.
- Methods to compact nano-powders without sintering nanosized particles to large particles are underdeveloped, reducing any benefits of nano-sizing.
- Soldering metal contacts in thermoelectric parts slows production and increases labor costs.

Market Impact



Historical Trends and Future Opportunities

PROJECTED MARKET DEMAND FOR THERMOELECTRIC MATERIALS WITH A ZT OF 1 AND 2 (THROUGH 2025)

	Density	2005 World Market	ZT ≈ 1 TEG @ 0.35 watt/gram (W/gm)		ZT ≈ 2 TEG @ 4.9 W/gm	
	(g/cm^3)	(tonnes)	(tonnes/ year)	Market Share	(tonnes/ year)	Market Share
Bismuth	9.78	5,200	61	1.20%	4.3	0.10%
Tellurium	6.24	113	39	34.20%	2.8	2.40%
Selenium	4.79	1,350	30	2.20%	2.1	0.20%
Germanium	5.32	90	33	36.60%	2.4	2.60%
Silicon	2.33	5,100,000	14	0.00%	1	0.00%
Gallium	5.91	63	37	58.10%	2.6	4.20%
Antimony	6.68	117,000	41	0.00%	3	0.00%

The table shows a projected material demand through the year 2025 based on 2005 world market values for thermoelectric generator (TEG) materials with figures of merit (ZT) of both 1 and 2. Gallium, germanium, and tellurium make up the largest shares of the world market supply and place tremendous pressure on material supply and price. The physical configuration of higher ZT materials is smaller and results in the use of less materials. These materials are expected to gain greater market penetration in the future. As a result, the demand for semiconductor materials will be lower.[12]

Materials compound discovery has played an important role in reducing the overall cost of thermoelectric devices. While there have been some reductions in manufacturing and labor costs, materials scientists have mainly focused on reducing the cost of materials through substitution. Compared to n-type Bi_2Te_3 (bismuth-telluride), which was developed in the 1950s and 1960s, new materials such as Co-Ni-Sb (cobalt-nickel-antimony) skutterudite are less expensive.

Thermoelectric Materials

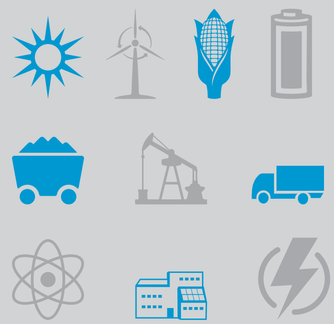
Higher Figure of Merit (ZT)

The efficacy of thermoelectric devices is measured by a dimensionless variable called the "figure of merit," or "ZT." Thermoelectric materials with high electrical conductivity, a high Seebeck coefficient, and low thermal conductivity have greater thermodynamic efficiencies and ZTs. Increasing the ZTs of these materials will improve the efficiency of waste heat harvesting, offering widespread opportunities to increase efficiency.

GAPS AND LIMITATIONS TO OVERCOME

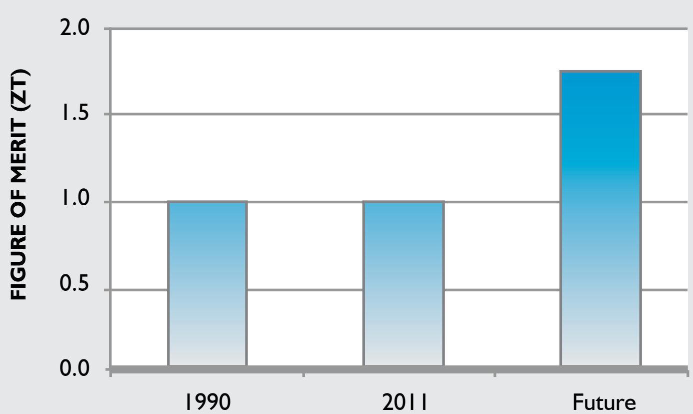
- The process of doping with p-type semiconductor materials hinders the reliable and reproducable construction of thermoelectrics with high conversion efficiencies due to the self compensation of native defects.
- The current toxicity of thermoelectrics reduces their potential for large-scale use.
- Current materials and structures lack high ZT performance, and therefore produce low energy yields or require high production volumes to be affordable.

Market Impact



Historical Trends and Future Opportunities

ZT OF COMMERCIALLY AVAILABLE THERMOELECTRIC MATERIALS



The current ZT of commercial thermoelectrics is equal to about 1 and has improved little over the past 20 years.[13] Further advances in thermoelectric technologies and processing techniques have the potential to increase the ZT to about 1.8 due to new methods of raw material purification and advances in nanomanufacturing techniques.[14]

Figure of Merit (ZT)

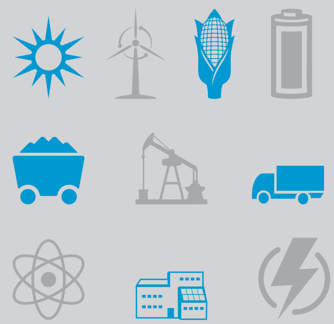
- 1990: 1
- 2011: 1
- Future: 1.8

Thermoelectric Materials

Sealants

Sealants are used on thermoelectric generators to prevent moisture from degrading the performance of the thermoelectric element. Some thermoelectric materials have only demonstrated durability for space applications operating in vacuum environments; the long-term durability of these materials in air and at high temperatures has not been demonstrated. To enable the use of thermoelectric materials in automotive and industrial applications, thermoelectric elements will require coatings to protect them from oxidation at operating temperatures of 600°C and higher. In addition, these sealants must also survive thermal cycling, which requires excellent adhesion and a coefficient of thermal expansion that matches that of the materials the sealant is intended to protect.[15]

Market Impact

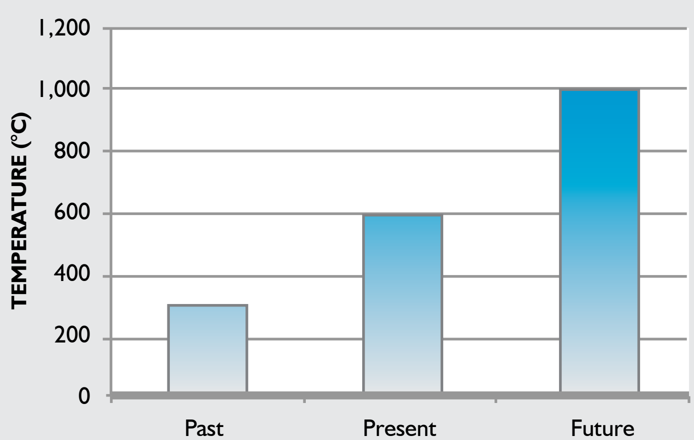


GAPS AND LIMITATIONS TO OVERCOME

- Sealants require high thermal stability at around 1,000°C to be reliable in commercial applications.
- Effective sealants of thermoelectric generators cannot guarantee long life at high temperatures or resist thermal cycling.
- There is insufficient fundamental understanding of the mechanisms and kinetics of the degradation of thermoelectric materials from elements in the atmosphere.
- Oxidation barriers with high-temperature capabilities for thermoelectric materials do not have the necessary thermomechanical durability.

Historical Trends and Future Opportunities

TEMPERATURES AT WHICH THERMOELECTRIC SEALANTS ARE THERMALLY STABLE



Typical epoxy-based sealants, an earlier form of thermoelectric sealants, are limited to temperature operation lower than 300°C. Current thermoelectric materials presenting a ZT greater than 1 oxidize in the presence of air and moisture at 600°C; today's sealants are effective up to this temperature limit. Future advancements in thermoelectric sealants must enable their use in harsh environments, such as in engines and industrial processes, at approximately 1,000°C.[16]

Thermal Stability (°C)

- Past: 300°C
- Present: 600°C
- Future: 1,000°C

Thermoelectric Materials

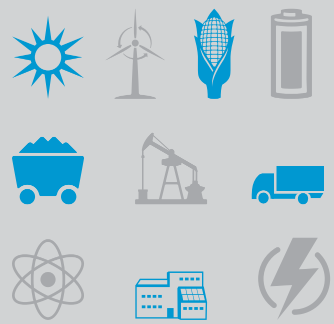
Substitute Materials

Common thermoelectric materials, such as bismuth telluride, contain toxic materials that are environmentally hazardous and difficult to recycle. Substitute materials, such as oxides and skutterudite thermoelectrics, consist of more environmentally friendly materials with high thermoelectric performance potential. Oxide thermoelectrics are composed of a superlattice structure that exhibits good electrical conductivity and low thermal conductivity. With further advances, their ZTs have the potential to improve to the level of common thermoelectrics. Because oxide thermoelectrics are less susceptible to oxidation, they may be suited for high-temperature operating environments.

GAPS AND LIMITATIONS TO OVERCOME

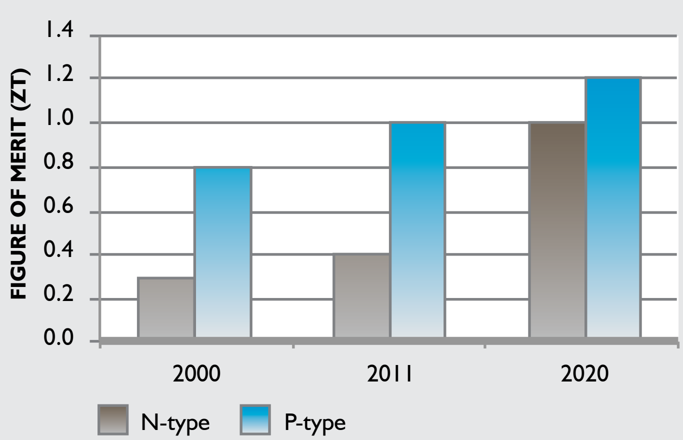
- Few p-type materials devices are currently available, and synthesis of p-type materials with the desired properties is challenging.[17]
- Materials design and property prediction capabilities do not yet allow scientists to narrow the list of potential thermoelectric materials.

Market Impact



Historical Trends and Future Opportunities

FIGURES OF MERIT FOR N-TYPE AND P-TYPE THERMOELECTRICS



The ability for oxide thermoelectrics to substitute for telluride-type thermoelectric materials depends on improvements in ZT for low-temperature applications. Current n-type oxide thermoelectrics carry a ZT of 0.4, which has increased from 0.3 in the past 10–20 years. This value is expected to increase to 1.0 over the next 10 years. Ten to 20 years ago, the ZT of p-type oxide thermoelectrics was 0.8. Their current ZT of 1.0 is expected to increase to about 1.2 over the next 10 years.[18]

ZT of N-type

- 2000: 0.3
- 2011: 0.4
- 2020: 1

ZT of P-type

- 2000: 0.8
- 2011: 1
- 2020: 1.2

R&D Priority Activities: Thermoelectric Materials

To overcome the gaps and limitations within the thermoelectric materials breakthrough opportunities, the MSE community must focus their efforts on improving the ZT of current thermoelectrics, identifying substitute materials, improving processing techniques, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Sealants** • Demonstrate effective sealing techniques (e.g., welding) on the generator level to operate thermoelectric elements in argon or in a vacuum at 600°C. • Develop a fundamental understanding of the mechanisms of degradation of thermoelectric materials in a vacuum and in air. • Develop an oxidation-protective coating for thermally stable thermoelectric materials. **Substitute Materials** • Develop new synthetic routes for the purification of low-cost, low-purity raw materials to develop low-cost, high-purity materials. • Consolidate the multiple steps involved in manufacturing substitute materials. **Crosscutting** • **Develop a range of thermoelectric polymers to enable wide-scale application of weight-optimized components for use in defense, automotive, and commercial applications.**
MID TERM (2–5 YEARS)	**Higher Figure of Merit (ZT)** • **Develop highly conductive thermoelectric materials compatible with additive manufacturing systems to enable corrosion-resistant, highly functional polymer designs for multifunctional components with structurally integrated power and communication circuits.** **Sealants** • Develop a cost-effective process to create a thermally stable, sealed generator at 600°C. • Demonstrate effective encapsulation of thermally stable thermoelectric materials in isothermal, thermal-gradient, and thermo-cycling conditions. • Develop a cost-effective oxidation barrier coating process for thermoelectric materials. **Substitute Materials** • Develop new low-cost thermoelectric materials with higher ZTs. • Advance new compacting processes in response to advances in nano-manufacturing.
LONG TERM (5–10 YEARS)	**Higher Figure of Merit (ZT)** • **Develop capacitance materials compatible with additive manufacturing methods to enable structurally integrated electrical energy storage systems.** **Sealants** • **Develop an oxidation barrier coating for thermoelectric materials operating at 1,000°C.** • Demonstrate effective sealing techniques at the generator level to operate thermoelectric elements in argon or vacuums at 1,000°C. **Substitute Materials** • Develop low-cost thermoelectric materials based on abundant, easily accessible materials (e.g., oxides).

*The experts identified the **bolded activities** as high priority.

PHASE-STABLE METALLIC MATERIALS

Increasing the efficiency of electricity generation requires materials that can withstand harsh conditions, such as temperatures greater than 650°C, radiation, and the presence of aggressive substances, including sulfur, hydrogen, chlorine, and water. It is critical to use advanced techniques to develop phase-stable metallic materials that retain their strength, ductility, and dimensional stability when exposed to these conditions. The opportunity for these advances to ensure that electricity demand is met in an efficient, cost-effective, and environmentally friendly way provides quantifiable justification for pursuing R&D of phase-stable metallic materials.

Market Opportunity: Electricity Generation

In 2010, the total U.S. energy consumption for electricity generation by the electric power sector was 39,579 TBtu,[19] 40% of total U.S. energy consumption.[20] Approximately 88% of this electricity was generated using steam turbine engines (61% of generating capacity) or gas turbine engines (27% of generating capacity).[21] Incorporating advanced phase-stable metallic materials capable of withstanding elevated inlet temperatures and harsh operating environments into the design of these turbines could greatly improve the efficiency of U.S. electricity generation. For example, a 1% reduction in fuel consumed by U.S. power-generating gas and steam turbines would save 348 TBtu of energy,[22] $400 million in fuel costs[23] to major investor-owned electric utilities (which represent only a portion of U.S. power producers), and 22 MMT of CO_2 emissions from coal and natural gas combustion.[24]

Breakthrough Opportunities

The MSE community can advance phase-stable metallic materials by developing and improving next-generation steels, next-generation nickel-cobalt (Ni-Co), irradiation-resistant materials, and next-generation zirconium (Zr) cladding. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow phase-stable metallic materials to make significant contributions toward addressing energy, environmental, and economic needs.

Phase-Stable Metallic Materials

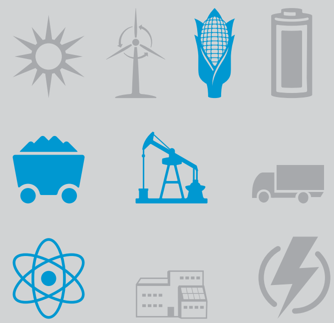
Next-Generation Steels

Steel is composed of iron and property-altering alloying elements. Next-generation steels must contain alloying elements that allow the steel to be phase-stable in extreme high-temperature environments. Some of the most promising steel compositions for use in demanding operating conditions are 9-chromium martensitic alloys, which have higher thermal conductivity and lower thermal expansion than their austenitic counterparts.

GAPS AND LIMITATIONS TO OVERCOME

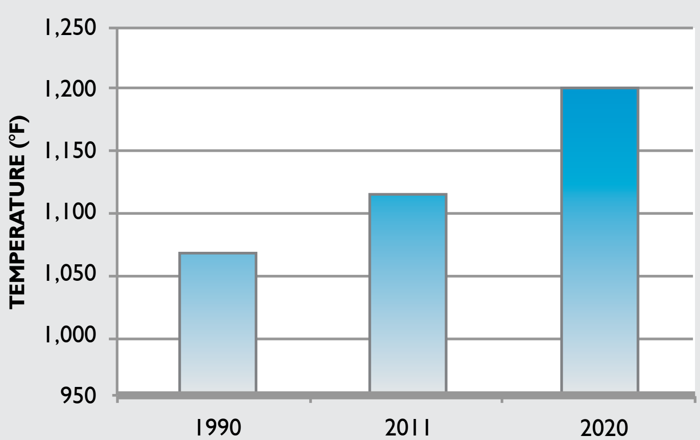
- Today's steels cannot withstand the temperature that alternate alloys can endure in steam turbine applications (about 1,400°F).
- Current steels are unable to safely reach operating lives of 250,000 hours in high-temperature and high-pressure environments.

Market Impact



Historical Trends and Future Opportunities

TEMPERATURE AT WHICH STEELS ARE THERMALLY STABLE



In the past 20 years, the use of new 9-chromium steels has increased the temperature stability of steels from about 1,065°F to 1,115°F. Further improvements to this steel in the next 5–10 years are expected to increase thermal stability to 1,200°F.

Thermal Stability (°F)

- 1990: 1,065°F
- 2011: 1,115°F
- 2020: 1,200°F

Phase-Stable Metallic Materials

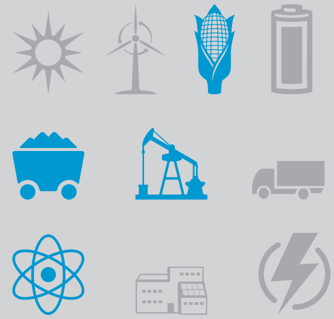
Next-Generation Nickel-Cobalt

Nickel-based alloys are classified as superalloys due to their ability to maintain strength and resist creep, corrosion, and oxidation at high temperatures. Adding cobalt to nickel-based alloys helps promote the growth of nickel-aluminum and nickel-titanium intermetallics, which have an ordered austenitic or face-centered cubic crystal structure also known as the gamma-prime phase. This addition of cobalt improves the ability for nickel-based alloys to maintain their strength and resist degradation in high-temperature, high-pressure environments, such as those in steam turbines in coal-fired power plants.

GAPS AND LIMITATIONS TO OVERCOME

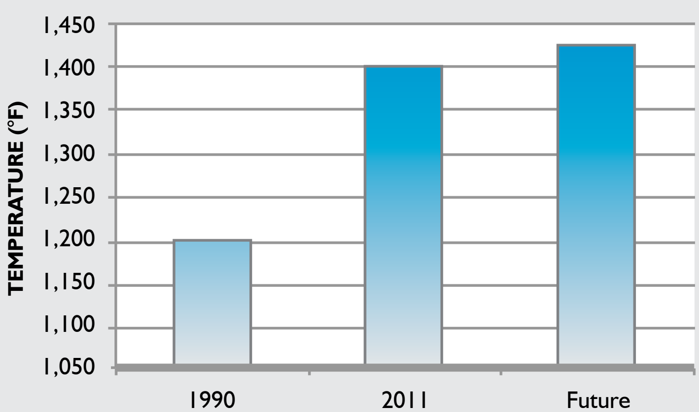
- Because nickel-cobalt (Ni-Co) alloy ingots are resistant to deformation at high temperatures, they are not well suited for hot-work processing.
- High levels of cobalt are not desired in alloys for nuclear applications because cobalt can damage pressurized water reactors if released from the structure.
- Nickel-based superalloys can fracture at high temperatures in high-pressure steam turbines.

Market Impact



Historical Trends and Future Opportunities

TEMPERATURE AT WHICH NICKEL-COBALT ALLOYS ARE THERMALLY STABLE



Over the past 20 years, Ni-Co alloys have increased their thermal stability from 1,200°F to 1,400°F. Future advances in Ni-Co alloys have the potential to raise the operating temperature to approximately 1,425°F, while still remaining phase-stable.

Thermal Stability (°F)

- 1990: 1,200°F
- 2011: 1,400°F
- Future: 1,425°F

Phase-Stable Metallic Materials

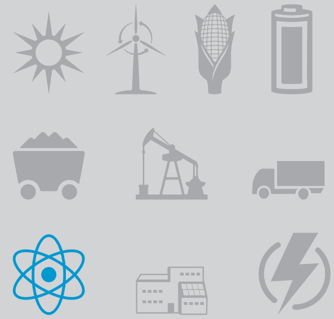
Irradiation-Resistant Materials

Irradiation-resistant materials—often stainless steel hard facings—are strong, stiff materials that are able to resist deformation and dimensional swelling when exposed to radiation. Therefore, these materials are commonly used in nuclear reactors to increase the overall efficiency of nuclear electricity generation and increase the lifetime and uptime of a plant. They are also easy to recycle and dispose of when they reach the end of their useful life.

GAPS AND LIMITATIONS TO OVERCOME

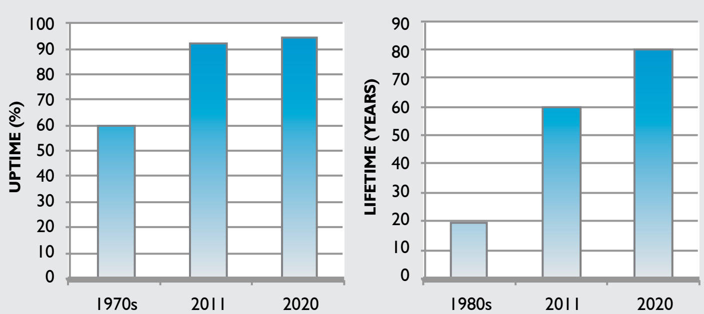
- Corrosion in the reactor causes cobalt from irradiation-resistant hard facings to enter the cooling stream, potentially discharging the poisonous compound into nearby water supplies.
- Irradiation-resistant hard facings also contain chromium and molybdenum to raise the corrosion and oxidation resistance of stainless steels. Lowering or altering the amount of these alloys to reduce the risk of introducing them into the nuclear reactor cooling stream may result in adverse effects. Materials scientists must find a balance between the need for high alloy content to resist corrosion and the need to avoid cooling stream contamination.

Market Impact



Historical Trends and Future Opportunities

NUCLEAR REACTOR UPTIME AND LIFETIME



Reactor uptime and lifetime are key metrics that reflect the benefits of increased irradiation resistance. The removal of impurities from irradiation-resistant materials has increased reactor uptime from 60% to 92% since the 1970s.[25] Changing the alloy composition (e.g., decreasing chromium and molybdenum concentrations) has also increased reactor lifetime from 20 to 60 years since the 1980s.[26] In the next 10 years, uptime is expected to increase to 94% and lifetime is expected to increase to 80 years.

Uptime

- 1970s: 60%
- 2011: 92%
- 2020: 94%

Lifetime

- 1980s: 20 years
- 2011: 60 years
- 2020: 80 years

Phase-Stable Metallic Materials

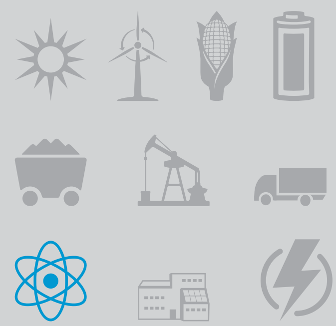
Next-Generation Zirconium Cladding

Nuclear fuel rods require fuel cladding with isotropic properties, high corrosion resistance, high thermal conductivity, and a low ability to absorb neutrons. Zirconium (Zr) is the dominant choice for metallic cladding in existing nuclear fission power plants because it exhibits excellent mechanical properties, corrosion resistance in hot water, and low thermal neutron capture.

GAPS AND LIMITATIONS TO OVERCOME

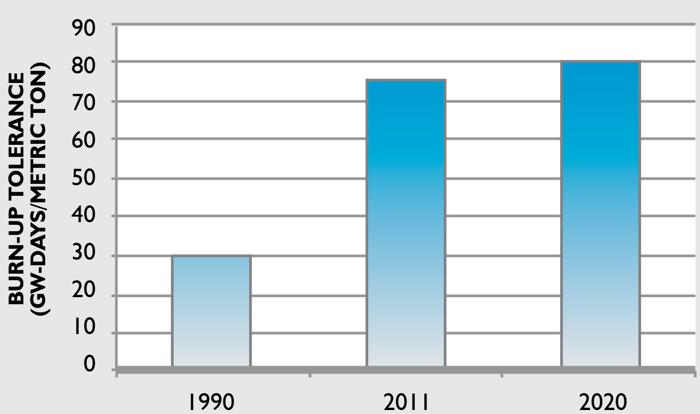
- Today's cladding materials have inadequate toughness and corrosion resistance. Corrosion in Zr alloys leads to a loss in ductility, causing lower mechanical stability. No existing cladding can withstand the doses of radiation associated with high fuel burn-up levels.
- Zr alloys have some oxidation issues on the surface, causing the alloys to absorb hydrogen more easily.
- It is unknown whether Zr alloys will be able to withstand the increased operating temperatures of advanced nuclear fuel rods.

Market Impact



Historical Trends and Future Opportunities

BURN-UP TOLERANCE OF NUCLEAR FUEL CLADDING



The burn-up tolerance of nuclear fuel cladding, a measure of the energy extracted from a nuclear fuel source, has increased with each new generation of Zr alloys (generation 4 is in development). Over the past 20 years, average discharge burn-up levels have increased from about 30 gigawatt-days (GW-days)/metric ton to 75 GW-days/metric ton. In the next 10 years, strong economic incentives are expected to facilitate an increase in the burn-up tolerance of Zr cladding to 80 GW-days/metric ton.[27]

Burn-up Tolerance (GW-days/metric ton)

- 1990: 30 GW-days/metric ton
- 2011: 75 GW-days/metric ton
- 2020: 80 GW-days/metric ton

R&D Priority Activities: Phase-Stable Metallic Materials

To overcome the gaps and limitations within the phase-stable metallic materials breakthrough opportunities, the MSE community must focus their efforts on developing new alloys, improving materials data availability, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

<table>
<tr><td>NEAR TERM
(0–2 YEARS)</td><td>Next-Generation Steels
• Create high-strength, low-alloy steel for ultra-deep-well drilling.
Next-Generation Nickel-Cobalt
• Develop low-cost nickel superalloys for well completion and oil production activities.
• Gather long-term performance data (e.g., gamma prime coarsening in nickel-based superalloys) to improve understanding of how alloys developed for aerospace can transfer to stationary uses.
Next-Generation Zirconium Cladding
• Develop corrosion-resistant Zr alloys with reduced hydrogen pickup.
Crosscutting
• Conduct technology transfer of microwave heat treatment systems developed for radioactive waste handling.</td></tr>
<tr><td>MID TERM
(2–5 YEARS)</td><td>Next-Generation Steels
• Develop stress-corrosion-cracking-resistant stainless steel variants (e.g., AISI 304 and 316 steels) for reactor applications.
• Develop 1,200°F steels for use in power plant steam turbines.
Crosscutting
• Develop irradiation-resistant pressure vessel steels (e.g., A508 and A533 steels) (Next-Generation Steels and Irradiation-Resistant Materials).
• Create physics-based models to predict component lifetime in power plants.
• Develop high-strength titanium for long, low-pressure turbine blades.</td></tr>
<tr><td>LONG TERM
(5–10 YEARS)</td><td>Next-Generation Zirconium Cladding
• Identify alternate fuel cladding materials (e.g., silicon carbide metal-matrix composites).
Crosscutting
• Develop oxidation- and corrosion-resistant refractory alloys for next-generation gas turbines.
• Develop a materials database to enable more accurate computational design.
  » First principles, molecular dynamics data, and modeling are still under development and are needed to assess minor element additions to improve alloys.
• Use new phase diagrams to create more accurate thermomechanical processing and heat treating of steels.
• Develop metallic glasses and high-entropy alloys for coatings and functional materials.
• Create activation-resistant alloys for nuclear applications (i.e., extract niobium and other elements, tailor for nuclear-specific application and recycling).</td></tr>
</table>

*The experts identified the **bolded activities** as high priority.

SURFACE TREATMENTS

Surface treatments, such as thermal spraying and laser deposition, can enhance the damage tolerance of materials, protect materials from harsh service environments, and repair surface fatigue, which increases the service life of products and reduces the need to manufacture new parts. Improving the strength and tolerance of surface treatments for both new and restored parts in demanding service environments can extend the life and robustness of substrate materials. Opportunities to restore or remanufacture parts in transportation and electricity generation sectors provide quantifiable justification for pursuing R&D of surface treatments.

Market Opportunity: Transportation

Remanufacturing parts can reduce energy consumption to only 2%–25% of the energy required to manufacture new parts.[28] Given this potential for energy savings, surface treatments that extend material life have significant potential to benefit the U.S. transportation sector. According to a recent study from the International Academy for Production Engineering, 17 MBtu of energy is consumed while manufacturing one new diesel engine, while only 10% of that energy—1.8 MBtu—is required to remanufacture the engine.[29] Advanced surface treatments of ferrous- and aluminum-based vehicle engine components can reduce this energy consumption while also reducing emissions and overall vehicle cost. Remanufacturing 1 million engines instead of manufacturing new engines could result in 15 TBtu in energy savings,[30] with a total CO_2 emissions reduction of nearly 1 MMT.[31] In addition, this growth of the remanufacturing industry would create skilled labor jobs throughout the United States.

Market Opportunity: Electricity Generation

In 2010, the total U.S. energy consumption for electricity generation by the electric power sector was 39,579 TBtu,[32] 40% of total U.S. energy consumption.[33] Approximately 88% of this electricity is generated using steam turbine engines (61% of generating capacity), or gas turbine engines (27% of generating capacity).[34] Surface treatments can be used to improve the tolerance of steam and gas turbine blades to wear, corrosion, and fatigue, extending turbine life, increasing the efficiency of the turbine in comparison to turbines with untreated surfaces, and decreasing downtime in the electricity generating process. More energy-efficient gas and steam turbines can decrease the consumption of natural gas and coal for electricity generation, reducing emissions and fuel costs. For example, a 1% reduction in fuel consumption as a result of surface treatments in both U.S. power-generating gas and steam turbines used by the electric power sector could save 348 TBtu of energy,[35] $400 million in fuel costs to major investor-owned utilities (which represent only a portion of electric power producers),[36] and 22 MMT of CO_2 emissions from coal and natural gas combustion.[37]

Breakthrough Opportunities

The MSE community can advance surface treatment materials by focusing on part restoration and surface processing. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow surface treatments to make significant contributions toward addressing energy, environmental, and economic needs.

Surface Treatments

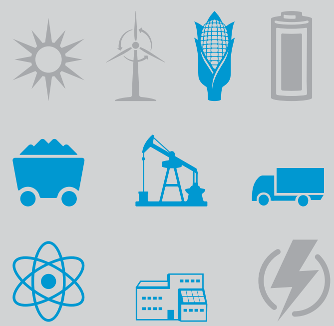
Part Restoration

Surface treatment materials for part restoration enable the remanufacturing of used system components, avoiding the need for the costly manufacturing of new components. Thermal spraying, the most common surface restoration technique, was developed in the 1950s and can be applied to a substrate through chemical, physical, or electroplating deposition techniques. Laser cladding techniques were introduced in the early 2000s; the two techniques are now being combined into laser-assisted thermal spray hybrid techniques to address diffusion bonding surface issues.

GAPS AND LIMITATIONS TO OVERCOME

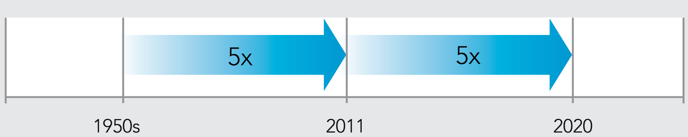
- Current laser cladding techniques are time-intensive and expensive, leaving the techniques greatly underdeveloped.
- Many companies do not have access to testing facilities that ensure proper surface adhesion/bonding.

Market Impact

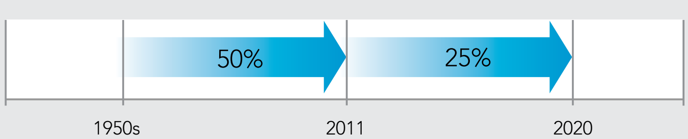


Historical Trends and Future Opportunities

IMPROVEMENT IN MECHANICAL DURABILITY OF RESTORED PARTS



INCREASE IN AMOUNT OF REMANUFACTURING



Advances in part restoration treatment can be measured by mechanical durability, which includes hardness, density, adhesive and cohesive strength, and wear and corrosion resistance. Mechanical durability has improved by 5x since the 1950s and is expected to improve by 5x over the next 10 years.[38]

Remanufacturing avoids a portion of the cost of manufacturing new parts. Remanufacturing has increased by 50% since the 1950s and is expected to increase by 25% over the next 10 years.[39]

Mechanical Durability

- 1950s–2011: 5x improvement
- 2011–2020: 5x improvement

Amount of Remanufacturing

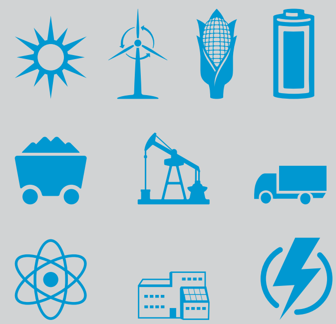
- 1950s–2011: 50% increase
- 2011–2020: 25% increase

Surface Treatments

Surface Processing

Surface treatments are applied to new parts to improve resistance to wear, corrosion, high temperatures, and fatigue, and ultimately to increase part life. Techniques for applying surface treatments include shot-peening, thermal sprays, and laser technologies. First-generation thermal sprays were developed in the 1950s, and laser cladding techniques were introduced in the early 2000s. The newest hybrid approaches combine laser processing with thermal spray to create diffusion bonds between the coating and substrates that increase bond strength and fatigue resistance.

Market Impact

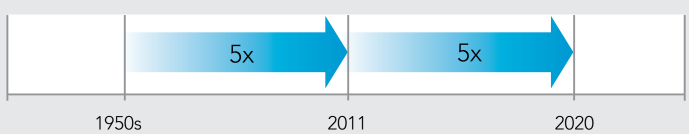


GAPS AND LIMITATIONS TO OVERCOME

- Current laser cladding surface processing techniques have slow processing rates and are too expensive, leaving the techniques greatly underdeveloped.
- Many companies do not have access to testing facilities necessary to ensure proper surface adhesion/bonding of parts.

Historical Trends and Future Opportunities

IMPROVEMENT IN MECHANICAL DURABILITY OF SURFACE-TREATED PARTS



Historical performance of surface processing treatments can be measured by mechanical durability, which includes hardness, density, adhesive and cohesive strength, and wear and corrosion resistance. These durability trends follow the same historical improvement as part restoration surface treatments. Mechanical durability has improved by 5x since the 1950s and is expected to improve by 5x over the next 10 years.[40]

Mechanical Durability

- 1950s–2011: 5x improvement
- 2011–2020: 5x improvement

R&D Priority Activities: Surface Treatments

To overcome the gaps and limitations within the surface treatments breakthrough opportunities, the MSE community must focus their efforts on identifying new surface treatment materials, advancing processing techniques, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Part Restoration** • **Create a user test facility for remanufactured parts testing.** **Surface Processing** • Identify coatings that are resistant to hot corrosion (i.e., oxidation assisted by salts) for use in engines. **Crosscutting** • **Develop lower-cost coating materials that are validated for use and have appropriate cost-performance specifications, rather than overdesigning coatings as happens today.**
MID TERM (2–5 YEARS)	**Part Restoration** • Develop resurfacing technologies for corrosion-resistant alloys. • Identify testing technologies for reconfigured parts that accurately predict long-term performance. **Surface Processing** • **Develop low-cost laser hybrid processing that can metallurgically bond surface layers.** • **Conduct highly accurate non-planar or larger-scale surface treating without damaging substrates (e.g., laser, high-density infrared, high-precision hybrid deposition).** • Develop non-chromate coatings for corrosion resistance. • Create powder-metallurgy coating technology for valves, pumps, and bearings (e.g., for cobalt-free bearings that require wear-resistant coatings). • Develop coatings for steam turbines that are capable of operating at temperatures above 1,400°F and resist erosion from oxidation products often formed in boiler tubes during shutdown. **Crosscutting** • Achieve better interface modeling of microstructures, starting by focusing on specific surface treatments (e.g., thermal barrier coatings).
LONG TERM (5–10 YEARS)	**Surface Processing** • **Develop ceramics for gas turbine parts (e.g., air foils).** • **Develop ultra-high-temperature (~1,600°F) thermal barrier coatings for oxy-combustion turbines.** » Develop new materials/coatings. » Reduce or lower oxygen penetration to base materials. » Ensure low thermal conductivity to protect base metal strength. » Tailor architecture to whole system. **Crosscutting** • Create thermomechanical processing of surfaces for crack removal and life extension.

*The experts identified the **bolded activities** as high priority.

LIGHTWEIGHT HIGH-STRENGTH MATERIALS

Decreasing the weight of a system component can reduce system load and increase efficiency but can also compromise the strength of the material. Advanced lightweight high-strength materials, such as composites, aluminum, magnesium, titanium, certain steel alloys, hybrid materials, and polymer-based materials, can reduce component weight without sacrificing robustness. Increasing the tolerance of these lightweight high-strength materials to wear and corrosion, reducing their cost, and streamlining manufacturing processes can increase their use in demanding energy applications. As a result, these advances can improve the energy and fuel efficiency of energy sectors. Opportunities to restore or remanufacture parts in transportation and electricity generation sectors provide quantifiable justification for pursuing R&D of lightweight high-strength materials.

Market Opportunity: Transportation

Because vehicles consume 70%–90% of their lifetime energy consumption during use,[41] the development of advanced lightweight high-strength materials has significant potential to benefit the U.S. transportation sector. A systems approach to vehicle weight reduction can optimize the use of lightweight high-strength materials, including magnesium, carbon-fiber composites, polymers, aluminum, and gradient materials, in vehicle design. By using this approach, automotive designers can develop lighter-weight vehicle designs that can increase fuel efficiency, reduce emissions, and decrease fuel costs while using smaller engines to achieve the same level of performance. A study from the Massachusetts Institute of Technology estimates that for every 10% reduction in vehicle weight, fuel economy could increase by 6% for cars and 8% for light-duty trucks.[42] Considering that the annual U.S. energy consumption of cars and light-duty trucks is above 16,000 TBtu,[43] reducing the vehicle weight of cars and light-duty trucks by 10% with lightweight high-strength materials could save 1,060 TBtu of energy,[44] 72 MMT of CO_2 emissions,[45] and $34 billion in fuel costs each year (assuming an estimated cost of motor gasoline of $3.98 per gallon or $31.84 per MBtu).[46]

Breakthrough Opportunities

The MSE community can advance lightweight high-strength materials by focusing on low-cost processing and synthesis and hybrid materials. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow lightweight high-strength materials to make significant contributions toward addressing energy, environmental, and economic needs.

Lightweight High-Strength Materials

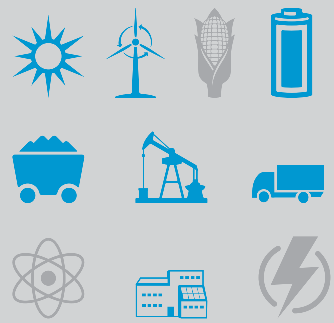
Processing and Synthesis

Lightweight high-strength materials, such as composites, aluminum, magnesium, titanium, high-strength steel alloys, hybrid materials, and polymer-based materials, are limited by costly and energy-intensive synthesis processes. For example, lightweight high-strength steels used in automotive applications (e.g., transformation-induced plasticity steel [TRIP] and twinning-induced plasticity steel [TWIP]) require complex, costly heat treatments.[47] To bring down the cost of these and other synthesis processes for lightweight high-strength materials, materials scientists must develop more efficient processes with fewer steps and reduced energy requirements.

GAPS AND LIMITATIONS TO OVERCOME

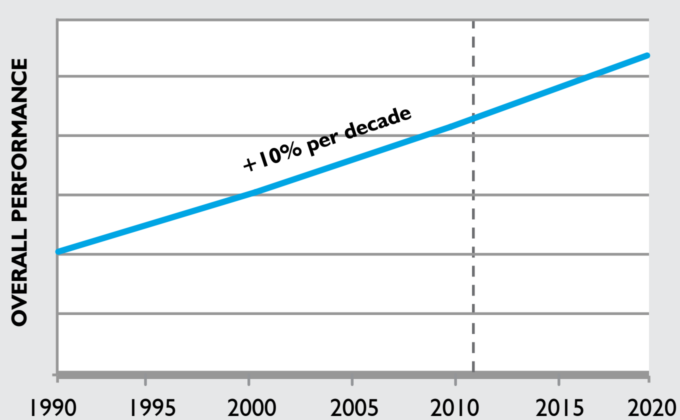
- Current processing and synthesis of lightweight alloys produces materials with inadequate wear and corrosion properties.
- No low-cost synthesis, processing, or manufacturing technologies exist for titanium, magnesium, and composites that can meet targeted costs and weight reductions as well as desired materials properties.

Market Impact



Historical Trends and Future Opportunities

OVERALL PERFORMANCE OF LIGHTWEIGHT HIGH-STRENGTH MATERIALS



Advances in the processing techniques of lightweight high-strength materials can be measured by overall performance improvements, which include advances in microstructural control, specific strength and stiffness, and fatigue resistance.[48] Performance of lightweight high-strength materials has improved at about 10% per decade for the past 20 years. This trend is expected to continue over the next 10 years.[49]

Overall Performance

- 1990–2011: 10% improvement per decade
- 2011–2020: 10% improvement

Lightweight High-Strength Materials

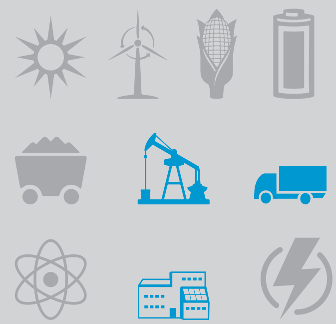
Hybrid Materials

Hybrid materials vary in structure and/or composition throughout a component, which causes a gradient or change in properties throughout the material. This variation is achieved by combining dissimilar materials via novel co-processing. These processes involve a combination of depositing powder metals onto a substrate with incremental changes in the powder composition, layering dissimilar materials in a single step (no secondary manufacturing), and using other structural marriage processes of advanced alloys in sheet, plate, or extruded form. Composites that have anisotropic properties and may be cast using a fiber preform that is infiltrated with resin—a type of co-casting—are also considered hybrid materials. Fiber metal laminate is a new class of metallic materials that combines metals, fibers, and matrix resins.

GAPS AND LIMITATIONS TO OVERCOME

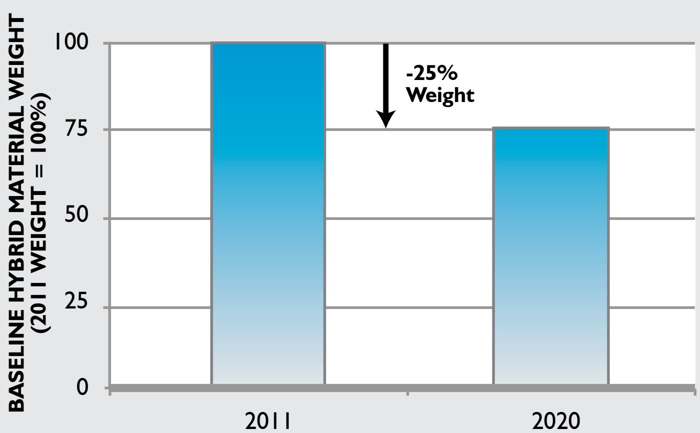
- Few integration strategies exist for dissimilar materials systems, such as automotive body structures. Interfacial properties of composites including dissimilar materials are unknown.
- Many of these processes are newly patented and have unknown impacts on the field of gradient materials.

Market Impact



Historical Trends and Future Opportunities

HYBRID MATERIAL WEIGHT REDUCTION



Hybrid materials are a relatively new technology. Major advancements in hybrid materials over the next 10 years are expected to yield a 25% decrease in weight and an increase in overall performance of specific strength, specific stiffness, and fatigue resistance.[50]

Overall Performance

- 2020: 25% weight reduction

R&D Priority Activities: Lightweight High-Strength Materials

To overcome the gaps and limitations within the lightweight high-strength materials breakthrough opportunities, the MSE community must focus their efforts on improving processing techniques, identifying new alloy designs, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Processing and Synthesis** • **Develop low-cost, improved processing methods of aluminum-, magnesium-, and metal-based composites for casting.** **Hybrid Materials** • **Improve wear resistance via a gradient-type approach or surface treatment of aluminum, magnesium, and other lightweight, high-strength materials.** • **Identify top transportation opportunities for custom optimized hybrid/gradient metallic systems.**
MID TERM (2–5 YEARS)	**Processing and Synthesis** • Improve machining processes for titanium alloys. **Gradient Materials** • **Develop new alloy designs with higher alloy retention for better recyclability.** • **Improve damage detection techniques for defects and mechanical reliability of all types of material systems.** • **Increase corrosion resistance of aluminum or magnesium via surface treatment and/or alloying approaches.** • Develop steels with higher strength and elongation (TWIP and TRIP) to improve the strength-ductility trade-off. **Crosscutting** • Improve thermal/diffusion modeling for designing hybrid/gradient materials.
LONG TERM (5–10 YEARS)	**Crosscutting** • Develop secondary manufacturing processes for gradient material components. • Develop next-generation polymers for use in cars.

*The experts identified the **bolded activities** as high priority.

NOTES

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3 BCS Incorporated for the U.S. Department of Energy (DOE) Industrial Technologies Program (ITP), *Waste Heat Recovery: Technology and Opportunities in U.S. Industry*, (Washington, DC: DOE ITP, 2008), 53, http://www1.eere.energy.gov/industry/intensiveprocesses/pdfs/waste_heat_recovery.pdf. Calculation: 222 TBtu = 1,478 TBtu * 15%.

4 Prepared by Energetics Incorporated for the Industrial Technologies Program, "Energy and Carbon Footprint: All Manufacturing Sectors," 2010, accessed August 29, 2011, http://www1.eere.energy.gov/industry/pdfs/mfg_footprint.pdf. Calculation: 42 $MMTCO_2$ = (222 TBtu/2,850 TBtu) * 544 $MMTCO_2$; calculation assumes offsite electricity is displaced, as compared to onsite generated electricity.

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6 U.S. Department of Energy (DOE) Vehicular Thermoelectric Generator (TEG) Project Objectives (presentation by John W. Fairbanks, *Vehicular Thermoelectrics: A New Green Technology*, DOE Thermoelectric Applications Workshop, Coronado, CA, January 3–8, 2011).

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8 Ibid. A 5% increase in fuel economy results in a 4.76% decrease in fuel consumption. Calculation: 781 TBtu = (8,831 TBtu + 7,572 TBtu) * 4.76%.

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12 Pacific Northwest National Laboratory and BCS Incorporated for the U.S. Department of Energy (DOE) Industrial Technologies Program (ITP), *Engineering Scoping Study of Thermoelectric Generator Systems for Industrial Waste Heat Recovery,* (Washington, DC: DOE, November 2006), http://www1.eere.energy.gov/industry/imf/pdfs/teg_final_report_13.pdf.

13 Ibid.

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15 Corning Incorporated, (PowerPoint presentation, U.S. Department of Energy, first meeting, May 23, 2011).

16 Ibid.; E. Godlewska et al., "Protective Coating to Suppress Degradation of CoSb3 Thermoelectric at Elevated Temperatures," *Ceramic Materials* 62, no. 4 (2010): 490–495; Jong-Ah Paik et al., "Aerogels as a Sublimation Suppression Layer for Thermoelectric Power System," (presentation, Materials Research Society 2005 Spring Meeting, San Francisco, CA, March 28–April 1, 2005).

17 The Minerals, Metals, & Materials Society (TMS) in support of the U.S. Department of Energy (DOE) Industrial Technologies Program, *Linking Transformational Materials and Processing For an Energy-Efficient and Low-Carbon Economy: Creating the Vision and Accelerating Realization* (Washington, DC: TMS, 2010), 18.

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20 Ibid, Table 2.1, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_3.pdf.

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22 U.S. Energy Information Administration (EIA), *Monthly Energy Review, May 2011* (Washington, DC: EIA, May 2011), Table 2.1, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_3.pdf; EIA, Form EIA-860, "Annual Electric Generator Report," http://www.eia.gov/cneaf/electricity/page/capacity/existingunits2008.xls. Calculation: 348 TBtu = 39,579 * (88%) * 1%; calculation assumes equal capacity factors of various generation technologies.

23 U.S. Energy Information Administration (EIA), *Electric Power Annual* (Washington, DC: EIA, April 2011), Table 8.1, http://www.eia.doe.gov/cneaf/electricity/epa/epat8p1.html.

24 U.S. Energy Information Administration (EIA), *Monthly Energy Review, May 2011* (Washington, DC: EIA, 2011), Table 12.1, http://www.eia.gov/totalenergy/data/monthly/pdf/sec12_9.pdf. Calculation: 22 $MMTCO_2$ = 1% * (1,828 $MMTCO_2$ + 399 $MMTCO_2$).

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30 Calculation: (17 MBtu – 1.8 MBtu) * 1,000,000 = 15.2 TBtu.

31 Calculated by examining energy consumption and CO_2 emissions in the transportation equipment industry (NAICS 336) based on *Energy and Carbon Footprints*, Department of Energy, Industrial Technologies Program, http://www1.eere.energy.gov/industry/pdfs/transport_footprint.pdf.

32 U.S. Energy Information Administration (EIA), *Monthly Energy Review, May 2011* (Washington, DC: EIA, 2011), Table 2.6, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_13.pdf.

33 U.S. Energy Information Administration (EIA), *Monthly Energy Review, May 2011* (Washington, DC: EIA, 2011), Table 2.1, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_3.pdf.

34 U.S. Energy Information Administration, Form EIA-860, "Annual Electric Generator Report," http://www.eia.gov/cneaf/electricity/page/capacity/existingunits2008.xls.

35 Calculation for natural gas consumption: 108 TBtu = 39,579 * (27.3%) *1% (calculation assumes equal capacity factors of various generation technologies); calculation for coal consumption: 240 TBtu = 39,579 TBtu * 60.7% * 1% (calculation assumes equal capacity factors of various generation technologies); 348 TBtu = 108 TBtu + 240 TBtu.

36 U.S. Energy Information Administration (EIA), *Electric Power Annual* (Washington, DC: EIA, April 2011) Table 8.1, http://www.eia.doe.gov/cneaf/electricity/epa/epat8p1.html.

37 U.S. Energy Information Administration (EIA), *Monthly Energy Review, May 2011* (Washington, DC: EIA, 2011), Table 12.1, http://www.eia.gov/totalenergy/data/monthly/pdf/sec12_9.pdf; Calculation for natural gas: 4 $MMTCO_2$ = 1% * 399 $MMTCO_2$; Calculation for coal: 18 $MMTCO_2$ = 1% * 1,828 $MMTCO_2$; 22 $MMTCO_2$ = 4 $MMTCO_2$ + 18 $MMTCO_2$.

38 A.S. Khanna et al., "Hard Coatings Based on Thermal Spray and Laser Cladding," *International Journal of Refractory Metals and Hard Materials* 27, no. 2 (2009): 485–491; Matthew Bray, Andrew Cockburn, and William O'Neill, "The Laser-Assisted Cold Spray Process and Deposit Characterization" *Surface and Coatings Technology* 203, no. 19 (2009): 2,851–2,857; Anders Hjörnhede and Anders Nylund, "Adhesion Testing of Thermally Sprayed and Laser Deposited Coatings," *Surface and Coatings Technology* 184, no. 2–3 (2004): 208–218; S. Sampath et al., "Role of Thermal Spray Processing Method on the Microstructure, Residual Stress and Properties of Coatings: An Integrated Study for Ni–5 wt.%Al Bond Coats," *Materials Science and Engineering:* A 364, no. 1–2 (2004): 216.

39 A. Boustini, "Remanufacturing and Energy Savings" (master's thesis, MIT, 2010); Energetics Incorporated, *A Roadmap for Recycling End-of-Life Vehicles of the Future* (Washington, DC: U.S. Department of Energy Office of Advanced Automotive Technologies/Argonne National Laboratory, 2001); Kenneth Peattie and M. Seitz, "Meeting the Closed-Loop Challenge: The Core of Remanufacturing," *California Management Review* 46, no. 2 (2004): 74–89; Vanessa Smith and Gregory Keoleian, "The Value of Remanufactured Engines: Life-Cycle Environmental and Economic Perspectives," *Journal of Industrial Ecology* 8, no. 1–2 (2004): 193–221; Robert Lund, *Remanufacturing: The Experience of the United States and Implications for Developing Countries* (Washington, DC: World Bank, 1984); William Hauser and Robert Lund, *Remanufacturing: Operating Practices and Strategies* (Brookline, MA: Boston University, 2008): 2.

40 A.S. Khanna et al., "Hard Coatings Based on Thermal Spray and Laser Cladding," *International Journal of Refractory Metals and Hard Materials* 27, no. 2 (2009): 485–491; Matthew Bray, Andrew Cockburn, and William O'Neill, "The Laser-Assisted Cold Spray Process and Deposit Characterization" *Surface and Coatings Technology* 203, no. 19 (2009): 2,851–2,857; Anders Hjörnhede and Anders Nylund, "Adhesion Testing of Thermally Sprayed and Laser Deposited Coatings," *Surface and Coatings Technology* 184, no. 2–3 (2004): 208–218; S. Sampath et al., "Role of Thermal Spray Processing Method on the Microstructure, Residual Stress and Properties of Coatings: An Integrated Study for Ni–5 wt.%Al Bond Coats," *Materials Science and Engineering:* A 364, no. 1–2 (2004): 216.

41 John L. Sullivan and Elisa Cobas-Flores, *Full Vehicle LCA's: A Review* (Warrendale, PA: SAE International, 2001).

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43 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls.

44 Ibid. A 6% increase in fuel economy results in a 5.66% decrease in car fuel consumption. An 8% increase in light-duty truck fuel economy results in a 7.41% decrease in fuel consumption. In 2008, cars consumed 8,831 TBtu and light-duty trucks consumed 7,572 TBtu. Calculation of energy savings for cars: 500 TBtu = 8,831 TBtu * 5.66%; Calculation of energy savings in light-duty trucks: 561 TBtu = 7,572 * 7.41%; 500 TBtu + 561 TBtu = 1,061 TBtu.

45 Ibid, Table 11.7, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table11_07.xls. In 2008, light-duty vehicles alone produced 1,113 MMT of CO_2. Calculation, assuming car CO_2 emissions make up 54% of total car and truck emissions, based on the fraction of energy consumed by cars compared to light-duty trucks: 54% = 8,831 TBtu/(8,831 TBtu + 7,572 TBtu). Then 34 $MMTCO_2$ = 1,113.3 $MMTCO_2$ * 5.66% * 54%; 38 $MMTCO_2$ = 1,113 * 7.41% * 46%; 34 $MMTCO_2$ + 38 $MMTCO_2$ = 72 $MMTCO_2$.

46 Ibid, Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls; U.S. Energy Information Administration (EIA), *Monthly Energy Review*, *June 2011* (Washington, DC: EIA, 2011), Table 9.4, http://www.eia.gov/totalenergy/data/monthly/pdf/sec9_6.pdf; EIA, *Annual Energy Review 2009*, (Washington, DC: EIA, August 2010), Appendix A, Table A1, http://www.eia.gov/totalenergy/data/annual/pdf/sec13_1.pdf; EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics," last updated July 5, 2011, accessed July 13, 2011, http://www.eia.gov/energyexplained/index.cfm?page=oil_home#tab2. Note that the price of motor gasoline is used in this example for simplicity purposes. Using diesel in these examples would yield different results because of differences in prices and heat content. Cost of motor gasoline based on $3.98 per gallon or $31.84 per MBtu, including taxes, (data from EIA, *Monthly Energy Review, May 2011*), energy content for motor gasoline of 5.253 MBtu per barrel (EIA, *Annual Energy Review 2009*), and a barrel to gallon conversion for petroleum products of 42 gallons per barrel (EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics").

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VI. NEW PARADIGM MATERIALS MANUFACTURING PROCESSES

It is fundamentally energy-intensive to manufacture materials such as steel and aluminum. Producing lower-volume materials, such as titanium and composites, can be even more energy-intensive due to the need for specialized processing techniques, increased mining and extraction energy requirements, and the complex chemistries and compositions of the final material. In addition to requiring a substantial amount of energy, the manufacturing of materials wastes resources during the production process and does not typically consider waste at the end of a product's life.

New paradigm materials manufacturing processes are needed to make the manufacturing of materials more sustainable. Minimizing the loss of both energy and materials in manufacturing processes is critical to improving process efficiency and cost-effectiveness. Increasing process yields, combining and streamlining steps, and recovering and recycling materials and energy will help minimize material and energy waste streams and produce higher-quality materials. Ultimately, these process innovations can reduce the cost, environmental impact, and energy requirements of energy generation, storage, and use across U.S. energy sectors.

The following pathways provide a guide for research and development (R&D) in the area of new paradigm materials manufacturing processes:

- Net-Shape Processing
- Additive Manufacturing
- Low-Cost Composites Manufacturing
- Energy-Efficient Metals Production

NET-SHAPE PROCESSING

Net-shape processing improves the manufacturing of hard-to-form materials. Techniques like thixocasting, rheo-casting, power metallurgy, net-shape forging, and laser processing can reduce material waste, thereby reducing energy requirements within processes such as melting, casting, and rolling. These techniques can also eliminate or reduce the number of processing steps, such as melting and remelting steps, and can achieve downstream savings in lightweight transportation manufacturing by producing metal components and composites with better materials properties. As a result, these improvements can increase efficiency and reduce costs in the energy sector. Opportunities in industrial processes and transportation sectors provide quantifiable justification for pursuing R&D of net-shape processing.

Market Opportunity: Industrial Processes

Industrial materials manufacturing uses a significant amount of energy. In 2006, the iron and steel industry consumed 1,481 trillion British thermal units (TBtu) of primary energy (excluding feedstocks) and emitted 62 million metric tons (MMT) of carbon dioxide (CO_2) using this energy. Similarly, the aluminum industry consumed 603 TBtu of primary energy (excluding feedstocks) and emitted 36 MMT of CO_2 using this energy.[1]

Near net-shape casting/strip casting is a net-shape processing technique that integrates casting and hot rolling into one step, reducing the need to reheat metal before rolling it.[2] Using this technique could greatly reduce the amount of energy consumed by these materials industries, as well as the associated CO_2 emissions and costs. For example, according to a 2004 Lawrence Berkeley National Laboratory study, using near net-shape casting/strip casting in the iron and steel sector has the potential to save 400 TBtu of primary energy per year in 2025 (100% market penetration). These calculations are based on the assumption that in 2025 the iron and steel sector will consume 1,578 TBtu.[3] Assuming the fuel saved is natural gas, this reduction in energy use equates to a potential savings of 16.7 MMT of CO_2 per year and $2.041 billion in energy cost savings (for a 400 TBtu reduction in 2025), and a potential savings of 6.7 MMT of CO_2 per year and $810 million in energy cost savings per year (for a 160 TBtu reduction in 2025).[4]

Market Opportunity: Transportation

Reducing vehicle weight is an important component of improving fuel economy. According to a study by the Massachusetts Institute of Technology (MIT), for every 10% reduction in vehicle weight, fuel economy could increase by 6% for cars and 8% for light-duty trucks.[5] Net-shape processing techniques can help to reduce the cost of processing metals, enabling the use of high-performance, lightweight metals in vehicles. For example, hot stamping of steel enables the production of complex, lightweight, strong components without the need for costly secondary processing and machining. Such advances in metals and materials processing could help displace some portion of the 8,831 TBtu consumed by cars and 7,572 TBtu consumed by light-duty trucks each year.[6] For example, if the weight of all vehicles in the U.S. car and light-duty truck fleet was reduced by 10%, the resulting energy savings would total 1,060 TBtu annually,[7] with a 72 MMT annual reduction in CO_2 emissions[8] and a $34 billion reduction in fuel costs.[9]

Breakthrough Opportunities

The materials science and engineering (MSE) community can advance net-shape processing by focusing on improving solid-state forming, powder metallurgy, and casting. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow net-shape processing to make significant contributions toward addressing energy, environmental, and economic needs.

Net-Shape Processing

Solid-State Forming

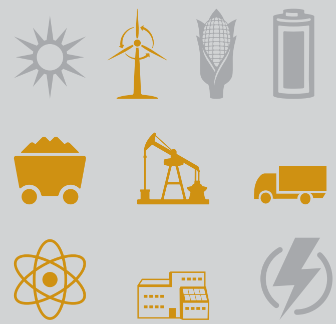
Solid-state forming is the shaping of wrought and worked materials into a net shape via processes such as stamping, forging, and sheet/bulk forming. Property control and heat treating can also be incorporated into solid-state forming, such as in hot stamping of steel, where quenching takes place in a die. The shape is largely produced when the material is warm and more formable and then quenched to a hard state, which would not be easily formed.

Complex, high-property components are often made by machining or assemblies, but are much more efficiently produced by controlling the state of the material and the process. Processes that enable more complex, efficient components include superplastic forming, hydroforming, hot gas forming, electromagnetic forming, hybrid electromagnetic forming, impulse forming, and advanced variants of current technologies such as blank-holder control in stamping and the applications of servo-presses. Advanced forming of materials in their desired microstructural state, as is the case in cold forging and impulse forming, also improves efficiency.

GAPS AND LIMITATIONS TO OVERCOME

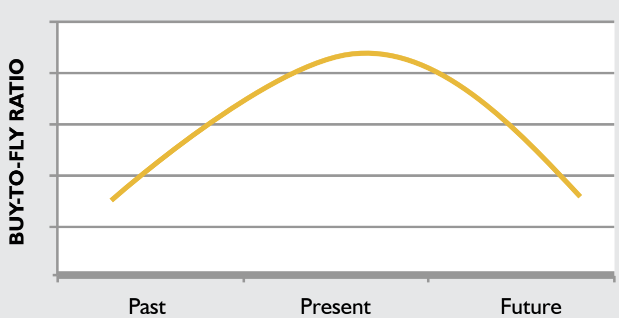
- There are few facilities that are equipped for advanced solid-state forming.
- Dies are needed for each new component. This adds cost and lead time to the net-shape process, favoring machined or assembled components.
- Many high strength-to-weight materials, such as magnesium, are particularly difficult to form via solid-state forming.
- Due to shortcomings in computational design, materials scientists are largely unable to tailor microstructures to needed specifications.

Market Impact



Historical Trends and Future Opportunities

FUTURE BUY-TO-FLY RATIO FOR SOLID-STATE-FORMED PARTS



The historical improvement of solid-state forming is best measured by the "buy-to-fly" ratio, which is the mass of material that is required to machine a part compared to the mass of material in the finished part. In the past, little secondary machining was needed, therefore little material was wasted. Today, high-speed machining is more prevalent and more material is wasted, which increases the buy-to-fly ratio. Advanced solid-state forming will enable the manufacture of parts without the need for additional machining, leading to an expected drop in the buy-to-fly ratio in the future.

Net-Shape Processing

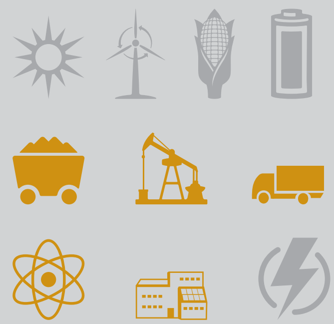
Powder Metallurgy

Powder metallurgy is the process of taking fine powders and bonding them into solid shapes via elevated temperatures and pressures. While extrusion, casting, and forging techniques involve solid-liquid phase changes during processing, powder metallurgy is more flexible because there is no need for phase control. Near net-shape processing of powders often generates parts that do not need secondary processing or machining, unlike other unfinished materials, such as metal ingots, that require such processing. Due to these processing advantages, there is currently interest in using powder metallurgy to combine dissimilar metals, known as functionally graded materials. Laser powder deposition and solid-state powder dynamic compaction are two energy-efficient and near-net manufacturing processes that will be used in the development and fabrication of functionally graded materials.

GAPS AND LIMITATIONS TO OVERCOME

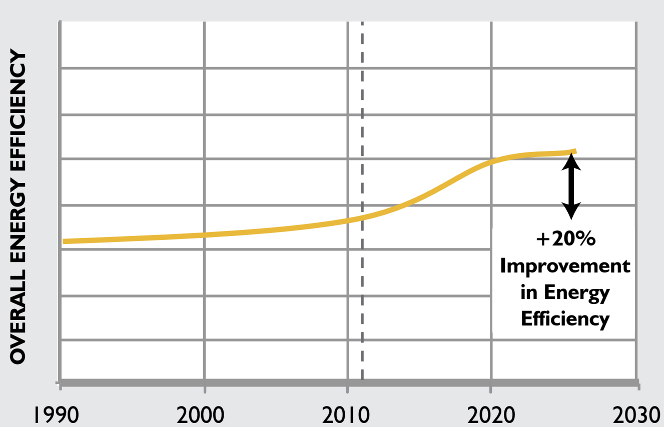
- Net-shape powder processing is hindered by batch processing and requires advances in continuous processing.
- Due to shortcomings in computational design, materials scientists are unable to tailor microstructures to needed specifications.

Market Impact



Historical Trends and Future Opportunities

ENERGY EFFICIENCY OF POWDER METALLURGY



The energy efficiency of powder metallurgy has been relatively stable over the past 20 years. Over the next 10 years, it is expected to improve by about 20% due to decreases in the costs of new powder metallurgy technologies and high-performance powder materials, as well as the movement from batch to continuous processing. After a rapid increase in energy efficiency over the span of a few years, the rate of change of energy efficiency is expected to level off.[10]

Energy Efficiency

- 1990–2011: Minimal
- 2011–2020: 20%

Net-Shape Processing

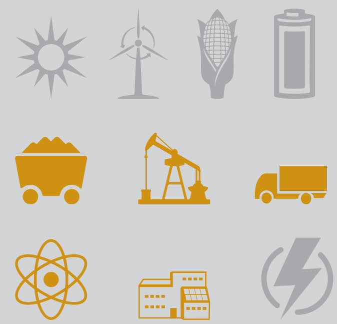
Casting

Casting is the process of pouring a liquid material into a mold and allowing it to solidify. Sand casting processes use silica (SiO_2) sand grains bonded with wet clay to surround a removable pattern. Investment casting, which is ideally used in the precision manufacture of turbine blades, golf club heads, and medical prostheses, uses a mold that is melted away, enabling manufacturing of parts with high complexity. In permanent mold and pressure die casting processes, a liquid is poured into a metallic cavity to solidify into a net-shape casting, and the mold can be reused to create additional parts. These parts have excellent surface finishes and dimensional accuracies, but have limited complexity and shape, and high costs for the molds and dies.[11]

GAPS AND LIMITATIONS TO OVERCOME

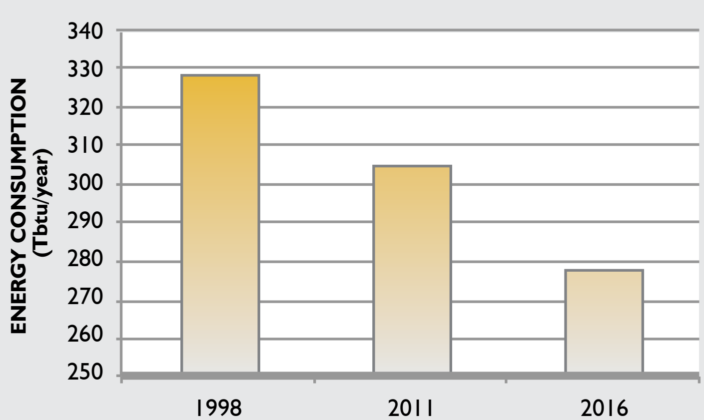
- Today's casting uses large amounts of material to reduce surface defects and eliminate warping.
- Due to shortcomings in computational design, materials scientists are largely unable to tailor microstructures to needed specifications.
- Entrapped gases in some casting processes result in undesirable porosity of parts. This effect can result from poor atmosphere control, improper venting, or turbulent flow of the liquid metal/slurry in the mold.

Market Impact



Historical Trends and Future Opportunities

ENERGY CONSUMPTION IN THE METAL CASTING INDUSTRY



Metalcasting is one of the most energy-intensive industries in the United States. Through advanced melting technologies, scrap reduction, and innovative casting processes, the metalcasting industry has and will continue to reduce energy consumption. In 1998, energy consumption in the metalcasting industry was 328 TBtu/year. Today, energy consumption is approximately 304 TBtu/year, and will effectively decrease at a rate of 5 TBtu/year to about 279 TBtu/year in the year 2016.[12]

Energy Consumption (TBtu/year)

- 1998: 328 TBtu/year
- 2011: 304 TBtu/year
- 2016: 279 TBtu/year

R&D Priority Activities: Net-Shape Processing

To overcome the gaps and limitations within the net-shape processing breakthrough opportunities, the MSE community must focus their efforts on developing new processing capabilities, advancing joining methods, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Solid-State Forming** • Adopt an alloy-to-part single melt approach to replace the master alloy/heat approach that is currently used by many cast alloys. **Casting** • Improve casting integrity using modeling techniques to boost production and limit rejects. **Crosscutting** • **Use innovative joining methods to improve dimensional control and enable forged and formed components to replace machined components and assemblies (fits all time ranges because this is an ongoing effort).**
MID TERM (2–5 YEARS)	**Solid-State Forming** • **Increase closed-loop, spring-back control and strain-distribution control for high-strength sheet metal components.** • **Improve room-temperature formability of magnesium-, titanium-, and aluminum-sheet metals by controlling crystallographic texture.** **Powder Metallurgy** • **Develop new nanomaterials (e.g., tooling and bearings) using spark plasma sintering techniques.** • **Develop a process for direct consolidation of titanium powder into tubular and structural shapes.** **Casting** • **Develop and commercialize a process for high-property, thin-walled, complex light metal castings.** • **Develop a metal casting technique that uses a high magnetic field to achieve wrought properties and improved yield.** **Crosscutting** • **Develop multi-material processing techniques.** • **Use innovative joining methods to improve dimensional control and enable forged and formed components to replace machined components and assemblies (fits all time ranges because this is an ongoing effort).**
LONG TERM (5–10 YEARS)	**Solid-State Forming** • **Develop processes that simultaneously improve both shape and material properties (e.g., variations of hot stamping, peen forming, and temperature-controlled stamping).** **Casting** • Develop sand-casting pattern techniques to replace additive manufacturing investment casting techniques. **Crosscutting** • **Use innovative joining methods to improve dimensional control and enable forged and formed components to replace machined components and assemblies (fits all time ranges because this is an ongoing effort).**

*The experts identified the **bolded activities** as high priority.

ADDITIVE MANUFACTURING

Additive manufacturing is a group of processes that builds up parts by adding material, often in layers. These processes enable the modification of a particular area of a part that requires a specific dimensional tolerance instead of modifying the entire part, helping to reduce energy-intensive finishing and heat treatment operations. As a result, these niche processes can improve hard-to-form, high-value products, such as tooling, medical devices, hip and joint implants, thermoelectric materials, and solar panels, and can aid in the repair and remanufacture of products. Implementing additive manufacturing can increase efficiency and reduce costs in the energy sectors. The opportunity to aid in the repair and remanufacturing of automotive parts provides quantifiable justification for pursuing R&D of additive manufacturing.

Market Opportunity: Transportation

Repairing and remanufacturing is one way that the automotive industry can reduce energy use and prevent the waste of end-of-life vehicle parts. Additive manufacturing can be used to remanufacture vehicle parts, which consumes 2%–25% of the energy required for the manufacture of new parts.[13] Capturing these savings by increasing the use of remanufactured parts could have substantial energy and emissions reduction benefits. For example, the manufacture of a new diesel engine requires 17 million Btu (MBtu) and the remanufacture of a similar engine requires only 10% of that energy (1.8 MBtu).[14] If one million engines were remanufactured instead of manufacturing new engines, an estimated 15 TBtu of energy[15] and 0.9 MMT of CO_2 emissions could be saved each year.[16] Additional savings could result from using additive manufacturing in the remanufacture of other vehicle parts.

Breakthrough Opportunities

The MSE community can advance additive manufacturing by focusing on improving metals manufacturing, polymers manufacturing, direct writing methods, and multifunctional manufacturing. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow additive manufacturing to make significant contributions toward addressing energy, environmental, and economic needs.

Additive Manufacturing

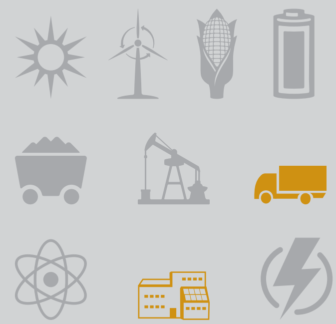
Metals Manufacturing

The design flexibility of metals additive manufacturing can improve the quality of complex, lightweight parts. Direct metal laser sintering (DMLS) is an additive manufacturing technology that uses a 3-D computer-aided design drawing as a blueprint for precisely melting metal powders together with a laser beam. Another type of additive manufacturing for metal parts is electron beam melting (EBM), which melts metal powder together one layer at a time with an electron beam inside a vacuum. In contrast to DMLS, EBM produces parts that are denser and void-free.

GAPS AND LIMITATIONS TO OVERCOME

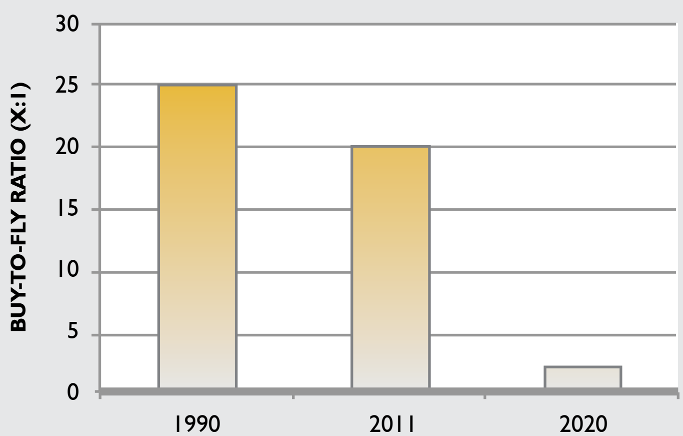
- While additive manufacturing techniques like EBM and DMLS produce higher-quality products than milling techniques, the processes are slow and extremely expensive for metal parts production.

Market Impact



Historical Trends and Future Opportunities

BUY-TO-FLY RATIO FOR METAL PARTS



Metal additive manufacturing technologies have improved the buy-to-fly ratio of metal parts, which is defined as the mass of material that is required to machine a part compared to the mass of material in the finished part. Machining improvements have changed the buy-to-fly ratio from 25:1 to 20:1 in the past 20 years. In the next 10 years, this ratio is expected to reach 2:1.[17]

Buy-to-Fly Ratio

- 1990: 25:1
- 2011: 20:1
- 2020: 2:1

Additive Manufacturing

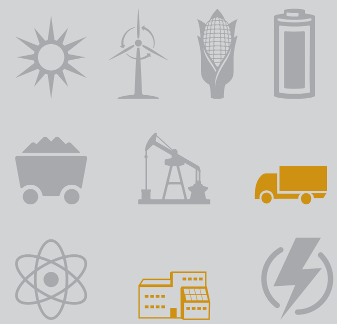
Polymer Manufacturing

Polymer additive manufacturing (also known as direct digital manufacturing [DDM] of polymers) can create new parts quickly, usually within a few hours to one day. Fused deposition modeling (FDM) is an additive manufacturing technology that uses 3-D computer-aided design drawing as a blueprint for creating thermoplastic parts. FDM technology has a precise extrusion head that deposits layers upon layers of thermoplastic resin to create a 3-D polymer part. Stereolithography (SL), another polymer manufacturing technology, produces thermoset polymer cross-sections by focusing an ultraviolet laser into a batch of photo-reactive resin.

GAPS AND LIMITATIONS TO OVERCOME

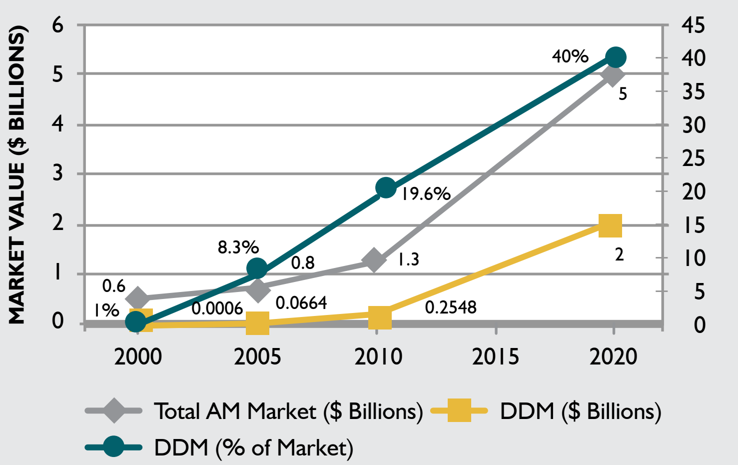
- FDM and SL processes require expensive machines that need major improvements to compete with conventional injection molding costs and production rates.
- Material options are limited and need to incorporate nanotechnologies to provide a wider range of design options.
- Designers are not yet optimizing parts based on the full capabilities of these systems to improve affordability and performance.
- Specialized software designed to optimize known product applications is underdeveloped.

Market Impact



Historical Trends and Future Opportunities

DIRECT DIGITAL MANUFACTURING MARKET VALUE



From 2003 to 2010, DDM has grown from 3.9% of the total additive manufacturing (AM) market to 19.6% of the market, according to *Wohlers Report 2011*. In the next 10 years, DDM has the potential to capture a significant percentage of the total additive manufacturing market.

The total value of the AM market has grown from $601.1 million in 2000 to $1.325 billion today. By 2020, the AM market is projected to reach $5.2 billion, according to Wohlers Associates, Inc.[18]

Additive Manufacturing

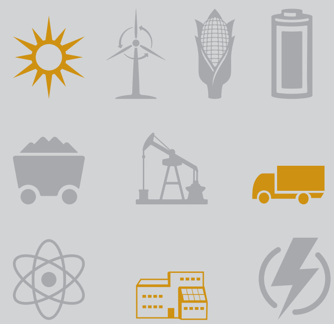
Direct Writing

Direct writing in additive manufacturing is an advanced printing method that enables the production of thermal coatings, dielectric materials, and laser-printed electronics at relatively low cost. This process is a large-scale production technique that allows the user to manufacture at the nanoscopic level. One example of direct writing is aerosol printing, which can be used to print nanoparticle inks such as silver, gold, or platinum in solar arrays.

GAPS AND LIMITATIONS TO OVERCOME

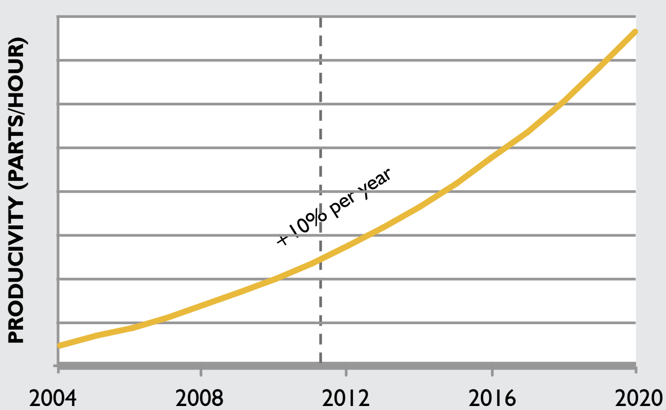
- Aerosol printing technologies and other deposition techniques have poor control of ink aggregation and size.

Market Impact



Historical Trends and Future Opportunities

PRODUCTIVITY OF DIRECT WRITING TECHNIQUES



When first used in 2004, direct writing technologies were slow, single-point delivery systems with poorly characterized materials. Since 2004, the rate of productivity of these technologies (parts/hour) has grown 10% per year due to advances in manufacturing and deposition techniques and improved deposition materials. This rate of improvement is expected to continue over the next 10 years.

Productivity (parts/hour)

- 2004–2011: 10% increase per year
- 2011–2020: 10% increase per year

Additive Manufacturing

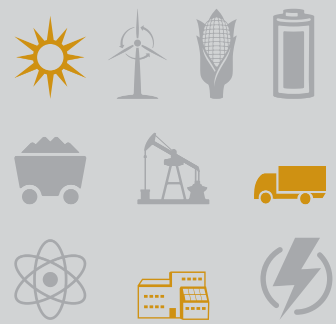
Multifunctional Manufacturing

Multifunctional additive manufacturing is the use of several manufacturing techniques to combine one or more materials into a single component that serves a number of functions, such as providing increased strength, corrosion resistance, and electrical conductivity. This process can increase the service life and efficiency of system components and may decrease part count and weight. Multifunctional manufacturing enables a single component to have a high grade of functional integration, positioning additive manufacturing to help meet the requirements of next-generation multifunctional structures and devices.[19]

GAPS AND LIMITATIONS TO OVERCOME

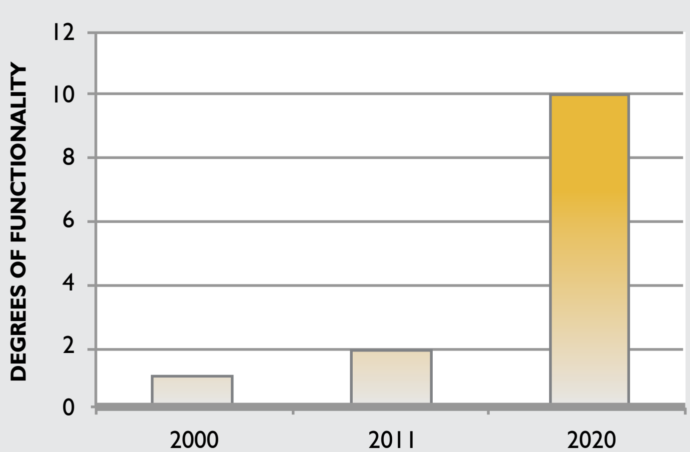
- Current multifunctional additive manufacturing methods are still in their infancy. These methods are currently slow and expensive, and will require major improvements to achieve regular and repeatable part production.
- Today's solar and thermoelectric materials are processed in batches rather than in a continuous manner. Low-cost processing of photovoltaics does not currently exist.

Market Impact



Historical Trends and Future Opportunities

DEGREES OF FUNCTIONALITY AVAILABLE THROUGH ADDITIVE MANUFACTURING



Improvements in multifunctional additive manufacturing can be measured by the maximum degree of functionality of a component. Materials scientists have only recently started to focus on the multifunctionality of materials to reduce system size, cost, and energy requirements. In the next 10 years, several macro- and micro-level design approaches will converge to increase embedded multifunctionality. As a result, the degree of functionality is expected to increase from 2 to 10 over the next 10 years.[20]

Degree of Functionality

- 2000: 1
- 2011: 2
- 2020: 10

R&D Priority Activities: Additive Manufacturing

To overcome the gaps and limitations within the additive manufacturing breakthrough opportunities, the MSE community must focus their efforts on developing new processing techniques, advancing analytical capabilities, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

<table>
<tr>
<td>NEAR TERM
(0–2 YEARS)</td>
<td>
Metals Manufacturing

Develop and advance automated spark plasma sintering techniques for the production of metal-matrix composites (e.g., silicon carbide, silicon nitride, tungsten carbide).
Develop closed-loop hardware/software to provide Ti-6Al-4V (titanium-aluminum-vanadium) material/part traceability for quality standards, thus improving yield numbers.

Polymer Manufacturing

Develop families of polymer compounds with nano-fillers that are compatible with additive manufacturing processes to create a wide spectrum of material properties.
Establish design rules to educate users on design optimization of additive manufacturing processes.
Increase machine throughput while maintaining or increasing system accuracy.

Direct Writing

Develop new inks and slurries for direct writing systems (fits all time ranges because this is an ongoing effort).

Multifunctional Manufacturing

Develop intricate microstructural designs using additive manufacturing to create multifunctional materials and embedded sensors with two or more functions.

Crosscutting

Set up additive manufacturing stations or areas for regional economic zones to lower shipping costs.

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MID TERM (2–5 YEARS)	**Metals Manufacturing** • **Develop a continuous process for titanium metal production, preferably in powder form.** **Polymer Manufacturing** • **Develop methods to increase throughput of additive manufacturing systems while increasing accuracy and in-situ process monitoring.** • Advance fused deposition modeling to create reinforced polymer materials for enhanced material properties. • Identify new processing methods to increase isotropic material properties. **Direct Writing** • **Develop new inks and slurries for direct writing systems (e.g., silver and copper inks) (fits all time ranges because this is an ongoing effort).** • Develop low-cost (e.g., printed) thermoelectric generators to exploit low-grade heat sources. **Multifunctional Manufacturing** • **Create an alternative file format to ".stl" to enable multi-material fabrication in a monolithic piece; less energy-intensive materials may be used functionally in place of a single energy-intensive material.** **Crosscutting** • **Develop larger chambers or multi-heads for direct metal deposition processes (Metals Manufacturing and Multifunctional Manufacturing).** • **Develop a system for sensing and controlling surface quality and residual stresses.** • Develop new manufacturing techniques for specific energy photovoltaic applications (e.g., copper-indium-gallium) (Direct Writing and Multifunctional Manufacturing). • Develop advanced additive manufacturing techniques for hybrid materials such as metal-ceramic, metal-metal, metal-polymer (Metals Manufacturing, Polymer Manufacturing, and Multifunctional Manufacturing).
LONG TERM (5–10 YEARS)	**Polymer Manufacturing** • Develop new finite element analysis predictive software that provides methods to analyze and optimize unique internal structures enabled by additive manufacturing. **Direct Writing** • **Develop large-scale printed energy storage batteries and capacitors (e.g., ones that may be used for wind farms).** • **Develop new inks and slurries for direct writing systems (fits all time ranges because this is an ongoing effort).** **Crosscutting** • **Create a residual stress analytical modeling system for non-vacuum-based additive manufactured systems; this will help predict residual stress or distortion of direct parts to increase yield numbers and increase part robustness.** • **Develop additive system techniques to integrate additive manufacturing systems seamlessly.**

*The experts identified the **bolded activities** as high priority.

LOW-COST COMPOSITES MANUFACTURING

Composite materials can provide reductions in weight, increased strength, and other performance benefits that can improve the efficiency of end products. However, the cost to produce these high-performance materials currently makes them prohibitive for use in many applications. Implementing process improvements that reduce steps and increase production yield can help to reduce the cost of processing metallic and non-metallic composites. As a result, these improvements can enable the increased use of composites to reduce energy use, emissions, and costs in energy sectors. Opportunities in transportation and wind power sectors provide quantifiable justification for pursuing R&D of composites manufacturing.

Market Opportunity: Transportation

In 2008, the U.S. transportation sector was responsible for approximately 28% (28,103 TBtu) of total U.S. primary energy consumption.[21] The same year, light-duty vehicles alone produced 1,113 MMT of CO_2.[22] Incorporating low-cost composites into vehicle design could help the automotive industry improve fuel economy and reduce tailpipe emissions without drastically increasing costs. An MIT study estimated that a 10% reduction in vehicle weight could increase fuel economy by 6% for cars and 8% for light-duty trucks,[23] which could save drivers $34 billion in fuel costs each year.[24] In addition, a 10% reduction in the weight of all vehicles in the U.S. car and light-duty truck fleet could result in a 1,060 TBtu annual reduction in energy[25] and a 72 MMT reduction in CO_2 emissions.[26]

Market Opportunity: Wind Power

The U.S. electric power sector produced 40% of total U.S. energy-related CO_2 emissions in 2010 (2,271 MMT),[27] and major investor-owned utilities, which represent only a portion of U.S. power producers, spent $40.2 billion on fuel in 2009.[28] Wind power represented a 2.3% share of 2010 U.S. electricity net generation (generating 94,647 million kilowatt-hours [kWh] of electricity).[29]

The use of carbon fiber composites to increase wind-turbine blade lengths can increase the overall efficiency, and therefore lower the cost, of wind power production. Rotor power grows with the square of the diameter of the turbine's blades, while the volume of material, and therefore its mass and cost, increases with the cube of the diameter.[30] As a result, low-cost composites could allow increases in turbine blade length, while significantly reducing weight penalties. Low-cost composite materials that allow for the cost-effective design of wind turbines could help wind power gain an even larger share in the U.S. electricity generation sector, reducing fossil fuel consumption, emissions, and costs. For example, if wind power gained an additional 1% market share of U.S. electric power sector production, it could displace 396 TBtu of electricity generation from other sources,[31] decrease CO_2 emissions by 23 MMT,[32] and reduce fuel costs of major investor-owned utilities (which represent only a portion of U.S. power producers) by $412 million per year.[33]

Breakthrough Opportunities

The MSE community can advance low-cost composites manufacturing by focusing on improving fibers manufacturing and developing advanced composite matrices. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow low-cost composites manufacturing to make significant contributions toward addressing energy, environmental, and economic needs.

Low-Cost Composites Manufacturing

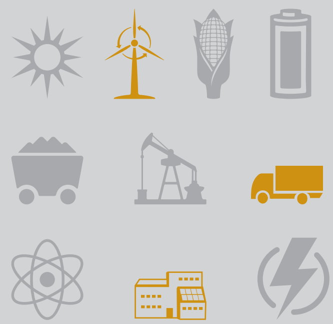
Fibers Manufacturing

Carbon fibers require less energy to manufacture and have fewer problems with corrosion than the metals they replace. They can also be used to reduce the number of parts in a system, decreasing system complexity. To be used more broadly in energy systems, materials scientists must work to reduce the manufacturing costs and energy inputs of fibers manufacturing.

GAPS AND LIMITATIONS TO OVERCOME

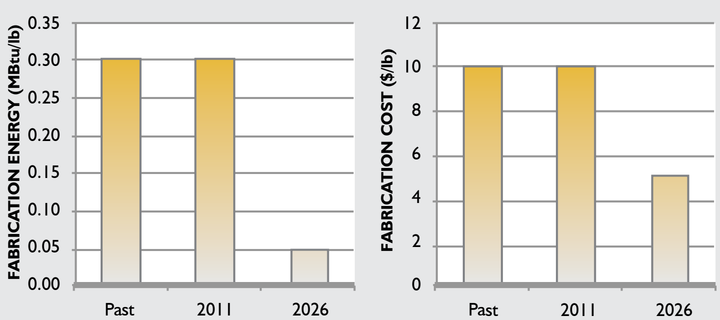
- Radical changes in the carbonization step of the carbon fiber production process are required to lower energy input. Lowering the cost of carbon fiber will be dependent on this factor.

Market Impact



Historical Trends and Future Opportunities

ENERGY REQUIREMENTS AND COSTS OF CARBON FIBER FABRICATION



Since the inception of using polyacrylonitrile (PAN) to replace rayon as a raw material for the manufacture of carbon fiber, there has been little-to-no improvement in carbon fiber fabrication cost and energy requirements. With major advancements in the next 15 years, the energy input of carbon fiber manufacturing can potentially drop from 0.30 MBtu/pound (MBtu/lb) to 0.05 MBtu/lb, and the cost is expected to drop from $10/lb to $5/lb.

Fabrication Energy

- Past/Present: 0.30 MBtu/lb
- 2026: 0.05 MBtu/lb

Fabrication Cost

- Past/Present: $10/lb
- 2026: $5/lb

Low-Cost Composites Manufacturing

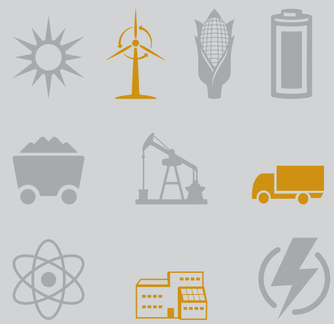
Composite Matrix Manufacturing

Composites, which contain a matrix and a reinforcement of a different material (e.g., fibers and particulates), offer a unique combination of properties (e.g., strength, rigidity, weight) that is not possible with individual materials. While polymer-matrix composites are ideal for carbon fibers, metal- and ceramic-matrix composite (MMC/CMC) systems are excellent materials for use in high-performance cutting tools, one of many useful applications. The advancement of MMC and CMC manufacturing methods have led to lower-cost, higher-quality cutting tools with complex compositions and greatly extended tooling life.

GAPS AND LIMITATIONS TO OVERCOME

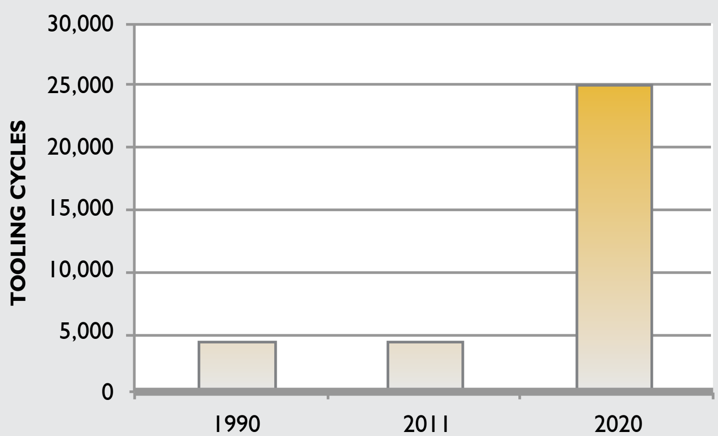
- Advanced MMCs, which have the ability to handle far more tooling cycles than today's current tooling standards, are not yet widely accepted by industry.
- CMCs offer great promise for use in mechanical seals but lack the ability to carry large amounts of deformation.

Market Impact



Historical Trends and Future Opportunities

INDUSTRIAL TOOLING CYCLES OF CUTTING TOOLS



For the past 20 years, cutting tools have had an industry standard of about 4,000 cycles before replacement. State-of-the-art MMCs and CMCs are beginning to demonstrate an ability to reach nearly 25,000 tooling cycles. In the next 10 years, these advanced cutting tools have the potential to become the new standard for tooling life, allowing industry to abandon the current tooling life of 4,000 cycles.

Tooling Cycles

- 1990: 4,000 cycles
- 2011: 4,000 cycles
- 2020: 25,000 cycles

R&D Priority Activities: Low-Cost Composites Manufacturing

To overcome the gaps and limitations within the low-cost composites manufacturing breakthrough opportunities, the MSE community must focus their efforts on automating fabrication processes, identifying new materials, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Composite Matrix Manufacturing** • **Develop new autoclave-free continuous processes (e.g., automation of fiber lay-up in resin transfer molding and vacuum-assisted resin transfer molding) that ensure accurate shape and orientation of polymer-matrix composites.** **Crosscutting** • **Develop automated panel lay-up forming to achieve a high production rate.**
MID TERM (2–5 YEARS)	**Fibers Manufacturing** • **Create fiber manufacturing processes that require less energy to create the final product.** **Crosscutting** • **Develop a high-volume production technology to reduce production cycle times.** • Automate the placement of core materials/components.
LONG TERM (5–10 YEARS)	**Fibers Manufacturing** • **Develop low-cost fiber feedstocks (e.g., by reducing energy input in fiber production or developing alternate precursors to pitch and PAN for carbon fibers).**

*The experts identified the **bolded activities** as high priority.

ENERGY-EFFICIENT METALS PRODUCTION

Improving the energy efficiency of metals production can help to reduce the costs and emissions associated with metals processing. Eliminating processing steps, reducing reheating needs, reducing equipment, and increasing production yields can help to reduce energy usage, equipment and tooling costs, and operation and maintenance costs.[34] As a result, energy-efficient metals production can increase efficiency and reduce costs in the energy sectors. Opportunities in transportation and industrial processes provide quantifiable justification for pursuing R&D of energy-efficient metals production.

Market Opportunity: Transportation

Using lightweight materials in vehicles is integral to improving vehicle fuel economy. Material advances and cost reductions in the primary production of lightweight metals can help to enable the use of high-performance, lightweight metals like aluminum, magnesium, titanium, and multi-material structures in vehicles. Such advances in metals production processes could help displace a portion of the annual 8,831 TBtu of energy consumed by cars and 7,572 TBtu of energy consumed by light-duty trucks.[35] For example, if the weight of vehicles in the whole U.S. car and light-duty truck fleet was reduced by 10%, the resulting energy savings would total 1,060 TBtu annually,[36] with a 72 MMT annual reduction in CO_2 emissions[37] and a $34 billion reduction in fuel costs.[38]

Market Opportunity: Industrial Processes

Manufacturing metals uses a significant amount of energy; in 2006, the iron and steel industry consumed 1,481 TBtu of primary energy (excluding feedstocks) and emitted 62 MMT of CO_2. The aluminum industry consumed 603 TBtu of primary energy (excluding feedstocks) and emitted 36 MMT of CO_2.[39] Process improvements such as using new materials for anodes and cathodes and insulating materials for furnaces and reactors can help to increase efficiency, as can direct reduction technologies that produce titanium in continuous processing, instead of batch processing. Developing new technologies for manufacturing steel and aluminum, such as direct reduction of iron ores, continuous casting of steel, and carbothermic reduction of aluminum, can also aid in efficiency improvements. A 10% reduction in the estimated energy consumption of the U.S. steel manufacturing sector would result in 148 TBtu in energy savings,[40] a 6.2 MMT reduction in CO_2 emissions,[41] and $489 million in savings for the steel manufacturing sector.[42] Similarly, a 10% reduction in the energy consumption of the aluminum manufacturing sector would result in 60 TBtu in energy savings,[43] a 3.6 MMT reduction in CO_2 emissions, and $175 million in savings for the aluminum sector.[44]

Breakthrough Opportunities

The MSE community can advance energy-efficient metals production by improving steel production, aluminum production, recycling technologies, and titanium production. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow energy-efficient metals production to make significant contributions toward addressing energy, environmental, and economic needs.

Energy-Efficient Metals Production

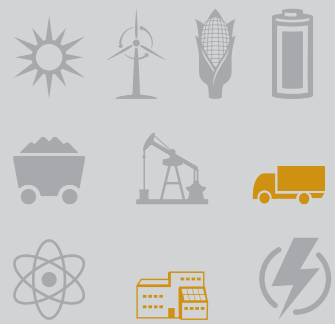
Steel Production

Steel is a widely accepted, low-cost material that is used in many parts of the economy, notably transportation and industrial structures. It consists of iron with small amounts of other elements that alter its properties. Losses of steel product can occur during steel manufacturing processes, including surface grinding, oxide inclusions, and vacuum arc remelting constrictions and excursions. Advancing these processing techniques can provide a greater yield of steel ingots.

GAPS AND LIMITATIONS TO OVERCOME

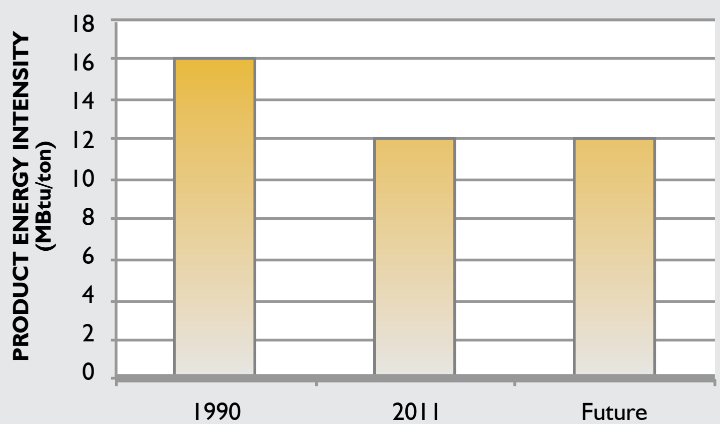
- There are currently no available multi-sensor, integrated spectrum devices or software for solid, liquid, and gas process control, such as metal ion sensors for molten metal processing.

Market Impact



Historical Trends and Future Opportunities

ENERGY INTENSITY OF NORTH AMERICAN STEEL PRODUCTION



The North American steel industry has continually reduced its energy intensity, minimizing the industry's footprint on the environment. Since 1990, energy intensities to make one ton of steel have been reduced by 30 percent, from 16 MBtu/ton to approximately 12 MBtu/ton. As a result of advances in today's steelmaking processes, the industry is approaching the limits defined by the laws of physics. Little improvement is expected in the future without major processing advancements.[45]

Product Energy Intensity

- 1990: 16 MBtu/ton
- 2011: 12 MBtu/ton
- Future: Minimal improvement

Energy-Efficient Metals Production

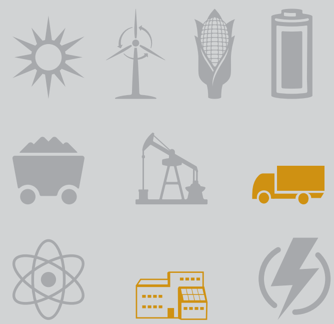
Aluminum Production

Aluminum is the most abundant metal in the earth's crust. It is lightweight, strong, and versatile, and has excellent corrosion resistance and electrical/thermal conductivities. Aluminum is extracted from aluminum oxide by electrolysis—a process that requires high levels of electrical energy with moderately high losses of materials within an aluminum electrolysis cell. Advancing these processes may lower the energy input of aluminum production and increase the product yield.

GAPS AND LIMITATIONS TO OVERCOME

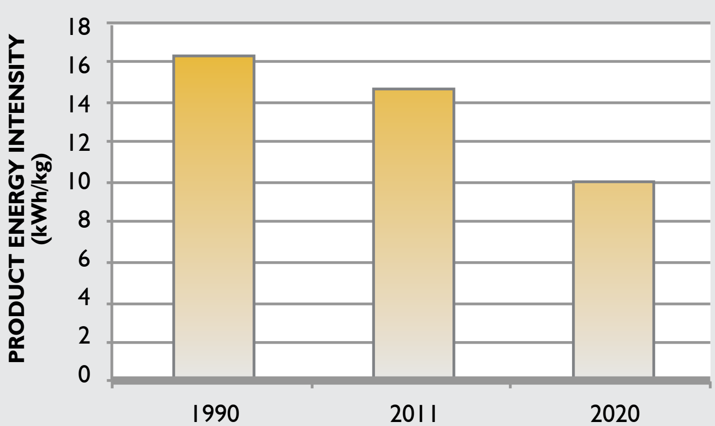
- There are currently no available multi-sensor, integrated spectrum devices or software for solid, liquid, and gas process control, such as metal ion sensors for molten metal processing.
- Carbothermic reduction, an alternative method of aluminum production that uses carbon as a reducing agent during a high-temperature chemical reaction, currently has many limitations, including the inability to attain the high temperatures required, materials of construction constraints, high carbon electrode consumption, inefficient separation of aluminum from carbon, and excessive losses of aluminum.

Market Impact



Historical Trends and Future Opportunities

ENERGY INTENSITY OF ALUMINUM PRODUCTION



The energy consumption of aluminum production has decreased from about 16.1 kWh/kilogram (kg) to 14.5 kWh/kg over the past 20 years. With additional improvements, this level is expected to drop to about 10 kWh/kg in the next 10 years.[46]

Product Energy Consumption

- 1990: 16.1 kWh/kg
- 2011: 14.5 kWh/kg
- 2020: 10 kWh/kg

Energy-Efficient Metals Production

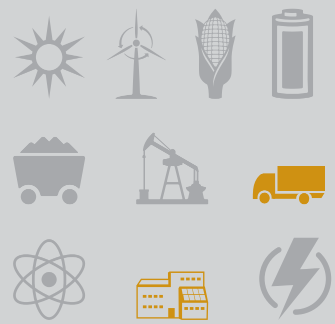
Recycling

Metals recycling technologies have the potential to reduce energy input and produce fewer emissions than creating new metal products. This reduction in energy input through refinement of manufacturing processes can lead to significant economic savings, reduced waste output, and increased metal yield due to fewer oxidative losses.

GAPS AND LIMITATIONS TO OVERCOME

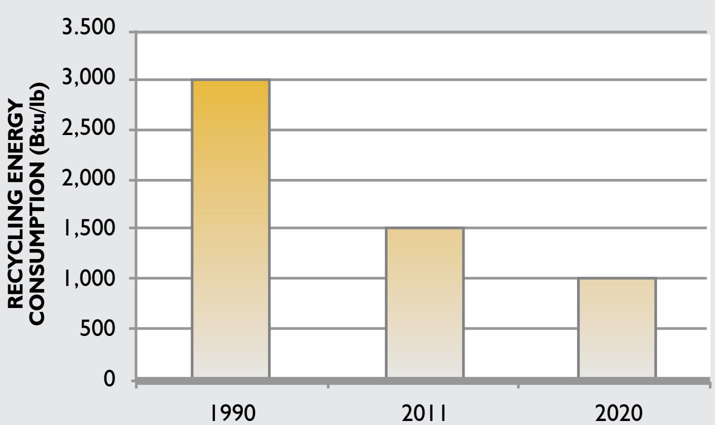
- Current recycling processes are incapable of converting dirty, low-grade materials to high-grade, pure materials. Systems to remove physical contaminants are ineffective and current elemental removal systems (e.g., selective separations) are inefficient.
- Recycling processes rely on inefficient combustion heating in thermal processing. There is a need for low-temperature recycling processes.

Market Impact



Historical Trends and Future Opportunities

ENERGY CONSUMPTION FOR ALUMINUM RECYCLING



Aluminum is one of the easiest metals to recycle and is much cheaper to recycle than mining and refining additional bauxite ores for new aluminum production. Over the past 20 years, energy input for recycling aluminum has dropped from 3,000 Btu/lb to 1,500 Btu/lb. Additional refinements in recycling are expected to lower energy consumption to 1,000 Btu/lb in the next 10 years.[47]

Recycling Energy Consumption

- 1990: 3,000 Btu/lb
- 2011: 1,500 Btu/lb
- 2020: 1,000 Btu/lb

Energy-Efficient Metals Production

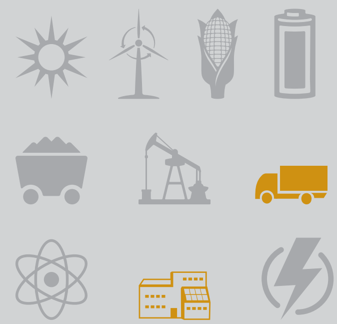
Titanium Processing

Titanium processing, which requires reduction, chlorination, and melting, is energy-intensive due to titanium's high melting point and sensitivity to environmental influences. Titanium naturally forms an oxide layer when exposed to atmospheric conditions, which causes loss of titanium product. Improving titanium processing will produce a greater yield of titanium and require less energy input. Titanium powder has become of growing interest to industry because it is relatively easy to use for processing titanium parts as opposed to starting with titanium ingots. Lately, it has been used extensively in manufacturing cookware and kitchenware, as well as critical aerospace components.

GAPS AND LIMITATIONS TO OVERCOME

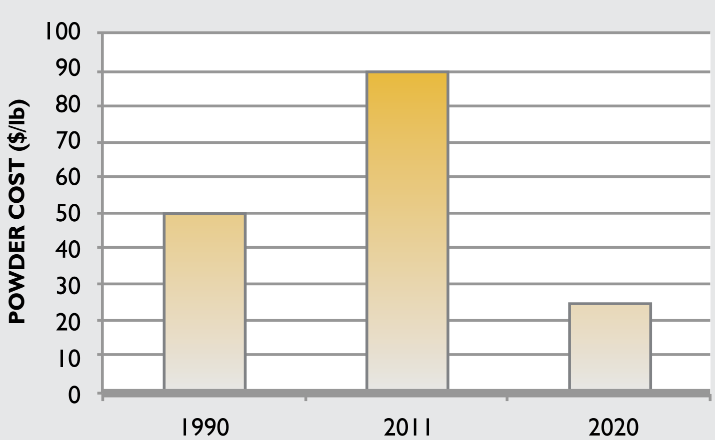
- There are currently no available multi-sensor, integrated spectrum devices or software for solid, liquid, and gas process control, such as metal ion sensors for molten metal processing.
- Altering any processing techniques would require changes to avert titanium's exposure to atmospheric conditions and may reduce the energy efficiency of the process.

Market Impact



Historical Trends and Future Opportunities

COST OF TITANIUM POWDER



The cost of titanium powder has nearly doubled over the past 20 years to approximately $90/lb. With major advances in titanium powder processing, it is possible that this cost may drop to $25/lb in the next 10 years.[48]

Powder Cost

- 1990: $50/lb
- 2011: $90/lb
- 2020: $25/lb

R&D Priority Activities: Energy-Efficient Metals Production

To overcome the gaps and limitations within the energy-efficient metals production breakthrough opportunities, the MSE community must focus their efforts on advancing existing processes, inventing new approaches to metals production, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Aluminum Production** • **Improve instrumentation for aluminum reduction cells, leading to better process control.** **Crosscutting** • Integrate thermal cycling to reduce energy loss from reheating.
MID TERM (2–5 YEARS)	**Aluminum Production** • **Develop new electrode materials for aluminum reduction cells.** **Titanium Processing** • **Develop a continuous process for titanium metal production, preferably in powder form.** • **Develop a titanium molten metal delivery system (i.e., closed-coupled gas atomization) that can lower the cost of production via a high-performance continuous process.** **Crosscutting** • Improve refractory development for aluminum and iron production (i.e., improve production, reduce heat input, reduce contamination) (Aluminum Production, Steel Production).
LONG TERM (5–10 YEARS)	**Steel Production** • **Develop a process for the direct reduction of iron ore using an electrolytic hydrogen or other non-carbon-reduction process.** **Aluminum Production** • **Develop novel electrochemistry processes for the production of aluminum and/or magnesium (e.g., lower-temperature ionic liquids).** **Recycling** • Identify alternative recycling strategies for all major manufacturing/construction materials to minimize energy requirements and greenhouse gas emissions. **Titanium Processing** • **Develop a continuous casting process for high-end alloys (e.g., titanium and nickel).** • Develop beta titanium alloy systems that take advantage of powder processing (e.g., laser-additive manufacturing, hot isostatic pressing, and near net-shape manufacturing). **Crosscutting** • **Advance scaling of melt facilities to increase product yield.** • **Develop a low-cost, high-property magnesium system for high-volume casting or sheet production.** • **Optimize the yield, use, and scale of vacuum-arc remelting and electroslag melting of high-end metals (e.g., iron, nickel, titanium); high-end alloys usually need multiple melting cycles (Steel Production, Titanium Processing).**

*The experts identified the **bolded activities** as high priority.

NOTES

1 Prepared by Energetics Incorporated for the Industrial Technologies Program, "Energy and Carbon Footprint: Iron and Steel," 2010, accessed August 29, 2011, http://www1.eere.energy.gov/industry/pdfs/steel_footprint.pdf.

2 Ernst Worrell, Lynn Price, and Christina Galitsky, *Emerging Energy-Efficient Technologies in Industry: Case Studies of Selected Technologies*, (Berkeley, CA: Lawrence Berkeley National Laboratory, 2004), http://ies.lbl.gov/iespubs/54828.pdf.

3 Ibid.

4 Prepared by Energetics Incorporated for the U.S. Department of Energy, Industrial Technologies Program 2010, "Manufacturing Energy and Carbon Footprints: Iron and Steel," http://www1.eere.energy.gov/industry/pdfs/steel_footprint.pdf. To estimate the carbon emissions associated with 400 TBtu and 160 TBtu in annual energy savings identified by the Lawrence Berkeley National Laboratory (LBNL) report, it is necessary to estimate an emissions factor for the industry. If in 2006, 1,481 TBtu of energy consumed by the sector resulted in 62 million MMT of CO_2, then it could be estimated that each TBtu produces 0.041864 MMT of CO_2/TBtu.Calculations: 0.041866 $MMTCO_2$/TBtu * 400 TBtu = 16.70 $MMTCO_2$; 0.041866 $MMTCO_2$/TBtu * 160 TBtu = 6.70 $MMTCO_2$; U.S. Energy Information Administration (EIA), *Monthly Energy Review, June 2011* (Washington, DC: EIA, 2011), Table 9.11, http://www.eia.gov/totalenergy/data/monthly/pdf/sec9_17.pdf; EIA, *Monthly Energy Review, June 2011* (Washington, DC: EIA, 2011), Table A4, http://www.eia.gov/totalenergy/data/monthly/pdf/sec13_4.pdf. To convert the energy savings identified by LBNL into energy cost savings, it is necessary to know which fuel is being saved by the near net shape/strip casting process. If for example, the reheating energy being displaced was in the form of natural gas, energy cost savings could be estimated by the following: Using the April 2011 average price of natural gas for industrial consumers of $5.23 per thousand cubic feet ($5.10 per MBtu), the 400 TBtu technical savings potential identified by LBNL could be approximated as $2,041 million in energy cost savings, and the 160 TBtu savings estimated by LBNL at 40% market penetration could be approximated as $810 million in energy cost savings per year. Calculations: $5.23 per thousand cubic feet converted into $5.10 per MBtu using a heat contents of natural gas of 1,025 Btu per cubic foot; 400 Tbtu * $5.10 per MBtu = $2,041 million in savings. 160 Tbtu * $5.10 per MBtu = $810 million in savings.

5 Lynette Cheah, John Heywood, and Randolph Kirchain, "The Energy Impact of U.S. Passenger Vehicle Fuel Economy Standards," (presentation, IEEE International Symposium on Sustainable Systems and Technology, Washington, DC, May 17–19, 2010), http://web.mit.edu/sloan-auto-lab/research/beforeh2/files/IEEE-ISSST-cheah.pdf (Note that the study assumed that powertrains are resized to maintain same acceleration performance when vehicle weight is reduced. Fuel consumption [or economy] refer to adjusted figures, which are revised upward [or downward] to better reflect actual, on-road figures, rather than dynamometer test results obtained in the laboratory); Lynette Cheah et al., "Factor of Two: Halving the Fuel Consumption of New U.S. Automobiles by 2035," in *Reducing Climate Impacts in the Transportation Sector*, edited by Daniel Sperling and James S. Cannon (New York: Springer, 2008), web.mit.edu/sloan-auto-lab/research/beforeh2/files/cheah_factorTwo.pdf.

6 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls.

7 Lynette Cheah, John Heywood, and Randolph Kirchain, "The Energy Impact of U.S. Passenger Vehicle Fuel Economy Standards," (presentation, IEEE International Symposium on Sustainable Systems and Technology, Washington, DC, May 17–19,); Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls. Assumes for every 10% weight reduction, fuel economy could increase by 6% for cars and 8% for light-duty trucks. A 6% increase in car fuel economy results in a 5.66% decrease in fuel consumption. An 8% increase in light-duty truck fuel economy results in a 7.41% decrease in fuel consumption. Calculations: Energy savings for cars = 500 TBtu = 8,831 TBtu * 5.66%; energy savings in light-duty trucks = 606 TBtu = 7,572 * 7.41%; 500 TBtu + 561 TBtu = 1,061 TBtu.

8 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 11.7, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table11_07.xls. In 2008, light-duty vehicles alone produced 1,113 MMT of CO_2. Calculations, assuming car CO_2 emissions make up 54% of total car and truck emissions, based on the fraction of energy consumed by cars compared to light trucks: 54% = 8,831 TBtu/(8,831 TBtu + 7,572 TBtu); 34 $MMTCO_2$ = 1,113.3 $MMTCO_2$ * 5.66% * 54%; 38 $MMTCO_2$ = 1,113 * 7.41% * 46%; 34 $MMTCO_2$ + 38 $MMTCO_2$ = 72 $MMTCO_2$.

9 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls; U.S. Energy Information Administration (EIA), *Monthly Energy Review, June 2011*, (Washington, DC: EIA, 2011), Table 9.4, http://www.eia.gov/totalenergy/data/monthly/pdf/sec9_6.pdf; EIA, *Annual Energy Review 2009* (Washington, DC: EIA, August 2010), Appendix A, Table A1, http://www.eia.gov/totalenergy/data/annual/pdf/sec13_1.pdf; EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics," last updated July 5, 2011, accessed July 13, 2011, http://www.eia.gov/energyexplained/index.cfm?page=oil_home#tab2. Note that the price of motor gasoline is used in this example for simplicity purposes. Using diesel in these examples would yield different results because of differences in prices and heat content.Cost of motor gasoline based on $3.98 per gallon or $31.84 per MBtu, including taxes, (EIA, *Monthly Energy Review, May 2011*), energy content for motor gasoline of 5.253 MBtu per barrel (EIA, *Annual Energy Review 2009*), barrel to gallon conversion for petroleum products of 42 gallons per barrel (EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics"). Calculations: $15.9 billion = $281.2 billion * 5.66%; $17.9 billion = $241.08 billion * 7.41%.

10 Bernard Williams, "Powder Metallurgy, A Global Market Review," *Market Review: IPMD 14th Edition 2010–2011* (Shrewsbury, UK: IPMD, 2011); P. Beiss, R. Ruthardt, H. Warlimont (eds.) *Powder Metallurgy Data* (Berlin, Heidelberg: Springer, 2003), 1.1–1.3; Y. Xiong et al., "A Streamlined Life Cycle Assessment on the Fabrication of WC–Co Cermets," *Journal of Cleaner Production* 16, no. 10 (2008): 1,118–1,126.

11 Donald R. Askeland and Pradeep P. Phulé, *The Science and Engineering of Materials, Fifth Edition* (Toronto, Ontario: Thomson, 2006).

12 U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE), Industrial Technologies Program (ITP), "Metalcasting E-SMARRT: Energy-Saving Melting and Revert Reduction Technology," n.d., http://www.e-smarrt.org/; DOE EERE ITP, "Energy-Saving Melting and Revert Reduction Technology," unpublished slide presentation.

13 John Sutherland et al., "A Comparison of Manufacturing and Remanufacturing Energy Intensities with Application to Diesel Engine Production," *CIRP Annals—Manufacturing Technology* 57, no. 1 (2008), 5–8.

14 Ibid.

15 Ibid.

16 Sutherland et al., "A Comparison of Manufacturing and Remanufacturing Energy Intensities," 5–8; Prepared by Energetics Incorporated for the U.S. Department of Energy Industrial Technologies Program, "Energy and Carbon Footprint: Transportation Equipment," 2010, accessed August 29, 2011, www1.eere.energy.gov/industry/pdfs/transport_footprint.pdf. Estimates an emission factor for the transportation equipment industry by examining energy consumption and CO_2 emissions in the transportation equipment industry (NAICS 336) from the energy footprints. Calculation: 54 $MMTCO_2$ per 904 TBtu of energy consumption = 0.05862 $MMTCO_2$ per TBtu. Therefore, 15 TBtu savings are equivalent to 0.05862 $MMTCO_2$ * 15 trillion Btu = 0.9 $MMTCO_2$.

17 David Bourell, Ming Leu, and David Rosen, eds., *Roadmap for Additive*

Manufacturing: Identifying the Future of Freeform Processing (Austin, TX: University of Texas at Austin, 2009), http://nextbigfuture.com/2009/10/roadmap-for-additive-manufacturing.html.

18 Terry Wohlers, *Wohlers Report 2011: Additive Manufacturing and 3D Printing State of the Industry* (Fort Collins, CO: Wohlers Associates, 2011).

19 L.D. Nayer, "Additive Manufacturing of Multifunctional Devices AMMD" (presentation at the Innovation for SME Partnering Event, Brussels, Belgium, May 17, 2011), http://www.cornet-era.net/portal/pics/3_innovation_for_sme/Partnering_Event_May_17_2011_Brussels/17_ammd.pdf; Joseph Beaman et al., *Additive/Subtractive Manufacturing Research and Development in Europe: Final Report,* (Baltimore, MD: World Technology Evaluation Center, Inc., 2004); M. Hedges et al., "New Method for Head-Up Display Realization by Mean of Chip On Board and Aerosol Jet Process" (presentation, Electronic System-Integration Technology Conference, Berlin, Germany, September 13–16, 2010); R. Plourde, "Aerosol Jet® Direct Write Technology, A Manufacturing Tool for Printed Electronics," PowerPoint presentation, http://www.isa.org/Content/Microsites530/Computer_Tech__Division/Home528/Passive_Wireless_Sensor_Workshop/Papers_Presentations/S7-P3_OptomecAJ.pdf.

20 B. P. Rice, A. Morgan, and K. Han, "Development of Multifunctional Materials for Additive Manufacturing" (presented at the Direct Part Manufacturing Workshop of the Midwest Society for the Advancement of Material and Process Engineering, Dayton, OH, March 29–30, 2011), http://www.midwestsampe.org/content/files/events/dpmworkshop/polymers/Polymers%20Rice.pdf; P. Dessert, "Additive Manufacturing of Nano-Materials: Cornerstone for the New Manufacturing Paradigm" (presented at the Rapid 2010 and 3-D Imaging Conferences & Exposition, Society of Manufacturing Engineers, Anaheim, CA, May, 2010); B. Zheng et al., "Powder Additive Processing with Laser Engineered Net Shaping (LENSÒ)," in Powder Metallurgy Research Trends, ed. Lotte Smit and Julia Van Dijk (Hauppauge, NY: Nova Science Publishers, 2009): 125–190.

21 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls.

22 Ibid, Table 11.7, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table11_07.xls.

23 Lynette Cheah, John Heywood, and Randolph Kirchain, "The Energy Impact of U.S. Passenger Vehicle Fuel Economy Standards," (presentation, IEEE International Symposium on Sustainable Systems and Technology, Washington, DC, May 17–19, 2010), http://web.mit.edu/sloan-auto-lab/research/beforeh2/files/IEEE-ISSST-cheah.pdf (Note that the study assumed that powertrains are resized to maintain the same acceleration performance when vehicle weight is reduced. Fuel consumption [or economy] refers to adjusted figures, which are revised upward [or downward] to better reflect actual, on-road figures, rather than dynamometer test results obtained in the laboratory); Lynette Cheah et al., "Factor of Two: Halving the Fuel Consumption of New U.S. Automobiles by 2035," in *Reducing Climate Impacts in the Transportation Sector*, edited by Daniel Sperling and James S. Cannon (New York: Springer, 2008), web.mit.edu/sloan-auto-lab/research/beforeh2/files/cheah_factorTwo.pdf.

24 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008,* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls; U.S. Energy Information Administration (EIA), *Monthly Energy Review*, *June 2011* (Washington, DC: EIA, 2011), Table 9.4, http://www.eia.gov/totalenergy/data/monthly/pdf/sec9_6.pdf; EIA, *Annual Energy Review 2009*, (Washington, DC: EIA, August 2010), Appendix A, Table A1, http://www.eia.gov/totalenergy/data/annual/pdf/sec13_1.pdf; EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics," last updated July 5, 2011, accessed July 13, 2011, http://www.eia.gov/energyexplained/index.cfm?page=oil_home#tab2. Note that the price of motor gasoline is used in this example for simplicity purposes. Using diesel in these examples would yield different results because of differences in prices and heat content).Cost of motor gasoline based on $3.98 per gallon or $31.84 per MBtu, including taxes, (data from EIA, *Monthly Energy Review, May 2011*), energy content for motor gasoline of 5.253 MBtu per barrel (EIA, *Annual Energy Review 2009*), barrel to gallon conversion for petroleum products of 42 gallons per barrel (EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics"). Calculations: $15.9 billion = $281.2 billion * 5.66%; $17.9 billion = $241.08 billion * 7.41%.

25 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls. In 2008, cars consumed 8,831 TBtu and light-duty trucks consumed 7,572 TBtu, A 6% increase in car fuel economy results in a 5.66% decrease in fuel consumption. An 8% increase in light-duty truck fuel economy results in a 7.41% decrease in fuel consumption. Calculations: Energy savings for cars = 500 TBtu = 8,831 TBtu * 5.66%; Energy savings for light-duty trucks = 561 TBtu = 7,572 * 7.41%; 500 TBtu + 561 TBtu = 1,061 TBtu.

26 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 11.7, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table11_07.xls. Calculations, assuming car CO_2 emissions make up 54% of total car and truck emissions, based on the fraction of energy consumed by cars compared to light trucks: 54% = 8,831 TBtu/(8,831 TBtu + 7,572 TBtu). Then 34 $MMTCO_2$ = 1,113.3 $MMTCO_2$ * 5.66% * 54%; 38 $MMTCO_2$ = 1,113 * 7.41% * 46%; 34 $MMTCO_2$ + 38 $MMTCO_2$ = 72 $MMTCO_2$.

27 U.S. Energy Information Administration, (EIA), *Monthly Energy Review, May 2011* (Washington, DC: EIA, 2011), Table 12.6, http://www.eia.gov/totalenergy/data/monthly/pdf/sec12_9.pdf.

28 U.S. Energy Information Administration (EIA), *Electric Power Annual* (Washington, DC: EIA, April 2011), Table 8.1, http://www.eia.doe.gov/cneaf/electricity/epa/epat8p1.html.

29 U.S. Energy Information Administration (EIA), *Monthly Energy Review, May 2011* (Washington, DC: EIA, 2011), Table 7.2a, http://www.eia.gov/totalenergy/data/monthly/pdf/sec7_5.pdf.

30 U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE), "20% Wind Energy by 2030: Increasing Wind Energy's Contribution to U.S. Electricity Supply," DOE/GO-102008-2567, (Washington, DC: DOE, July 2008), http://www1.eere.energy.gov/windandhydro/pdfs/41869.pdf.

31 U.S. Energy Information Administration, *Monthly Energy Review May 2011* (Washington, DC: U.S. Energy Information Administration, May 2011), Table 2.6, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_13.pdf. In 2010, the total U.S. energy consumption for electricity generation was 39,579 TBtu. Calculation: 396 TBtu = 1% * 39,579 TBtu.

32 U.S. Energy Information Administration (EIA), *Monthly Energy Review, May 2011*, Table 12.6 (Washington, DC: EIA, 2011), http://www.eia.gov/totalenergy/data/monthly/pdf/sec12_9.pdf; Ibid, Table 2.6, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_13.pdf. Calculation: 23 MMT = 1% * (39,579 TBtu/(39,579 TBtu - 924 TBtu)) * 2,271 MMT. (Based on average CO_2 emissions for non-wind production; wind technologies do not produce emissions when generating electricity.)

33 U.S. Energy Information Administration (EIA), *Electric Power Annual* (Washington, DC: EIA, April 2011), Table 8.1, http://www.eia.doe.gov/cneaf/electricity/epa/epat8p1.html; U.S Energy Information Administration (EIA), *Monthly Energy Review, May 2011,* Table 2.6, http://www.eia.gov/totalenergy/data/monthly/pdf/sec2_13.pdf. Calculation: $412 million = 1% * (39,579 TBtu/(39,579 TBtu - 924 TBtu)) * $40.2 billion in fuels purchased by major investor-owned utilities. (Based on average fuel costs for non-wind production; wind technologies do not incur fuel costs when generating electricity.)

34 Workshop discussion, New Paradigm Materials Manufacturing Processes—Energy Efficient Metals Production Impact Team Workshop, Warrendale, PA, June 20–21, 2011.

35 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls.

36 Lynette Cheah, John Heywood, and Randolph Kirchain, "The Energy Impact of U.S. Passenger Vehicle Fuel Economy Standards," (presentation, IEEE International Symposium on Sustainable Systems

and Technology, Washington, DC, May 17–19; Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008,* Table 2.6, (Washington, DC: U.S. Department of Energy, July 2010) http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls.. In 2008, cars consumed 8,831 TBtu and light-duty trucks consumed 7,572 TBtu. Assumes for every 10% weight reduction, fuel economy could increase by 6% for cars and 8% for light-duty trucks. A 6% increase in car fuel economy results in a 5.66% decrease in fuel consumption. An 8% increase in light-duty truck fuel economy results in a 7.41% decrease in fuel consumption. Calculations: Energy savings for cars = 500 TBtu = 8,831 TBtu * 5.66%; energy savings for light-duty trucks = 561 TBtu = 7,572 * 7.41%; 500 TBtu + 561 TBtu = 1,061 TBtu.

37 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008* (Washington, DC: U.S. Department of Energy, July 2010), Table 11.7, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table11_07.xls. Assumes car CO_2 emissions make up 54% of total car and truck emissions, based on the fraction of energy consumed by cars compared to light-duty trucks. Calculation: 54% = 8,831 TBtu/(8,831 TBtu + 7,572 TBtu); 34 $MMTCO_2$ = 1,113.3 $MMTCO_2$ * 5.66% * 54%; 38 $MMTCO_2$ = 1,113 * 7.41% * 46%; 34 $MMTCO_2$ + 38 $MMTCO_2$ = 72 $MMTCO_2$.

38 Oak Ridge National Laboratory, *Transportation Energy Data Book 29th Edition, Transportation Energy Use by Mode 2007–2008,* (Washington, DC: U.S. Department of Energy, July 2010), Table 2.6, http://cta.ornl.gov/data/tedb29/Spreadsheets/Table2_06.xls; U.S Energy Information Administration (EIA), *Monthly Energy Review*, *June 2011* (Washington, DC: EIA, 2011), Table 9.4, http://www.eia.gov/totalenergy/data/monthly/pdf/sec9_6.pdf; EIA, *Annual Energy Review 2009* (Washington, DC: EIA, August 2010), Appendix A, Table A1 http://www.eia.gov/totalenergy/data/annual/pdf/sec13_1.pdf; EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics," last updated July 5, 2001, accessed July 13, 2011, http://www.eia.gov/energyexplained/index.cfm?page=oil_home#tab2. Note that the price of motor gasoline is used in this example for simplicity purposes. Using diesel in these examples would yield different results because of differences in prices and heat content.Cost of motor gasoline based on $3.98 per gallon or $31.84 per MBtu, including taxes, (EIA, *Monthly Energy Review, May 2011*), energy content for motor gasoline of 5.253 MBtu per barrel (EIA, *Annual Energy Review 2009*), barrel to gallon conversion for petroleum products of 42 gallons per barrel (EIA, "Oil Crude and Petroleum Products Explained: Data and Statistics"). Calculations: $15.9 billion = $281.2 billion * 5.66%; $17.9 billion = $241.08 billion * 7.41%.

39 Prepared by Energetics Incorporated for the U.S. Department of Energy, Industrial Technologies Program, "Manufacturing Energy and Carbon Footprints: Iron and Steel," http://www1.eere.energy.gov/industry/pdfs/steel_footprint.pdf.

40 Ibid.

41 Ibid.

42 U.S. Census Bureau, "Annual Survey of Manufactures: Statistics for Industry Groups and Industries," accessed August 30, 2011, http://www.census.gov/manufacturing/asm/index.html. Calculations: $4.89 billion * 10% = 489 million; 1.75 billion * 10% = 175 million.

43 Prepared by Energetics Incorporated for the U.S. Department of Energy, Industrial Technologies Program, "Manufacturing Energy and Carbon Footprints: Iron and Steel," http://www1.eere.energy.gov/industry/pdfs/steel_footprint.pdf.

44 U.S. Census Bureau, "Annual Survey of Manufactures: Statistics for Industry Groups and Industries," accessed August 30, 2011, http://www.census.gov/manufacturing/asm/index.html. Calculations: $4.89 billion * 10% = 489 million; 1.75 billion * 10% = 175 million.

45 Steel Recycling Institute, "The North American Steel Industry Reduces Energy Intensity," 2011, accessed August 30, 2011, http://www.recycle-steel.org/Sustainability/Energy%20Reduction.aspx.

46 International Aluminum Institute, "Energy Use: Primary Aluminum," 2011, accessed August 30, 2011, http://www.world-aluminium.org/Sustainability/Environmental+Issues/Energy+use.

47 The Aluminum Association, "State Grant Supports Study of Aluminum Energy Efficiency," May 1, 2007, accessed August 30, 2011, http://www.aluminum.org/AM/Template.cfm?Section=New_Can_Stock_%28Class%29_Scrap_Receipts&TEMPLATE=/CM/ContentDisplay.cfm&CONTENTID=24688.

48 C.A. Lavender, V.S. Moxson, and V.A. Duz, *Cost-Effective Production of Powder Metallurgy Titanium Components for High-Volume Commercial Applications* (Washington, DC: DOE, October 2010), http://www.pnl.gov/main/publications/external/technical_reports/PNNL-19932.pdf.

VII. MATERIALS AND PROCESS DEVELOPMENT ACCELERATION TOOLS

Realizing materials science and engineering (MSE) innovation requires an integrated approach that can simultaneously propel research and development (R&D) in Functional Surface Technologies, Materials Integration in Clean Energy Systems, Higher-Performance Materials, and New Paradigm Materials Manufacturing Processes. Computer-aided simulation tools that are guided, validated, and verified by critical experiments can systematically accelerate the research priorities discussed in the past four chapters to maximize the impact that MSE can have on meeting the nation's energy and carbon reduction needs.

Materials and process development tools are critical to understanding the nature of materials, simulating system performance, and preventing detrimental defects and faults. Radical advances in collaborative databases and predictive modeling tools have allowed computational systems to not only model experimentally proven phenomena, but also simulate theoretical interactions that can direct laboratory work in the hypothesis stage. Computational modeling holds promise to transform MSE from an empirical, time-consuming, and costly endeavor into a more rapid materials design and development cycle based on the iterative interaction between computational and experimental tools.

The following pathways provide a guide for the R&D of tools that can accelerate materials and process innovation:

- Collaborative Databases
- Predictive Modeling of Material Performance
- Process Modeling Codes
- Integrated Computational Materials Engineering

COLLABORATIVE DATABASES

Collaborative materials databases include images and quantitative data that characterize the structure and properties of functional and structural materials (e.g., microstructure, conductivity, strength, diffusion, corrosion resistance, and viscosity). Increasing the comprehensiveness and usability of these databases can enable codes and models to simulate relevant materials and processes more accurately and can greatly accelerate the exchange of critical information and data needed for materials and process design. As a result, these advances can increase the efficiency and reduce the cost of test models and the resultant materials design and implementation, leading to economic and energy savings in nearly every energy sector.

Breakthrough Opportunities

The MSE community can advance collaborative databases by developing and improving both structural and functional materials databases. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow collaborative databases to make significant contributions toward addressing energy, environmental, and economic needs.

Collaborative Databases

Structural Materials Databases

Structural materials databases contain images and information about the structure and properties of various materials, including microstructure, strength, modulus, and thermal/electrical conductivity. These databases help materials scientists make informed decisions when selecting materials for a given application and provide critical input and validation for predictive computational models. This streamlined process greatly reduces trial and error, resulting in cost, time, and energy savings.

Historically, structural information about materials was recorded in only two dimensions, and eventually developed into data for 3-D analysis. Today, 4-D data adds a new level of accuracy by describing how material properties change over a given period of time. This analysis is especially applicable to the study of microstructural data.

The Materials Genome Initiative is a new, multi-stakeholder effort to develop an infrastructure to accelerate advanced materials discovery and deployment in the United States. Over the last several decades there has been significant federal investment in new experimental processes and techniques for designing advanced materials. This focused initiative will better leverage existing federal investments through the use of computational capabilities, data management, and an integrated approach to MSE.[1]

GAPS AND LIMITATIONS TO OVERCOME

- Newer data, particularly microstructural data, must be highly detailed to be comprehensive. This data requires massive storage that breaches the allowable limits of digital space. Therefore, the data is also difficult to transfer through current technology because of the bandwidth required (e.g., hours of upload/download to move from machine to machine, site to site). Data sharing and transfer may be a greater limitation than data storage.

Highly Impacted Materials and Processing Innovation Areas

Functional Surface Technologies

- Coatings

Materials Integration in Clean Energy Systems

- Joining Processes for Multi-Material Structures
- Composites with Structural Capabilities

Higher-Performance Materials

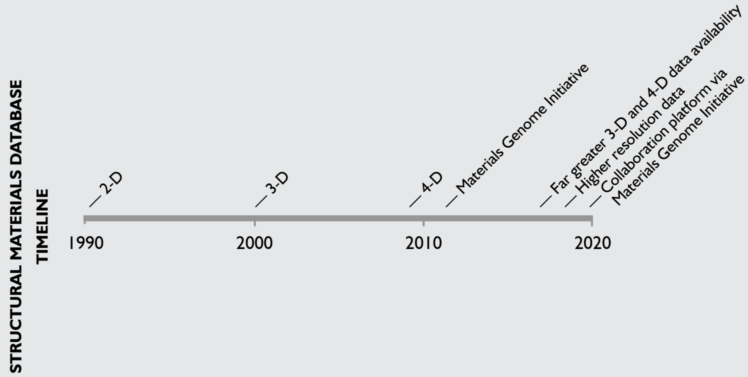
- Phase-Stable Metallic Materials
- Surface Treatments
- Lightweight High-Strength Materials

New Paradigm Materials Manufacturing Processes

- Net-Shape Processing
- Additive Manufacturing
- Energy-Efficient Metals Production

Historical Trends and Future Opportunities

EVOLUTION OF STRUCTURAL MATERIALS DATABASES



The key metrics of today's structural materials databases are population and resolution. Property data from approximately 10 years ago has not changed significantly, but the advancement of microstructural data requires updating with higher resolution. An increase in the population of 3-D and 4-D data is expected in the next 10 years.

Additionally, the Materials Genome Initiative will help enable a data exchange system that will allow researchers to index, search, and compare data to allow greater integration and collaboration.

Collaborative Databases

Functional Materials Databases

Functional materials databases hold extensive property data of materials and relevant systems such as solar photovoltaics, thermoelectrics, and fuel cells. Functional materials (sometimes known as "smart materials") are different from structural materials because load bearing and/or mechanical stability are typically not their primary function and environmental forces such as temperature and pressure may change their physical and chemical properties. The desired outcome may be energy capture, higher product yield, or improved system efficiency.

GAPS AND LIMITATIONS TO OVERCOME

- Currently there are no comprehensive systematic functional materials databases, but rather "islands" of databases with limited accessibility. Most of these are only published papers.

Highly Impacted Materials and Processing Innovation Areas

Functional Surface Technologies

- Catalysts
- Solar Materials
- Gas-Separating Membranes

Materials Integration in Clean Energy Systems

- Next-Generation Batteries and Fuel Cells

Higher-Performance Materials

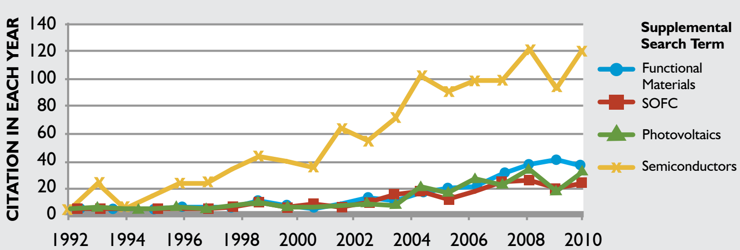
- Thermoelectric Materials

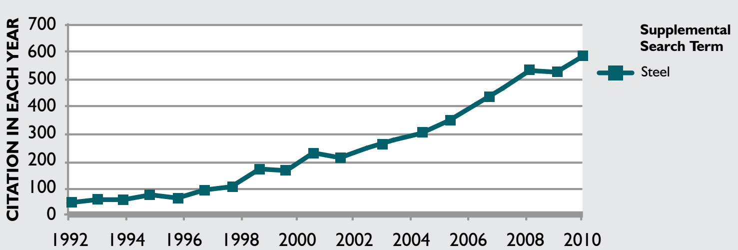
New Paradigm Materials Manufacturing Processes

- Additive Manufacturing

Historical Trends and Future Opportunities

NUMBER OF JOURNALS REFERENCING "FUNCTIONAL MATERIALS" AND OTHER KEYWORDS





These results are based on a search with the phrase "computational modeling" as opposed to "databases," as the latter implies a definition of the word that is too broad. A search of "steel" is used as a tool for comparison with a common structural material.

Functional materials databases significantly lag behind structural materials databases. The historical progression of functional materials databases may be represented by the number of citations that reference specific functional materials. Even though the future improvements in functional materials databases are expected to be minimal, they will be valuable as functional materials continue to make breakthroughs in materials properties and performance over the next 10 years.

R&D Priority Activities: Collaborative Databases

To overcome the gaps and limitations within the collaborative databases breakthrough opportunities, the MSE community must focus their efforts on expanding and improving the quality of data in databases, establishing database infrastructures and interfaces, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Structural Materials Databases** • **Establish fundamental databases for epoxy resin design and other polymers and for advanced metallics and composites systems.** • **Add topology/structure to databases and include a search function.** **Functional Materials Databases** • **Establish a database for nanoparticle synthesis that may be used for catalysis-based work.** **Crosscutting** • Link/condense existing materials databases for ease of access, reduced overlap, and increased gap identification.
MID TERM (2–5 YEARS)	**Structural Materials Databases** • Establish a database/infrastructure for lightweight high-strength materials and advanced metallics and composites. **Functional Materials Databases** • **Establish basic databases/infrastructure for photovoltaics, thermoelectrics, and fuel cells.** • **Enhance coatings and substrates databases intended for descriptive and predictive modeling.** **Crosscutting** • Integrate and input ab-initio and density functional theory output data into CALPHAD (CALculation of PHAse Diagrams) for the prediction of life-limited phases of alloy design models.
LONG TERM (5–10 YEARS)	**Structural Materials Databases** • Integrate pressure/volume/bulk modulus data into CALPHAD databases. **Functional Materials Databases** • Establish a database/infrastructure for electrolyte materials. • Establish a database/infrastructure for solid oxide fuel cell materials and membranes. **Crosscutting** • Establish more accurate low-temperature data for thermodynamic and kinetic models to assist with solving solid-state precipitation and life-limiting issues.

*The experts identified the **bolded activities** as high priority.

PREDICTIVE MODELING OF MATERIAL PERFORMANCE

Computer-assisted predictive modeling enables materials scientists to simulate the performance characteristics of materials in different operating environments and conditions. Prior to the use of predictive modeling, materials scientists observed materials after they failed, which is referred to as descriptive modeling. Improving predictive modeling of materials deformation, fracture and fatigue, and degradation can help prevent failure by facilitating the development of materials capable of resisting the mechanical and/or thermal loading, corrosion, oxidation, and wear/tribological effects of a given application. As a result, these advances can ensure that materials scientists select materials with properties that can withstand the operating conditions of a particular application, reducing the number of physical test models required and lowering the cost of manufacturing products.

Breakthrough Opportunities

The MSE community can advance predictive modeling of materials performance in the following areas: deformation and texture evolution, fracture and fatigue, and materials degradation. Addressing the gaps and limitations specific to each of these breakthrough opportunities will allow predictive modeling of materials performance to make significant contributions toward addressing energy, environmental, and economic needs.

Predictive Modeling of Material Performance

Deformation and Texture

Deformation of materials through thermodynamic, mechanical, and other influences can be computationally modeled, which is more efficient and cost-effective than using descriptive trial and error techniques. Some of the predictive modeling techniques used for deformation and texture of parts are finite element analysis, phase field modeling, atomistic modeling, and multi-scale and multi-physics modeling. Deformation and texture predictive modeling can improve the safety, efficiency, lifetime, and speed of market readiness of system components.

GAPS AND LIMITATIONS TO OVERCOME

- Predictive modeling techniques depend on the integration and accuracy of materials databases, which must be expanded and corrected to produce valid deformation results.
- The accuracy of model validation can be decreased by outdated data.

Highly Impacted Materials and Processing Innovation Areas

Materials Integration in Clean Energy Systems

- Joining Processes for Multi-Material Structures
- Composites with Structural Capabilities

Higher-Performance Materials

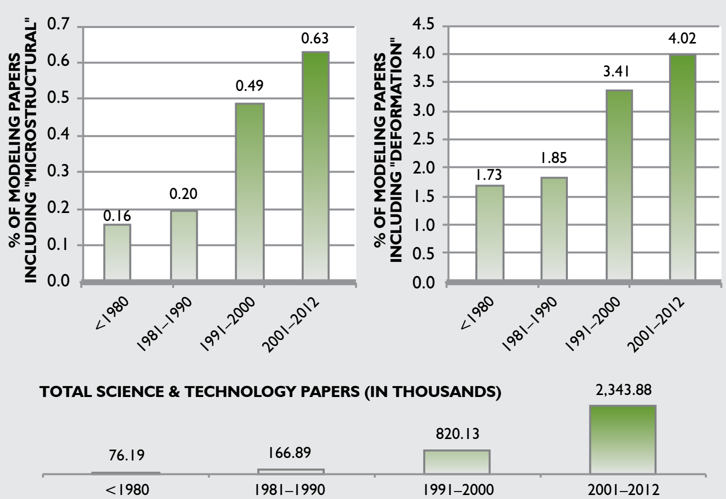
- Phase-Stable Metallic Materials
- Surface Treatments
- Lightweight High-Strength Materials

New Paradigm Materials Manufacturing Processes

- Net-Shape Processing
- Energy-Efficient Metals Production

Historical Trends and Future Opportunities

PERCENTAGE OF TECHNICAL PAPERS ON MODELING THAT ADDRESS MICROSTRUCTURE AND DEFORMATION



Over the past 60 years, descriptive techniques for understanding deformation and texture have advanced into predictive techniques. The number of references to research involving computational modeling and simulation of deformation and microstructural effects shows that the field has been rapidly growing over the last few decades. The graphs represent the percentage of science and technology papers that contain the search terms "deformation" and "microstructural." Over the next 10 years, there is expected to be an exponential increase in the number of references to deformation and texture modeling codes in response to more accurate predictive models.[2]

Predictive Modeling of Material Performance

Fracture and Fatigue

Predictive modeling of materials fracture and fatigue involves the probabilistic science and behavior of defects and accelerated void coalescence. By properly simulating voids in a model, the ability to predict fatigue life and failure locations becomes more accurate and reliable. A cutting-edge predictive mechanistic framework enhances scientists' understanding of failure mechanisms, and therefore awards them the tools to build efficient, optimized parts. The computational modeling of fracture and fatigue in metals has made a dramatic transition from descriptive to predictive over the past decade.

GAPS AND LIMITATIONS TO OVERCOME

- Numerical approaches in predictive modeling codes need major improvements so modeling codes can accurately simulate voids to predict fatigue failure locations.
- Fracture models need extensive and accurate validation from experiments.

Highly Impacted Materials and Processing Innovation Areas

Functional Surface Technologies

- Gas-Separating Membranes

Materials Integration in Clean Energy Systems

- Joining Processes for Multi-Material Structures
- Composites with Structural Capabilities

Higher-Performance Materials

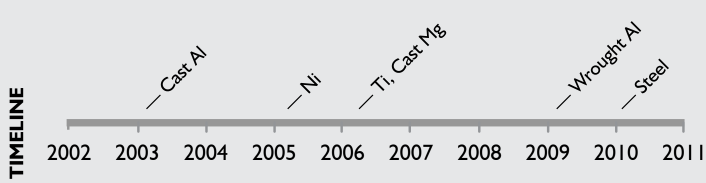
- Phase-Stable Metallic Materials
- Surface Treatments
- Lightweight High-Strength Materials

New Paradigm Materials Manufacturing Processes

- Additive Manufacturing

Historical Trends and Future Opportunities

MICROMECHANICS FATIGUE NUCLEATION SIMULATION



In the area of fatigue modeling, a major improvement in predictive capability has involved addressing the early stages of high-cycle fatigue, including crack nucleation and microstructurally short crack growth.

In 2003, micromechanical modeling of plasticity-based damage at fatigue nucleants (e.g., pores and inclusions in cast automotive aluminum alloys) demonstrated nucleation-controlled high-cycle fatigue life.[3] Since 2003, additional predictive simulations of micromechanics fatigue nucleation have been applied to nickel (Ni), titanium (Ti), magnesium (Mg), wrought aluminum (Al), and steel. Future predictive simulations will focus on developing more accurate codes and simulating other advanced metal alloy systems.

Predictive Modeling of Material Performance

Materials Degradation

Predictive modeling of materials degradation enables materials scientists to quantify the approximate lifetime of a part in response to influences such as wear and corrosion. Uncertainty quantification can determine the accuracy of degradation modeling, allowing materials scientists to determine the margin of error of a degradation prediction. Accurate data and predictive degradation modeling can significantly reduce the amount of test time required to develop and certify nuclear fuels, which typically takes 20 years from inception to certification.

GAPS AND LIMITATIONS TO OVERCOME

- Corrosion models and irradiation-damage models currently lack coupling with accurate and extensive databases to provide improved materials lifetime predictions.
- Uncertainty quantification methods must be improved to allow predictive models to simulate reactor irradiation conditions if linked with appropriate component physics experiments.

Highly Impacted Materials and Processing Innovation Areas

Functional Surface Technologies

- Catalysts
- Solar Materials
- Coatings

Materials Integration in Clean Energy Systems

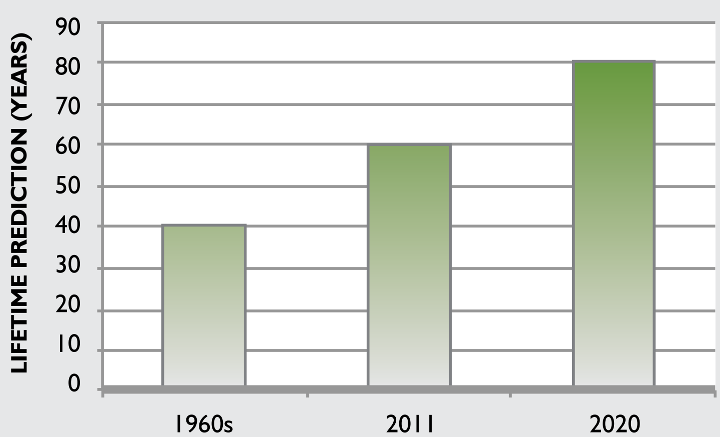
- Next-Generation Batteries and Fuel Cells
- Joining Processes for Multi-Material Structures
- Composites with Structural Capabilities

Higher-Performance Materials

- Phase-Stable Metallic Materials
- Surface Treatments
- Lightweight High-Strength Materials

Historical Trends and Future Opportunities

NUMBER OF YEARS OF SERVICE LIFE THAT CAN BE PREDICTED VIA MODELING



A key metric for measuring the historical advances of materials degradation modeling is the maximum number of years of a part's lifetime that scientists can accurately predict. In the 1960s, maximum predictable lifetime for a part was 40 years. With materials degradation modeling codes, today's lifetime prediction has increased to 60 years. In the next 10 years, scientists may be able to predict the lifetime of a part up to 80 years.

Lifetime Prediction

- 1960s: 40 years
- 2011: 60 years
- 2020: 80 years

R&D Priority Activities: Predictive Modeling of Material Performance

To overcome the gaps and limitations within the predictive modeling of materials performance breakthrough opportunities, the MSE community must focus their efforts on creating new methodologies, advancing computational codes, and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Crosscutting** • **Create a statistical representation of microstructural evolution in codes for the prediction of material performance.**
MID TERM (2–5 YEARS)	**Fracture and Fatigue** • Develop robust methodologies for combining phenomenological material models with crystal plasticity results (e.g., room-temperature-, warm-, and hot-forming of magnesium sheet alloys). • Incorporate fracture into component simulations under impact conditions. • Develop reliable fracture models (e.g., cohesive zone) that can be validated by experiments. **Materials Degradation** • **Develop a coatings "degradation predictor" for energy technologies.** **Crosscutting** • **Develop practical and computationally efficient approaches in coupling multiphysics and multi-scale modeling of materials performance.** • **Establish probabilistic strategies for extending part life that account for microstructural variances.** • Integrate and input ab-initio and density functional theory output data into CALPHAD for the prediction of life-limited phases of alloy design models. • Integrate codes for the interaction of coatings and substrates.
LONG TERM (5–10 YEARS)	**Materials Degradation** • **Improve the coupling of CALPHAD-type databases into corrosion models and irradiation-damage models.**

*The experts identified the **bolded activities** as high priority.

PROCESS MODELING CODES

Process modeling codes are used in the predictive modeling of material processes to optimize process efficiency and to determine the properties of resulting materials and components. Simulating processes like stamping, forging, or gas-pressure forming before using them to manufacture materials provides insight into ways to optimize processes, such as improving heat balance or the loading of furnaces for heat treatment. Using process modeling codes to improve materials processes prior to manufacture can drastically increase the efficiency and lower the costs of materials manufacturing processes.

Breakthrough Opportunities

The MSE community can advance process modeling codes by focusing on microstructural evolution and materials performance, materials/compound discovery, and process manufacturing and component performance. Addressing the gaps and limitations specific to each of these breakthrough opportunities will identify a path forward for maximizing the economic, environmental, and energy benefits of process modeling codes in energy markets.

Process Modeling Codes

Microstructural Evolution and Materials Performance

Evolution of microstructure can be modeled with modeling codes that use principles from thermodynamics and kinetics, as well as data from forging, casting, and other processes to predict how microstructure will evolve and affect materials performance. Using process modeling codes to understand the evolution of microstructure during the synthesis of materials accelerates the development of products and reduces costs. The development of thermodynamic and kinetic databases for practical materials, such as thermoelectric materials with high figures of merit (ZT) and copper iridium gallium selenide (CIGS) photovoltaics, is an important precursor to modeling microstructural evolution in materials during processing and service.[4]

GAPS AND LIMITATIONS TO OVERCOME

- There is currently a lack of composition- and temperature-dependent property data, especially at low temperatures.
- There is a lack of data on interfacial energies of materials microstructures.

Highly Impacted Materials and Processing Innovation Areas

Functional Surface Technologies

- Coatings

Materials Integration in Clean Energy Systems

- Joining Processes for Multi-Material Structures
- Composites with Structural Capabilities

Higher-Performance Materials

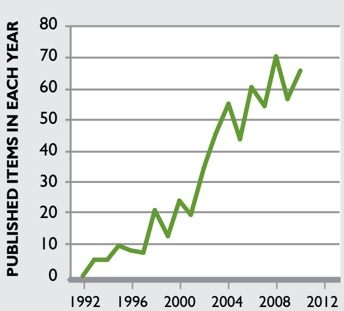
- Thermoelectric Materials
- Phase-Stable Metallic Materials
- Surface Treatments
- Lightweight High-Strength Materials

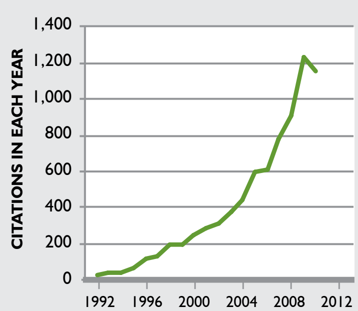
New Paradigm Materials Manufacturing Processes

- Net-Shape Processing
- Additive Manufacturing
- Low-Cost Composites Manufacturing
- Energy-Efficient Metals Production

Historical Trends and Future Opportunities

PUBLICATIONS AND CITATIONS THAT INCLUDE THE SEARCH TERM "THERMO-CALC"





Process modeling codes for microstructural evolution are relatively scarce and have improved little in the past 20 years. However, a more appropriate representation of the historical improvement of these process modeling codes is the number of publications and citations that use the thermodynamics, diffusion, and kinetics software called "Thermo-Calc." There has been a dramatic increase in the number of publications and citations that discuss microstructural evolution codes and databases since the 1990s. The number of publications and citations is expected to increase exponentially over the next 10 years.[5]

Process Modeling Codes

Materials/Compound Discovery

Process modeling codes captured in atomic-scale calculations aim to enable materials scientists to predict materials properties and crystal structures, validate other codes, and discover new materials and compounds. The use of fundamental codes can lead to the identification of previously unknown trends and correlations and can be expanded to give way to new compound predictions.

GAPS AND LIMITATIONS TO OVERCOME

- The prediction of new compounds can be impeded by the difficulty of predicting the correct crystal structure.
- Scientists lack robust kinetics codes for building new compounds and structures.

Highly Impacted Materials and Processing Innovation Areas

Functional Surface Technologies

- Catalysts

Materials Integration in Clean Energy Systems

- Next-Generation Batteries and Fuel Cells

Higher-Performance Materials

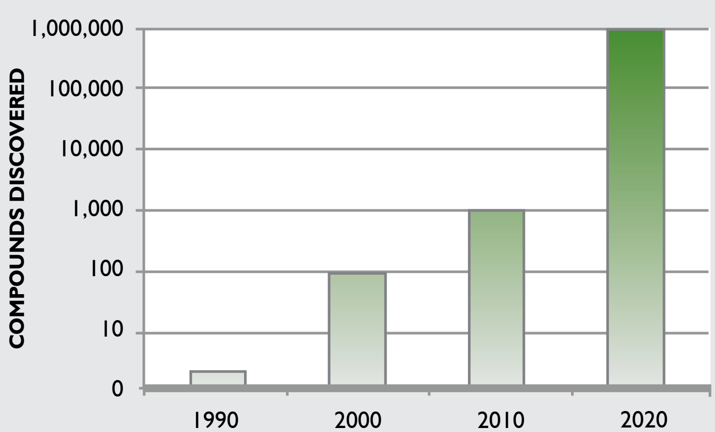
- Thermoelectric Materials
- Phase-Stable Metallic Materials

New Paradigm Materials Manufacturing Processes

- Additive Manufacturing

Historical Trends and Future Opportunities

COMPOUNDS DISCOVERED FROM DENSITY FUNCTIONAL THEORY CALCULATIONS



Discovery of new compounds has increased exponentially with the growth of atomic-scale calculations such as density functional theory (DFT). The number of new compound discoveries will continue to increase over the next 10 years with the improvement of kinetic codes and methods of predicting crystal structures are improved.[6]

Compounds Discovered

- 1990s: 1–2
- 2000: Hundreds
- 2011: Thousands
- 2020: Millions

Process Modeling Codes

Process Manufacturing and Component Performance

Materials scientists can model manufacturing processes using finite element simulation technology, including stamping, forging, or gas-pressure forming, and can model component performance through crash impact, noise, and vibration simulations. The use of such codes can significantly lower manufacturing costs and the need to conduct laboratory tests.

GAPS AND LIMITATIONS TO OVERCOME

- There is a lack of physics-based constitutive material models for finite element simulations, particularly for metals. The finite element programs have advanced considerably, but the materials models used in the software are lacking.

Highly Impacted Materials and Processing Innovation Areas

Functional Surface Technologies

- Solar Materials

Materials Integration in Clean Energy Systems

- Next-Generation Batteries and Fuel Cells
- Joining Processes for Multi-Material Structures
- Composites with Structural Capabilities

Higher-Performance Materials

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New Paradigm Materials Manufacturing Processes

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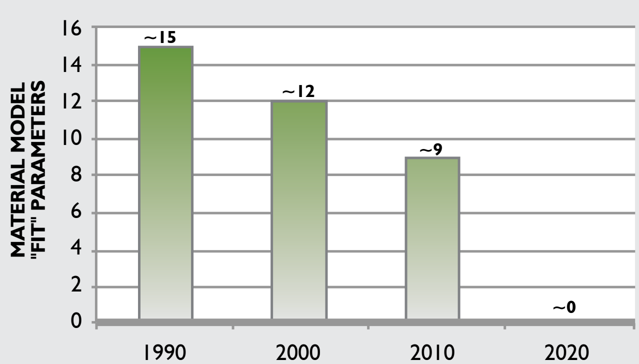
Historical Trends and Future Opportunities

NUMBER OF FIT PARAMETERS REQUIRED OF MATERIALS MODELS



Improvement of material constitutive models can be measured by the elimination of fit parameters. This metric indicates the ability for the material model to accurately predict the physical response of the material in simple experiments and complex forming processes. Around 2000, a crystal plasticity model required about 15 fitting parameters. Remaining parameters must be generated through fits to experimental data. In the next 10 years, materials scientists are expected to be able to predict these material properties from physics-based models, thereby entirely eliminating the need for data fitting.[7]

Material Model Fit Parameters

- 1990: ~15
- 2000: ~12
- 2010: ~9
- 2020: ~0

R&D Priority Activities: Process Modeling Codes

To overcome the gaps and limitations within the process modeling code breakthrough opportunities, the MSE community must focus their efforts on developing new modeling capabilities and methodologies and pursuing other R&D activities provided in the following table. The table divides the priority activities for each research initiative by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	**Microstructural Evolution and Materials Performance** • Develop process modeling codes that integrate finite elements and microstructural tools.
MID TERM (2–5 YEARS)	**Microstructural Evolution and Materials Performance** • Develop robust methodologies for combining phenomenological material models with crystal plasticity results (e.g., room-temperature-, warm-, and hot-forming of magnesium sheet alloys). • Incorporate fracture into component simulations under impact conditions. • Develop reliable fracture models (e.g., cohesive zone) that can be validated by experiments. **Process Manufacturing and Component Performance** • **Develop physics-based material constitutive models with integrated experimentation and data generation for multi-axial straining (over a broad range of strain rates, temperatures, etc.) for metals and polymers. In addition, combine such models with interfacial constitutive models when deformation involves contact (e.g., tool/workpiece interface).** • Improve the integration of models over various length scales. **Crosscutting** • **Develop the ability to model compounds of polymers and metals with nano-fillers.** • **Integrate models and databases for welding and joining issues of dissimilar materials (Microstructural Evolution and Materials Performance, Process Manufacturing and Component Performance).** • Develop scale-dependent thermodynamics models.
LONG TERM (5–10 YEARS)	**Microstructural Evolution and Materials Performance** • **Create multi-scale codes that link density functional theory and kinetic Monte Carlo codes for microstructural evolution.** **Crosscutting** • **Develop methods to analyze finite element predictive performance for unique additive manufacturing internal structures.** • **Introduce composition-dependent models and data into higher-level process modeling codes for casting, deformation, etc. (Microstructural Evolution and Materials Performance, Process Manufacturing and Component Performance).** • Improve models and databases for composition-dependent properties.

*The experts identified the **bolded activities** as high priority.

INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING

Integrated computational materials engineering (ICME) combines the previous three initiatives to help build system components and entire systems. ICME aims to accurately simulate the complete materials and component development process, from integrating basic material properties to simulating manufacturing, in order to reduce the number of physical test models needed. For example, Ford has a "virtual aluminum castings" program that uses computer simulations for the production of engine components, from manufacturing and machining simulations to real-life conditions such as high temperatures and stresses. This process saves Ford millions of dollars in product development.[10]

Addressing the gaps and limitations specific to ICME will identify a path forward for maximizing the economic, environmental, and energy benefits of materials in energy markets.

Integrated Computational Materials Engineering

ICME Platforms

ICME platforms integrate materials information that is captured in computational tools with engineering product performance analysis and manufacturing process simulations.[8] ICME enables researchers and engineers to model materials-related processes (e.g., oxidation, joining, welding, and brazing) and component production across the entire manufacturing cycle. It also allows materials scientists to model accelerated degradation of materials during their use.

GAPS AND LIMITATIONS TO OVERCOME

- It is only possible to predict materials properties such as phase constitution, chemistry, and reactivity for a limited number of systems compared with the full range of possible combinations of compositions.
- Computational modeling has not yet been able to provide a thorough understanding of the relationships among materials history, microstructure, and properties. In addition, materials scientists' ability to control microstructures is underdeveloped.

Highly Impacted Materials and Processing Innovation Areas

Functional Surface Technologies

- Catalysts
- Coatings

Materials Integration in Clean Energy Systems

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- Joining Processes for Multi-Material Structures
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New Paradigm Materials Manufacturing Processes

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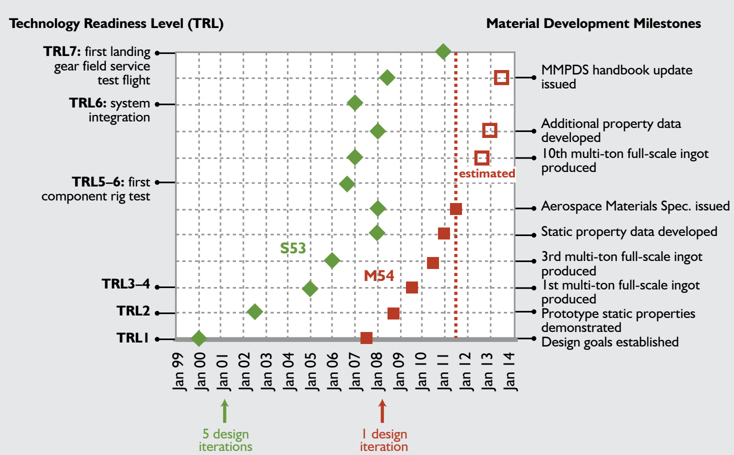
- Energy-Efficient Metals Production

Historical Trends and Future Opportunities

COMPUTATIONAL MATERIALS QUALIFICATION ACCELERATION



ICME modeling platforms have the ability to accelerate the qualification of materials and products. The development timeline of QuesTek's landing gear steels is a documented example. The Ferrium S53 took 8.5 years from paper to flight qualification, with five design iterations. The high-toughness Ferrium M54 for carrier-based planes (for use by the Naval Air Systems Command) is on schedule to qualify for flight in 5 years with a single design iteration.[9]

The figure to the left is a flight qualification timeline showing the faster development time of the M54 system.

R&D Priority Activities: Integrated Computational Materials Engineering

To overcome the gaps and limitations of ICME, the MSE community must focus their efforts on expanding ICME capabilities and usability and pursuing other R&D activities provided in the following table. The table divides the priority activities for ICME by the time frame in which they are estimated to impact U.S. energy sectors: near term (0–2 years), mid term (2–5 years), and long term (5–10 years).

NEAR TERM (0–2 YEARS)	• **Develop a high-profile ICME example to show its applicability to energy problems (e.g., fuel cells, batteries, heat exchangers, or wind turbines).**
MID TERM (2–5 YEARS)	• **Advance and accelerate the qualification of high-temperature alloys.** • **Introduce materials design for novel joinability (e.g., automobile industry spot welding).** • **Advance materials design for additive manufacturing of magnesium and transformation-induced plasticity steels.** • **Integrate models and databases for welding and joining issues of dissimilar materials.** • **Develop inverse methodologies for materials design.** • Develop simulation-based design of nano-dispersion-enhanced thermoelectric materials. • Integrate the "I" with "CME". » Prove that ICME offers value beyond the archival literature with key case studies, specifically within the energy sector. » Develop procedures for simulating an entire material within an overall component materials design and development cycle (not just one or two phases in a material). • Develop a data infrastructure for next-generation steels, nickel-cobalt, and zirconium.
LONG TERM (5–10 YEARS)	• **Develop concurrent design of a material and its applicable component within an energy application area.** • Develop a few web-based ICME platforms that will be available from anywhere there is an internet connection.

*The experts identified the **bolded activities** as high priority.

NOTES

1 National Science and Technology Council (NSTC), "Materials Genome Initiative for Global Competitiveness," (Washington, DC: NSTC, 2011).

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5 Internet search conducted using ISI Web of Knowledge. Thompson Reuters, "ISI Web of Knowledge" accessed June 22, 2011, http://www.webofknowledge.com.

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8 Committee on Integrated Computational Materials Engineering, National Research Council, *Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security* (Washington, DC: National Academies Press, 2008).

9 C.J. Kuehmann and G. B. Olson, "ICME: Success Stories and Cultural Barriers," *Integrated Computational Materials Engineering,* ed. S. Arnold and T. Wong (Materials Park, OH: ASM International, forthcoming 2011); Charles J. Kuehmann, Herng-Jeng Jou, and Chris Kern, "From Concept to Flight: An Example of Computational Design and Qualification for Aerospace Structural Alloys," (paper presented at the 1st World Congress on Integrated Computational Materials Engineering, Seven Springs, PA, July 10–14, 2011).

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VIII. THE PATH FORWARD

The previously published *Vision Report of the Energy Materials Blue Ribbon Panel* and *Opportunity Analysis for Materials Science and Engineering* have culminated in the identification of a set of important areas for materials science and engineering (MSE) product and process innovation. The innovations outlined in this *Innovation Impact Report* identify materials and processing breakthroughs that can radically reduce the cost, environmental impact, and energy requirements of energy generation, storage, and use across the United States. If realized, these MSE advances have the opportunity to significantly impact the United States' progress toward enhanced sustainability and economic growth.

As a next step, it is important to identify key pathways that integrate the research and development priority activities in this report into a coherent approach that leverages the highest-value opportunities and addresses the most critical needs. Especially important will be the advancement and use of materials and process development acceleration tools to decrease the time and cost of translating materials and process discoveries into real-world commercial applications.

IX. APPENDIX

ACRONYMS AND ABBREVIATIONS

°C	degrees Celsius
°F	degrees Fahrenheit
AISI	American Iron and Steel Institute
Al	aluminum
AM	additive manufacturing
bcm	billion cubic meters
Bi	bismuth
Btu	British thermal units
CALPHAD	CALculation of PHAse Diagrams
CdTe	cadmium telluride
cermet	ceramic-metal composite material
CIGS	copper indium gallium selenide
CMC	ceramic-matrix composites
Co	cobalt
CO_2	carbon dioxide
CSP	concentrated solar power
DDM	direct digital manufacturing
DFT	density functional theory
DMLS	direct metal laser sintering
DMMC	discontinuous metal-matrix composite
EBM	electron beam melting
FDM	fused deposition modeling
FSW	friction stir welding
FT	Fischer-Tropsch
GW-days	gigawatt-days
ICE	internal combustion engine
ICME	Integrated Computational Materials Engineering
IIT	innovation impact team
kg	kilogram
kWh	kilowatt-hour
LBNL	Lawrence Berkeley National Laboratory
lbs	pounds
LFW	linear friction welding
MBtu	million British thermal units
Mg	magnesium
MIT	Massachusetts Institute of Technology
MMC	metal matrix composites
MMT	million metric tons
MSE	materials science and engineering
Ni	nickel
nm	nanometer
PAN	polyacrylonitrile
PV	photovoltaics
R&D	research and development
Sb	antimony
SiC	silicon carbide
SL	stereolithography
SOFC	solid oxide fuel cell
TBtu	trillion British thermal units
TEG	thermoelectric generator
Ti	titanium
TMS	The Minerals, Metals, & Materials Society
TRIP	transformation-induced plasticity
TWIP	twinning-induced plasticity
V	vanadium
Wh	watt-hour
ZT	figures of merit
Zr	zirconium

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