Materials Research Constellation

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Overview:

Materials science uses the principles of chemistry, physics, and engineering to address societal needs and practical problems. Major technology areas including electronics, nanotechnology, biotechnology, medicine, civil infrastructure, energy, metal production, aerospace, and others rely on innovations in materials research. As an indication of the potential impact of materials research, more than half of the Grand Challenges for Engineering defined by the National Academy of Engineering are directly tied to advances in materials.

Materials research is ubiquitous across the Missouri S&T campus with some aspect of research on materials occurring in a majority of the departments on campus. Since the founding of our campus as the Missouri School of Mines and Metallurgy in 1870, materials research and education have been an integral part of the institution. By its nature, materials research is highly interdisciplinary and involves a combination of experimental, theoretical, and computational approaches.

Definition

The traditional materials research paradigm is expressed as the composition, structure, properties, and performance tetrahedron. Materials research is diverse, ranging from the fundamental science of metals, ceramics, and polymers to the applied research and development of materials for specific applications. Materials research spans many orders of magnitude in scale from the electronic structure of individual atoms to the largest infrastructure projects yet conceived. For the purpose of this strategic planning exercise, materials research is defined as any study involving the chemistry, physics, and engineering of materials that include metals, ceramics, and polymers, as well as composites containing any one of those types of materials, that may be in the form of solids, liquids, gases, or plasmas.

Current Strengths

The long history of materials research at Missouri S&T has led to several strengths including:

- Infrastructure for materials research including the center’s state-of-the-art characterization facilities, common-use equipment in departments or research centers, and highly specialized capabilities in the individual faculty research laboratories;
- A majority of income from royalties on licensed patents come from materials-based patents;
- Demonstrated success in entrepreneurial efforts that utilize materials research (e.g., Brewer Science and Mo-Sci);
- Materials research is pervasive at Missouri S&T, with collaborations and research efforts spanning across departments and colleges;
- Some of the most highly regarded scholars on our campus are involved in materials research.

Key areas of strength within materials research are summarized in the table that accompanies this document. In general, investigators continue to pursue funding opportunities in areas of existing strength.

Resource Needs

Key resources needed for future growth in materials research include human resources, faculty time, awareness of expertise, and research infrastructure. Each is addressed briefly below.

Human Resources

Research is conducted by a combination of students, staff, and faculty. Each have a key role in successful research. Some actions that are needed to ensure viable levels of personnel are available to conduct research are:

- Recruit qualified graduate students in sufficient numbers to provide students for funded research projects. This includes an adequate number of domestic students for projects that require U.S. persons and to fully utilize funds available for U.S. persons such as Chancellor's Distinguished Fellowships and GAANN fellowships.
- Provide staff support for key research needs such as research specialists to operate instruments and facilities, administrative staff to assist with activities purchasing and grant management, and trained technicians to support laboratory-based research
- Recruit and retain top-quality faculty in key research areas
- Promote research excellence through policies and incentives

Faculty Time

Aligning research expertise with opportunities and preparing quality proposals takes dedicated effort. Actions that would enable faculty to devote more time to pursuing opportunities are:

- Minimize administrative and bureaucratic burden on faculty by maximizing utilization of staff resources
- Increase resources and training to support teaching activities such as GTAs and teaching faculty to reduce teaching burden on productive faculty
- Provide adequate and timely support through the Office of Sponsored Programs, academic departments, and research centers for preparation and submission of proposals and management of grants
- Streamline pre-award processes for proposals
- Train faculty to take advantage of available resources
- Increase training for department or center staff who support proposal preparation to reduce the time required from faculty for administrative aspects of proposal preparation

Awareness of Research Expertise Areas

The grand challenges for materials research require broad, cross-disciplinary knowledge coupled with deep understanding in specific areas to address needs. Important considerations include:

- Facilitate communication among faculty on campus to build collaborations and teams
- Hire new faculty in key areas to complement existing faculty expertise and fill critical gaps in expertise
- Coordinate "cluster" hires across departments for strategic research areas
- Develop a program to increase numbers of research faculty in key areas
- Market existing research expertise and successes locally and nationally

Research Infrastructure

Materials research requires state-of-the-art analytical equipment and specialized laboratory facilities. Future growth of research necessitates expansion of laboratory space and capabilities. Some needs include:

- Dedicate centralized laboratory space to research clusters
- Build new, dedicated research space
- Increase professional staff support for major research instrumentation and computational facilities
- Coordinate and support effort to acquire key analytical equipment
- Acquire new analytical equipment to complement capabilities in core facilities

Roadmap for the Future

Materials research is a key area for future growth due to its multidisciplinary and cross-cutting nature. New opportunities constantly emerge for materials research based on the constant push for increased efficiency, longer operating life, higher operating temperatures, and new technologies, all of which require new and improved materials. Materials research also addresses a number of grand challenges such as those defined by the National Academy of Engineering or similar forward-looking groups, which requires large multidisciplinary teams. Strategies suggested for growth of materials research are listed below.

1. **Continue to aggressively pursue single-investigator grants:** Single investigator grants in areas of faculty expertise are a fundamental part of academia. Single investigator grants and the accompanying research help faculty establish scholarly reputations, which can be an important part of receiving tenure and gaining promotion through the academic ranks. In addition, strong individual scholarly reputations are needed when building teams to compete for larger, collaborative grant opportunities. Faculty should continue to pursue individual grants to help cultivate a strong academic reputation.
2. **Align priority areas with Kummer Institute:** Materials research will benefit from synergy with the Kummer Institute in several areas. For example, materials research has great potential to promote local and regional economic development as has been demonstrated through entrepreneurial efforts such as Brewer Science and Mo-Sci. Likewise, materials research can support a number of the planned research thrust areas for the institute. Aligning closely with the roadmap for the institute may benefit materials research through additional faculty hiring, establishing new collaborations, and access to new facilities.
3. **Explore emerging areas:** Broadening the scope of expertise and establishing new research areas is important to sustaining a high level of research activity. Seed funding from internal sources and exploratory grants from external agencies can enable research into new materials and applications as well as facilitating development of collaborative teams.
4. **Utilize National user facilities:** Performing research at national user facilities can leverage existing funding and provide access to powerful research tools that can enhance the quality of materials research. Many of these facilities are free to use. In addition, this activity can establish new collaborations since results obtained at such facilities are often published jointly with scientists from those laboratories.
5. **Establish new consortia:** Consortia involving industry, government laboratories, and/or other universities can be established in areas of research strength to facilitate larger

research efforts (e.g., EMC Lab and PSMRC). Consortia can facilitate large research efforts and enhance external visibility.

6. **Increase external collaborations**: Productive collaborations with researchers at other institutions can enhance research. Collaborations can provide access to expertise and equipment not available locally to increase the quality of research while also enhancing the external visibility of the faculty involved and the institution.
7. **Pursue large grant opportunities**: Faculty should be encouraged to lead or participate in large, multi-disciplinary teams. Support for such efforts can be in the form of working with a grant writer, staff assistance with completion of the application package, and minimizing logistical barriers to collaborative research are needed. Some specific targets for large grants are:
    a. Department of Transportation, university transportation center focused on materials
    b. Department of Energy, Energy Frontier Research Center focused on nuclear materials
    c. National Science Foundation Materials Research Science and Engineering Center focused on transparent conducting oxides; Engineering Research Center focused on additive manufacturing
    d. Department of Defense Multidisciplinary University Research Initiative grant focused on ultra-high temperature ceramics.

Metrics

The effectiveness of activities should be assessed using metrics such as research expenditures of individual faculty, research teams, or centers; scholarly publications; impact of scholarly works; external awards or recognition such as society fellowship or membership in national academies; patent royalties; numbers of PhD students graduated. When investments are made, activities can be assessed based on return on investment such as the ratio of external funding to internal funding (e.g., seed grants, start-up packages).

Area	Description	Existing Strengths	Faculty/Department
Materials for extreme environments	Discover, design, and study fundamental behavior of materials capable of withstanding conditions beyond the capabilities of existing materials.	• Global recognition as leaders plus highly cited papers on ultra-high temperature ceramics • Unique equipment for testing mechanical, electrical, and thermal properties at extreme temperatures • Broad range of funded projects in areas that include hypersonics, nuclear energy, and concentrated solar power	Bill Fahrenholtz*/MSE Arezoo Emdadi/MSE Greg Hilmas/MSE Joseph Graham/Nuclear Vadym Mochalin/Chemistry Alex Chernatynskiy/Physics Haiming Wen/MSE Jeremy Watts/MSE
Computational Materials Science	Design, discover, and optimize novel electronic, photonic, optical, and quantum materials; advanced alloys and ceramics; prediction of process-structure-property-performance relationships in structural and functional materials	• High throughput computational materials design to support the Materials Genome Initiative • Pioneering research and world-wide collaborations on amorphous transparent semiconductors • The Center for High Performance Computing (HPC) provides campus and state-wide computing capabilities through NSF-MRI-funded Foundry cluster • Experience and established collaborations in Integration Computational Materials Engineering (ICME) and multi-scale multi-disciplinary modeling, such as DFT, CALPHAD, phase-field/phase-field crystal and FEM	Julia Medvedeva*/Physics Arezoo Emdadi/MSE Yijia Gu/MSE Alex Chernatynskiy/Physics Chenglin Wu/CArE
Materials informatics	Machine-learning assisted materials design	• The Center for High Performance Computing (HPC) Research provides computing capacity through the Forge and the Numerically Intensive Computing (NIC) Cluster • Optimization of material/chemical properties • Prediction scaled-up material properties with artificial intelligence	V.A. Samaranayake*/Math Aditya Kumar/MSE Jinling Liu/EMSE Taghi Sherizedeh/Mining Sanjay Madria/CS Mike Hilger/BIT
Materials Workforce Development	Organize and deliver educational materials, training workshops, internship and research opportunities, as well as conduct outreach to candidates and stakeholders.	• Only US institution with degree programs in both ceramic and metallurgical engineering • Offers graduate certificates in materials for extreme environments, iron and steel metallurgy, and advanced engineering materials as resident and distance programs • Lead institution for national hypersonics materials curricula development funded by ONR/OUSD	David Lipke*/MSE Joseph Newkirk/MSE Bill Fahrenholtz/MSE Greg Hilmas/MSE Wayne Huebner/MSE Scott Miller/MSE Kelley Wilkerson/MSE Mike Moats/MSE

Low dimensional materials	Synthesis, fundamental physics and chemistry, and rational design of applications of low-dimensional materials in optoelectronics, quantum computing, biology and medicine, advanced composites, energy, and catalysis	• Highly cited papers on 0D (nanodiamond) and 2D (2D transition metal carbides/nitrides - MXenes) • Patents on nanodiamond functionalization and composites • Pioneering work on fundamental chemistry and physics of 0D and 2D materials • Active funding from federal agencies and industry, great potential for internal and external collaborations • Expertise in atomic layer deposition including pioneering work on deposition on porous materials and particles	Vadym Mochalin*/Chemistry Manashi Nath/Chemistry Alex Chernatynskiy/Physics Risheng Wang/Chemistry Anthony Convertine/MSE Chenling Wu/CAE Sutapa Barua/Chemical Eng. Xinhua Liang/Chemical Eng Fateme Rezaei/ChE Ali Rownaghi/ChE
Photonic Materials	Design, characterization, and applications of novel photonic materials and nanostructures, optical metamaterials, and quantum emitters	• Highly recognized journal publications on optical metamaterials especially chiral plasmonic metasurfaces • Demonstrated the world's thinnest optical holograms with nanopatterned 2D material monolayer • Advanced equipment for charactering optical properties of photonic materials and optical metamaterials	Xiadong Yang*/MAE Jie Gao/MAE
Topological materials	Discovery and study of new electronic materials that are promising for new science and technology development.	• One of the pioneers in topological materials synthesis • Developed new technique in synthesizing and fabricating the new materials • Worldwide collaboration in the studies of topological materials	Yew San Hor*/Physics
Metal additive manufacturing	Design of new alloys and new processes for additive manufacturing and optimization of metal additive manufacturing processes for enhanced performance	• Commercial and unique custom printers including a custom printer designed for new alloy research • Original developers of hybrid manufacturing and recognized leader in metal additive manufacturing in the U.S. due to long history of successful research • State-of-the-art infrastructure for metal additive manufacturing housed in a new showcase laboratory • Modeling and simulation of metal additive manufacturing • Large core of faculty working in this area with numerous funded projects.	Joe Newkirk*/MSE Yijia Gu/MSE Laura Bartlett/MSE Ming Leu/MAE Frank Liou/MAE Ron O'Malley/MSE Haiming Wen/MSE K. Chandrashekhara/MAE

Ceramic additive manufacturing	Development of new ceramic additive manufacturing methods to produce dense ceramics; fundamental research on ceramic feedstocks and structure-property relations of ceramics produced by additive manufacturing	• Developed and patented new additive manufacturing processes including ceramic freeze form fabrication and ceramic on demand extrusion (CODE) • Seminal studies of structure-property relations in ceramics produced by additive manufacturing • Unique facilities for materials agnostic printing, densification, and characterization including materials for extreme environments	Greg Hilmas*/MSE Ming Leu/MAE JeremyWatts/MSE Fateme Rezaei/ChE Ali Rownaghi/ChE
Energetic materials	Experimentation and computational research and performance testing of existing materials, creation of new energetic materials	• Experience with sensitivity testing of energetic materials for heat, friction, impact and ESD • Surface, underground and chamber test facilities • Broad range of funded projects including additive manufacturing of high explosives and shaped charge liners, explosibility of dusts and powders, and propellant mixing	Catherine Johnson*/Explosives
High Pressure-High Temperature Synthesis	Synthesis of new materials or metastable phases using the high pressure, high temperature environment produced by detonation	• Dedicated test chamber for materials synthesis • Federal explosives license with fully trained faculty and staff • Experience with explosive compaction and synthesis of nanodiamond and non-oxide ceramic nanopowders	Bill Fahrenholtz*/MSE Catherine Johnson/Mining Vadym Mochalin/Chemistry
Infrastructure materials	Design, characterization, and application of conventional and innovative infrastructure materials for planning, design, construction, forensics, and repair sustainable built environment.	• Strategic investment area for Missouri S&T • Global recognition as leaders plus highly cited papers on infrastructure material • State-of-the-art equipment for testing rheological, mechanical, structural, and durability properties of construction and infrastructure materials • National/international recognized experts in asphalt, concrete, geotechnical materials areas • Broad collaborations from diverse disciplines with long history of successful acquisition of external funding from state DOTs, USDOT, and industry • Major infrastructure investment with the Clayco ACML ($7M laboratory with >$3.5 M research equipment).	Jenny Liu*/CAE Kamal Khayat*/CAE Xiong Zhang/CAE Magdy Abdelrahman/CAE Mohamed ElGawady/CAE John Myers CAE Kwame Awuah-Offei/MNE Dimitri Feys/ CArEE Aditya Kumar/MSE Hongyan Ma/CAE Thomas Shuman/Chemistry Lesley Sneed/CAE Grace Yan/CAE Bob Wu/CAE

Steel production	Development and prototyping of next generation steels with superior mechanical properties, manufacturing process development for improved production efficiency and product quality and advanced sensing technologies for sensing in extreme manufacturing environment	• Peaslee Steel Manufacturing Research Center (PSMRC) with financial support from 18 industry members • Fully equipped steel foundry for producing pilot quantities of steel and non-ferrous alloys and castings • Lab and pilot scale hot and cold rolling facilities • Fully equipped materials testing laboratory with Gleeble and other specialized testing equipment. • Access to Advanced Materials Characterization Laboratory (AMCL) and other specialized characterization equipment (SEM-AFA, Cathodoluminescence, etc.) • Modeling and simulation software • Expertise in steelmaking, casting, refractory systems, thermomechanical processing, and microstructure-property relationships	Ron O'Malley*/MSE Laura Bartlett/MSE Jeff Smith/MSE Jie Huang/ECE Mario Bucheley/MSE Simon Lekakh/MSE K. Chandrashekhara/MAE
Metal casting	Modeling, design, production, and finishing of high performance and lightweight alloys.	• Dedicated foundry and joining laboratory for lab-scale and pilot-scale processing • Thermodynamic and kinetic simulation capabilities • Atomistic simulations to design compositions and predict fundamental properties and phase stability • Full analytical support for composition and inclusion analysis • Induction and vacuum induction melting • Sand/permanent molding and investment casting	Laura Bartlett*/MSE Julia Medvedeva/Physics
Glass	Design new compositions and produce functional forms that solve engineering problems, and. develop physics-based models to predict composition-structure-property relationships	• International reputation for specialty glass science and technology • Laboratory infrastructure for preparing and characterizing glasses • Strong interdisciplinary collaborations involving glasses for additive manufacturing, optical sensors, biomedical applications • S&T alumni in positions of influence in all sectors of US glass industry	Richard Brow*/MSE Aditya Kumar/MSE Julia Medvedeva/Physics Ali Rownaghi/ChE

Biomaterials	Synthesis an in vitro / in vivo evaluation of for use in constructing artificial organs, prostheses, controlled drug/gene delivery, and tissue engineering	• Dedicated animal vivarium and animal staff scientist for conducting animal experiments / surgeries • State of the art in vitro analysis equipment (e.g. confocal microscopes, flow cytometers) • Biosafety level 2 cell culture synthetic wet laboratories focused on biomaterial synthesis • Licensed patent portfolio of materials for biomedical applications	Anthony Convertine*/MSE Richard Brow/MSE Hu Yang, ChemE Yue-Wern Huang, Biology Nuran Ercal, Chemistry Julie Semon, Biology
Cement chemistry	Design and discovery of new cementitious materials with near-zero carbon footprint and unprecedented properties (high strength; high workability; enhanced durability in extreme climactic conditions)	• Broad range of funded projects from state, federal, and private entities (e.g., NSF, DOE, and DOT) • State-of-art equipment to characterize various physicochemical characteristics of cementitious materials • Unique equipment to: monitor reaction kinetics; determine evolutions of rheological properties and mechanical properties; assess durability of cementitious formulations • Unique first principles- and artificial intelligence-based methods to predict and optimize properties of cementitious formulations	Aditya Kumar*/MSE Hongyan Ma/CAE Monday Okoronkwo/Chem Eng Kamal Khayat/CAE
Raw material supply	Improving the sustainable supply of raw materials for modern infrastructure and manufacturing needs through technological and policy innovations. Synergistically supports Materials, Manufacturing, Infrastructure and ReNEWs pillars	• Broad range of funded projects from state, federal, and private entities (e.g., NSF, DOE, and DOT) • O'Keefe Institute focused on entire raw material supply chain • Can address entire supply chains within one university • Submitted 4 proposals this summer to State Dept and DOE/AMES Critical Materials Institute • Significant network with major mining companies • History of industrial and international funding	Mike Moats*/MSE Lana Alagha/MNE Kwame Awuah-Offei/MNE Suzie Long/EMGT Marek Locmelis/GGPE Alanna Krolikowski/PolySci Mark Fitch/CAE
Nuclear materials	Design, development, fabrication and testing of materials used in nuclear energy applications and in extreme radiation environments	• Campus nuclear research reactor, campus radioactive materials licenses and authorized laboratories • Existing research projects funded by DOE and NASA, and strong research partnerships with DoE laboratories • Expertise in advanced nuclear materials development, irradiation experiment design, post-irradiation examination, and computational modeling of nuclear fuel properties	Joseph Graham*/Nuclear Eng Haiming Wen/MSE Alex Chernatynsiky/Physics

Environmentally-friendly corrosion inhibitors	Replacements materials for cadmium and chromium compounds	• Patents for chromate replacements licensed commercially • History of working with DoD and industrial partners on large projects • Continued effort to reduce environmental footprint of corrosion mitigation in DoD and DoE platforms	Bill Fahrenholtz*/MSE Tom Schuman/Chemistry Matt O'Keefe/MSE
Materials for energy and environment	Materials for sustainable production of clean water and energy, catalysis, CO_2 storage, and energy conversion/storage	• Ability to tailor porosity from nano to macro scale in polymers and other materials • Fundamental studies of adsorption and diffusion in many different materials • Different approaches involving nanomaterials, catalysis, porous materials, and others • Patent applications for catalyst preparation by ALD • Design of new materials for energy storage and conversion	Fateme Rezaei*/ChE Xinhua Liang/ ChE Hongyan Ma/CArE Ali Rownaghi/ChE Angela Lueking/ChE Daniel Forciniti/ChE Jee C. Wang/ChE Partho Neogi/ ChE Monday Okoronkwo/ChE Muthanna Al Dahhan/Che Amitava Chouhury/Chemistry Manashi Nath/Chemistry Jonghyun Park/MAE Jay Switzer/Chemistry Julia Medvedeva/Physics

* Denotes lead on input for the research pillar assessment