Materials laboratories of the future for alloys, amorphous, and composite materials

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In alignment with the Materials Genome Initiative and as the product of a workshop sponsored by the US National Science Foundation, we define a vision for materials laboratories of the future in alloys, amorphous materials, and composite materials; chart a roadmap for realizing this vision; identify technical bottlenecks and barriers to access; and propose pathways to equitable and democratic access to integrated toolsets in a manner that addresses urgent societal needs, accelerates technological innovation, and enhances manufacturing competitiveness. Spanning three important materials classes, this article summarizes the areas of alignment and unifying themes, distinctive needs of different materials research communities, key science drivers that cannot be accomplished within the capabilities of current materials laboratories, and open questions that need further community input. Here, we provide a broader context for the workshop, synopsize the salient findings, outline a shared vision for democratizing access and accelerating materials discovery, highlight some case studies across the three different materials classes, and identify significant issues that need further discussion.

Materials laboratories of the future: A community vision

Over a decade ago, the Materials Genome Initiative sounded a clarion call to discover, manufacture, and deploy advanced materials twice as fast and at a fraction of the cost compared to conventional methods.[1,2] In the past decade, the centrality of materials solutions to many of the defining problems of our generation has become even more urgent in a world that is struggling to accelerate the energy transition in the face of an unprecedented climate emergency[3] and coming to terms with the limits of planetary boundaries and natural resources.[4] To achieve and accelerate the vision of the Materials Genome Initiative and to rapidly bridge the continuum of invention—innovation—manufacturing—deployment, materials laboratories of the future will need to integrate tools across the materials development continuum, ranging from materials prediction and simulations to synthesis/processing, characterization, and manufacturing.[1,5] Solutions are needed to not only discover materials with the desired functionalities, but will also need to consider low energy, environmentally friendly manufacturing routes, and end-of-life and upcycling strategies. Solutions will require grappling with the implications and opportunities of artificial intelligence (AI),[6] poised at the beginning of a paradigm shift in how objects are manufactured, used, and

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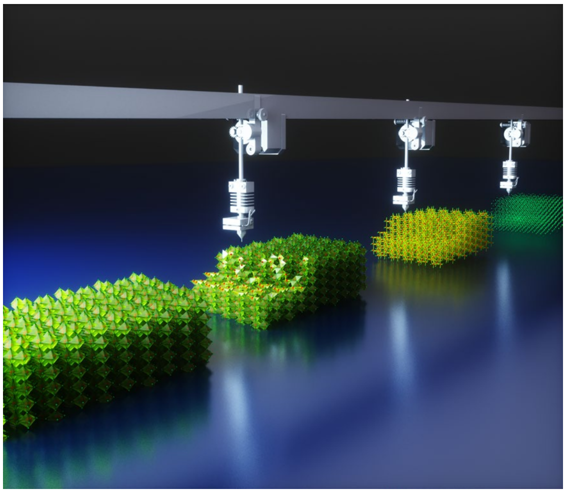

Figure 1. A vision for materials laboratories of the future that structure materials with atomic precision across decades of length scales.

recycled. Transformative tools are required across this continuum to expand the frontiers of materials characterization in time, space, energy, and to deterministically structure materials across decades of length scales (**Figure 1**).

In response to these urgent challenges and to develop a community vision for the materials laboratories of the future, the US National Science Foundation (NSF) Division of Materials Research (DMR) supported a hybrid workshop on November 7–8, 2022, at The University of Chicago, which was attended by 51 researchers from across academia and national laboratories. The workshop emphasized three important classes of materials: alloys, amorphous materials, and composite materials. The workshop was part of a three-part series, with each workshop individually and collectively seeking to thread together needs and opportunities across different classes of materials to establish a blueprint for ensuring US leadership in materials innovation over the next decade and beyond. The other two workshops focused on the distinctive needs and opportunities of (a) soft materials, polymers, and biomaterials and (b) materials with long-range order.

Workshop participants were prompted to describe one materials problem they want to solve in the next 10 years and the instrument or infrastructure capability needed to solve it. Lodestar talks on AI/machine learning (ML) tools to accelerate characterization,[7,8] laboratory-based x-ray absorption and emission spectroscopy,[9] and democratized access to electron microscopy through remote operation[10] provided succinct summaries of the state of the art, identified critical gaps, channeled emerging needs of stakeholders, and set the stage for extensive discussions and breakout groups whose summary findings are provided in subsequent sections.

Broader context for reimagining materials laboratories

Alloys, amorphous, and composite materials encompass a massive design space where causal relationships between compositional/structural degrees of freedom and the resulting properties are complex. The lack of long-range order and enormous diversity of constituent elements lends considerable complexity to such materials classes but also affords unparalleled opportunities for emergent properties and dynamical materials transformations. In such materials, design rules for assembling atoms within larger building blocks and for interfacing and collating singular or multiple building blocks into macroscopic objects remain to be defined with adequate granularity.

Our vision for the workshop was informed and shaped by several previous initiatives. The US Department of Energy (DOE) Office of Science, Office of Basic Energy Sciences (BES) organized a "Basic Research Needs Workshop for Innovation and Discovery of Transformative Experimental Tools: Solving Grand Challenges in the Energy Sciences" in 2016.[11] The workshop addressed a broad scope of topics including chemical reactions and transformations in functional environments, far-from-equilibrium imaging, deciphering spatiotemporal heterogeneity in materials, and transformative tools integrating modeling and experimentation. However, the last eight years have seen transformative advances in the role of automation, AI/ML, and deep learning in constraining, fusing, and guiding experiments and simulations that were only briefly touched upon in 2016. These topics were emphasized to a much greater extent in our workshop. Other workshops that were somewhat narrower in scope but have produced valuable inputs include a workshop funded by the National Institute of Standards and Technology and the Office of Naval Research on the role of AI in accelerating the development of materials and manufacturing innovations organized by The Minerals, Metals & Materials Society.[12] The National Academies of Sciences, Engineering, and Medicine hosted a workshop on emerging opportunities in materials science enabled by AI and ML on July 16–17, 2019, in Washington, DC.[13] Their report provides a broad perspective on the role of data science in materials design and manufacturing.

Other initiatives have focused more narrowly on specific techniques, such as an NSF-sponsored workshop on electron microscopy organized by Cornell University,[14] a National Academies of Sciences, Engineering, and Medicine workshop on ultrafast spectroscopy with high-brilliance laser sources,[15] and a workshop funded by the DOE and the National Institutes of Health (NIH) on magnetic resonance spectroscopy and imaging.[16] Our 2022 workshop was the first of its kind to bring together alloys, amorphous, and composite materials (e.g., high-entropy materials, glasses, metallic glasses, amorphous oxide semiconductors, nanocomposites, polycrystalline materials, and metal–organic frameworks [MOF]) under one roof to explore their distinctive challenges and opportunities.

The workshop also emphasized key workforce development and equitable access themes, which are inextricably interwoven with technical challenges and opportunities in instrumentation and infrastructure.[17–19]

Unifying themes and divergent needs across alloys, amorphous, and composite materials

Although there are workflows that have been advanced and integrated, including notable recent advances in robotic synthesis and high-throughput platforms,[20,21] Bayesian-based closed-loop methods,[22–24] and integrated workflows fusing data analytics, imaging, and simulations,[8,25–27] there is much that needs to be achieved to accurately encode physics and chemistry in AI and deep learning algorithms, to extract new design principles on the fly from experimental data, develop realistic, mixed-representation models across length scales, and to embrace complexity of form and function in materials design. Embedding autonomous experimentation loops within materials design workflows, pivoting between exploration and exploitation, and developing human/machine cohesion methods represent key frontiers.

Precision materials synthesis—the three-dimensional (3D) structuring of matter across length scales as sketched in Figure 1—remains a key priority, from an improved understanding of thermomechanical processing of alloys to solution-phase crystal growth, with a view toward deriving a greater understanding of reaction trajectories to achieve improved control of synthetic outcomes (i.e., phase purity, new states of matter, and scalable processing). All three communities represented in the workshop have a strong interest in nonequilibrium pathways,[28–30] predictive control of reaction trajectories, and improved understanding of synthesis/processing/fabrication/manufacturing, albeit the length scale that is of most interest varies across communities (e.g., atomistic control versus microstructure or macroscopic function).

The structure of complex interfaces and their dynamical evolution under realistic operational conditions remains a challenge across the alloys, amorphous, and composite materials communities. Interfaces show an incredible range of diversity in composition, structure, and 3D topology. The details of structure and connectivity along the interface–interphase continuum underpin transport phenomena and many emergent properties. Understanding defect and interface structure is of pivotal importance to deterministically mediating charge and mass transport in many modern technological applications. Yet there remain substantial deficiencies in experiments and simulations that limit the precision to which interfaces and interphases can be structured and systematically modulated.

Common concerns across the three materials communities focused on growing inequities in capabilities and challenges with training a diverse workforce with existing underfunded patchwork models. Although summer schools, internships, and workshops represent important constitutive elements of the materials science ecosystem, there was concern that such initiatives are ad hoc, fragmented, and heavily oversubscribed. As advanced instrumentation becomes more expensive, multimodal capabilities become imperative, and there is increased consolidation of instrument manufacturers, new paradigms are needed to ensure equitable and democratized access. Related concerns focused on costs and expertise needed to build data toolsets and infrastructure. Although the centrality of data to materials research is now well established, gaps remain in defining standards, quality control, and key interoperable and reusable aspects of Findable, Accessible, Interoperable, and Reusable (FAIR) principles.[31,32] The transformations wrought by data science, AI, automation, and multimodal capabilities have engendered across materials communities an unprecedented openness to new collaborative models for maintaining and accessing midscale physical and data infrastructure (for instance, the A-Lab at Lawrence Berkeley National Laboratory and materials acceleration programs leveraging robotic materials synthesis platforms at the University of Toronto, Liverpool, Georgia Tech, and Carnegie Mellon),[21,33–36] which in turn should inspire new funding mechanisms and modes of distributed access.

Some notable distinctions and differentiators also came to the fore between the alloys, amorphous, and composite materials communities, some of which were further echoed in discussions with the organizers of the other workshops. First, the costs of experimentation are different and often are related to the complexity of chemistry—"high-throughput" has very different meanings across different communities. Second, sample scales and form factors of most interest vary widely—from "bulk" materials or macroscopic samples to single crystals and thin films. This, in turn, results in some common threads but different emphases on defect structure and its evolution. From the perspective of materials characterization and instrumentation needs, different communities have varying emphasis on average versus local structure. Finally, not all communities are in the same place concerning integration with AI/active-learning or automation. Different research communities bring different cultures of contributing to and accessing shared regional or national user facilities. Addressing the needs of different materials research communities will be critical to designing the next generation of midscale infrastructure.

Key science drivers for materials laboratories of the future

Critical challenges in alloys, amorphous materials, and composite materials include being able to observe and understand them at the level of atoms and electrons under realistic operating conditions, and explore the dynamical evolution of complex forms of matter at relevant time scales. Such understanding is imperative to deterministically direct flows of charge, energy, and mass as required for applications in modern technologies. Effective utilization of new toolsets will require not only overcoming technical obstacles and integration of traditionally siloed workflows but also the

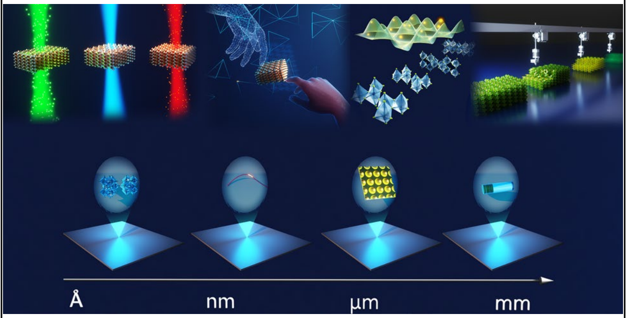

Figure 2. A community vision for materials laboratories of the future: a schematic depiction of the aspirations of the alloys, amorphous, and composite materials research communities.

training of a next-generation workforce with the interdisciplinary skills to address the challenges and take advantage of the opportunities afforded by transformative and generational changes in automation, artificial intelligence, scale-bridging modeling, and instrument development.[2,18,19] The following emerged as the most crucial science drivers that cannot be accomplished within the capabilities of current materials laboratories (**Figure 2**):

1. Real-time atom-by-atom manipulation of matter and "on-the-fly" modification of reaction trajectories or pathways during synthesis to arrive at desired structural or microstructural outcomes;
2. understanding and establishing deterministic control of nonequilibrium pathways, and learning design rules for stabilizing metastable phases of matter;
3. multimodal 3D atom-precise understanding of the structural evolution of matter in response to application of different fields (e.g., optical excitation, high strain rate deformation, and thermal excitation) under realistic operational conditions, and mapping of dynamical structural evolution to principles of device function;
4. embedding AI in nontrivial tasks to understand new physics and chemistry, propose and explore scientific hypotheses, and effectively interface with human intelligence; and
5. multifidelity design and interfacing of experiments and models, and the ability to "zoom-in/zoom-out" as required to understand phenomena at different length scales.

In the following sections, we provide brief vignettes of recent advances, describe a blueprint for realizing these ambitious goals, and make note of key gaps and opportunities.

Case studies of materials laboratories of the future

To set the stage for broader discussions, we present brief highlights from the recent literature that exemplify the promise of integrated workflows and multimodal characterization in materials laboratories of the future. We provide examples from three materials classes and research communities represented at our workshop.

Alloys: High-throughput synthesis and characterization of metals via compositionally heterogeneous coupons

The vast design space of metallic materials—including, but not limited to, composition, phase fraction, and microstructure—is often in direct conflict with their synthesis and processing. Traditional manufacturing has been optimized to produce a single composition into a uniform material with a prescribed microstructure. As a result, existing workflows are not amenable to materials discovery. New approaches are needed to produce different materials within a single batch and efficiently map out thermal/mechanical treatments.

Spatial tailoring of materials composition is a particularly promising approach. Complex phase diagrams can be rapidly discovered by locally varying the composition, either as regions with discrete compositions or as gradients.[37] These insights can then be combined with localized heating for prescribed time intervals,[38] to rapidly determine time–temperature–transformation diagrams. Finally, local materials properties can be extracted using surface-based techniques. However, emerging synthesis approaches are poised to accelerate these workflows even more.

Powder-based additive manufacturing is a useful class of techniques to rapidly fabricate spatially tailored materials. Using laser-directed energy deposition (L-DED), a suite of compositions can be immediately deposited by modulating the feed rate from different powder hoppers. A significant benefit of L-DED is that samples are easily made in ASTM/ISO geometries with microstructures that are representative of industrial materials.[39] Furthermore, as-fabricated samples can be integrated with mechanical test frames for automated bulk testing.[40] These integrated testing concepts are extendable to evaluating other materials properties, such as oxidation kinetics.

A recent study (**Figure 3**)[41] demonstrated a high-throughput oxidation test that used spatially tailored in both the specimen and environment. Test coupons were fabricated with spatially tailored compositions via L-DED and then oxidized under a thermal gradient. This approach overcame the sluggish batchwise nature of oxidation testing by enabling every temperature of interest to be evaluated simultaneously (at a single partial pressure and time). After testing, the activation energy was characterized in a single step by quantifying the oxide film thickness versus temperature. Composition variations in the coupon were modest to avoid interdiffusion effects, but this feature could be exploited in dissimilar systems to understand additional chemical effects. This study is but one example of how heterogeneous materials can be leveraged in novel workflows in laboratories of the future.

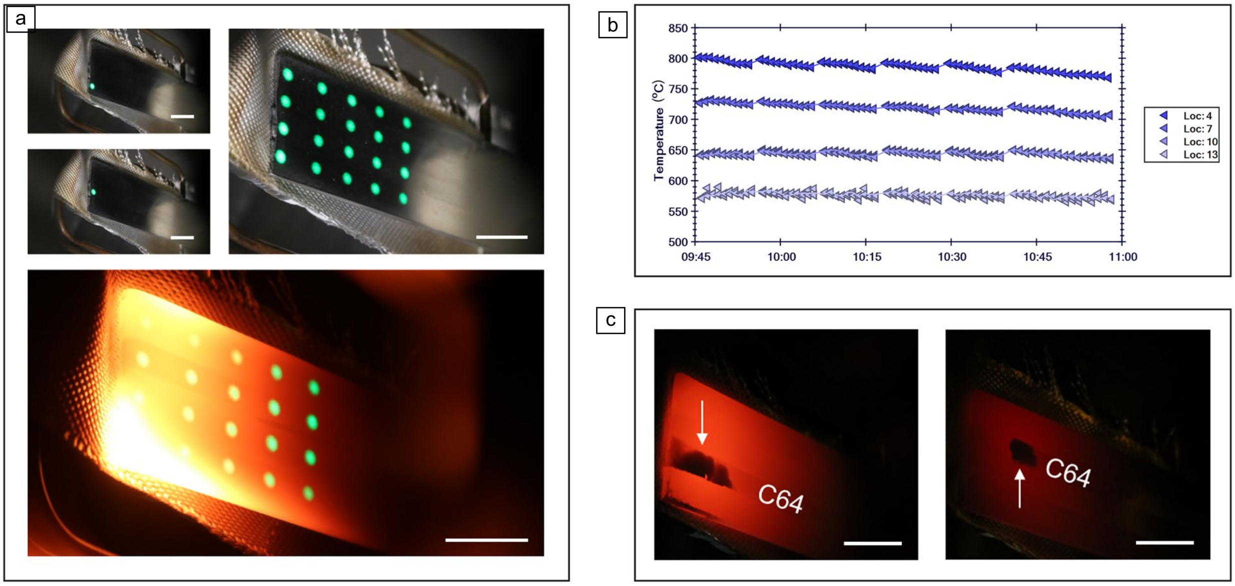

Figure 3. High-throughput oxidation testing using a compositionally heterogeneous coupon under a thermal gradient. (a) Multimaterial coupon, before and during test, consisting of four different steels deposited via laser-directed energy deposition. Green laser spots indicate regions where a multiwavelength hyperspectral pyrometer collects thermal data (before and during testing). (b) Representative temperature versus time in minutes from the pyrometer, highlighting steady-state temperature readings. (c) Spalling oxide on Ferrium C64 steel during cooling. Scale bars = 2 cm.

Amorphous materials: Time-resolved coherent scattering of dynamics in disordered systems

Dynamics in liquids and glasses are temporally and spatially complex, involving 15 or more orders of magnitude in time and nanometer to subnanometer length scales. This complexity poses major challenges for characterization, simulation, and theory. However, manipulating dynamics offers synthesis routes to new materials for a vast range of applications, from organic light-emitting diode displays to gears and springs.

Time-resolved coherent scattering, in the form of x-ray photon correlation spectroscopy (XPCS), electron correlation microscopy (ECM), and related techniques, has made significant progress in unraveling this complex behavior across length scales and has provided insights into dynamic transformations. Early experiments with coherent soft x-ray beams were limited to studying colloids and large molecules, but high energy, coherent electron beams, and hard x-ray beams provide access to atomic scattering in liquids and glasses.

For systems in (metastable) equilibrium, XPCS yields the structural relaxation time, τ, over a wide range of time and temperature. For example, XPCS experiments measuring $\tau(T)$ for a sodium silicate glass found that, well below its glass-transition temperature, T_g, τ values are orders of magnitude faster than bulk properties would suggest.[42] The shortest τ values were attributed to "liquid-like" regions trapped inside the glass, which are not predicted by theories of glass formation but could influence mechanical properties. ECM yields $\tau(T)$ over a narrower range of time and temperature but with subnanometer spatial resolution. ECM produced the first images of nanoscale domains with varying τ within a supercooled liquid,[43] as shown in **Figure 4**. Understanding the growth of these domains is central to validating and developing systematic theories of the glass transition.

These methods reveal discrete events arising from stochastic, activated processes for systems out of equilibrium. For example, XPCS measurements on metallic glasses show that stress, even in the elastic regime, causes a variety of irreversible structural relaxation events to occur.[44] These events continue over surprisingly long times and break otherwise universal aging behavior. ECM experiments show that thermal aging events in glasses are spatially heterogeneous and intermittent in time, and that deliberate nanoscale variations in composition, as in a nanoglass, can be used to control aging.[45] Higher brightness sources and faster detectors will bring greater insights into dynamics in disordered systems provided by these experiments. However, data from such experiments will be prodigious in quantity and complexity, requiring integration with emerging AI/data science methods in materials laboratories of the future to maximize impact.

Composite materials: Cryo-FIB/EM-enabled structural and chemical analyses of composite materials of synthetic and biological origins

The proper processing and functioning of many composite materials rely on carefully designed interfaces and/or interphases across many length scales, where detailed knowledge

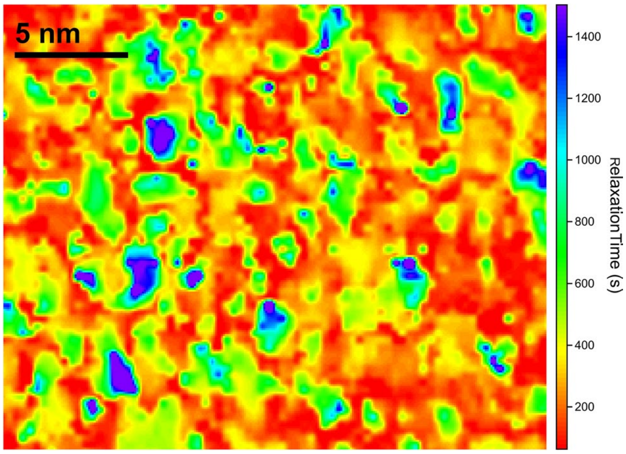

Figure 4. Electron correlation microscopy map of the structural relaxation time of supercooled $Pd_{43}Cu_{27}Ni_{10}P_{20}$ held 4 K above T_g. The dynamics are strongly spatially heterogeneous: While much of the sample has a relaxation time of ~200 s typical for a liquid near T_g, some nanoscale regions have relaxation times up to 1500 s. The map has been up-sampled from the original 62 × 74 pixel size for presentation and smoothed to reduce noise.

of the structure, chemistry, and dynamics is critical. These interfaces and interphases often involve materials with starkly different properties such as liquid/solid interfaces, organic/inorganic interfaces, and cellular/mineral interfaces. Understanding interfacial and interphasic structure poses significant challenges for conventional electron microscopy techniques such as scanning electron microscopy (SEM) and (scanning) transmission electron microscopy ([S]TEM), as they are limited to vacuum- and electron-beam-stable solid materials. Cryogenic electron microscopy, which was originally developed in the 1980s for characterizing biological specimens in their native aqueous states, has recently found increasing use for studying a range of beam-sensitive materials, particularly composites. Moreover, by combining with cryo-focused ion beam (FIB) milling, site-specific (S)TEM specimens from hydrated, beam-sensitive "soft" materials can be prepared and studied in bulk, thin films, or particulate form.

One particular group of materials that can benefit from this technique is energy-storage and conversion materials that are inherently heterogeneous. For example, Zachman et al.[46] utilized cryo-FIB and *in situ* liftout to prepare electron-transparent lamella of the anode–electrode interface of lithium-metal batteries in their native state and subsequently performed detailed structural and chemical analyses of the interface using cryo-STEM and electron energy-loss spectroscopy (**Figure 5**a). They uncovered two dendrite types coexisting on the lithium anode, each with a distinct morphology and composition. As another example, the surfactant-mica interface studied by Long et al. (Figure 5b)[47] can also be characterized by this approach. In contrast to bulk samples where cryo-FIB milling of (S)TEM lamella is required prior to liftout, particle-based specimens can be directly transferred to TEM grids from a cryo stage and subsequently cryo-FIB milled. Zhou et al. utilized this methodology to study the ultrastructure of highly beam-sensitive MOF crystals with atomic resolution (Figure 5c–g).[48] Samples milled at cryogenic temperature clearly showed reduced FIB milling damage and hence enabled high-resolution imaging (Figure 5c–d).

In addition to synthetic materials, cryo-FIB/EM has recently enabled important new insights for understanding the formation mechanisms of biomineralized materials by providing structural and chemical information at the biomineralization front under close-to-native conditions.[49,50] For example, utilizing cryo-FIB-based serial sectioning and SEM imaging, Raguin et al. analyzed the calcium-rich intracellular vesicles in 3D within the forming bone tissue of a chick embryo femur (Figure 5h–i).[51] Capua-Shenkar et al. utilized a similar approach to investigate the formation pathways of the organic crystalline cholesterol, which plays a critical role in the development of atherosclerosis (Figure 5j–l).[52] The authors showed that the nucleation and growth of cholesterol crystals are strongly associated with the intracellular and extracellular lipid droplets and multilamellar bodies. Finally, using cryo-FIB milling and, subsequently, cryo-TEM tomography, Kadan et al. revealed the nanoscale membrane-calcite crystal interfacial architecture in unicellular coccolithophores and further pointed out the importance of extreme confinement in biomineralization (Figure 5m–n).[53] With advances in data science approaches and developments in instrumentation[54] and workflow,[55] cryo-FIB/EM-based analyses stand poised to play a critical role in materials laboratories of the future for characterizing various soft–hard interfaces in composite materials of both synthetic and biological origins.

Reimagining the materials instrumentation, infrastructure, and innovation ecosystem

Invention and innovation in materials science are tightly interwoven with instrumentation and infrastructure. Our vision in convening this workshop was to bring together a diverse community of researchers in this endeavor to ensure the representation of stakeholders from across the NSF DMR community spanning technical areas, materials classes, types of institutions, researcher career stages, and diversity of researcher backgrounds. To systematically reimagine materials laboratories of the future, the participants undertook deep dives into the following overarching themes:

1. Integrating infrastructure and instrumentation in materials laboratories of the future: embedding AI/ML in closed-loop make, measure, model cycles
2. Bridging length and time scales in modeling and measurement
3. Interrogating dynamical transformations of materials in functional environments and far from equilibrium
4. Atom-precise assembly across length scales
5. Workforce development needs

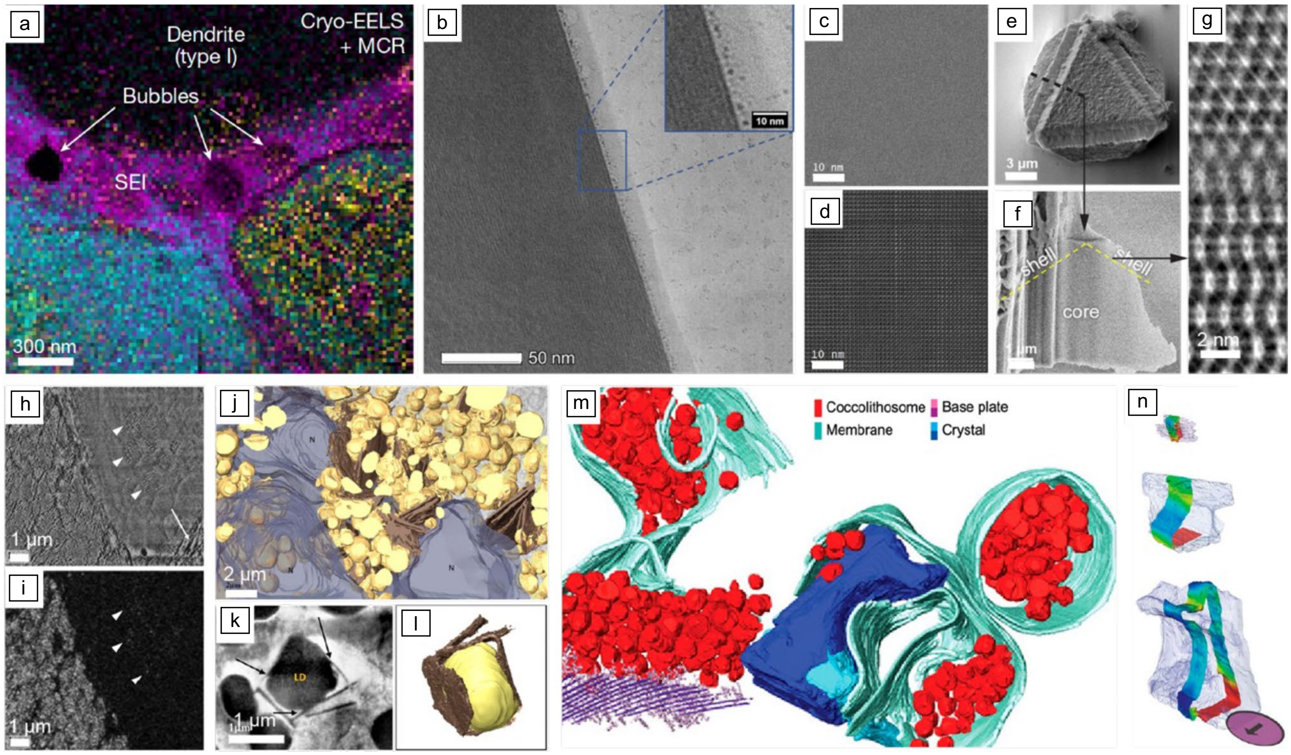

Figure 5. Cryo-focused ion beam (FIB)/EM analyses of synthetic and biological materials. (a) Spectroscopic mapping by cryo-scanning transmission electron microscopy-electron energy-loss spectroscopy (STEM-EELS) of the liquid/solid interface in a lithium-metal battery.[46] (b) Cryo-TEM image of the surfactant-mica interface.[47] High-resolution transmission electron microscopy images of HKUST-1 metal–organic framework (MOF) specimens prepared via FIB milling at (c) room and (d) cryogenic temperatures.[48] (e) An octahedron-shaped MOF crystal with a core–shell structure, corresponding (f) TEM specimen prepared via cryo-FIB milling, and (g) STEM image of the core–shell interface.[48] (h) The mixed Inlens/secondary electron and (i) corresponding backscattered electron images showing the intracellular vesicles containing mineral precursors (arrowheads).[51] (j) Three-dimensional rendering of the atherosclerotic lesions based on cryo-FIB/SEM tomography data sets, showing lipid droplets in yellow, cholesterol crystals in brown, and cell nuclei in light purple.[52] (k) Two-dimensional slice image and (l) 3D view of individual crystals attached to a lipid droplet.[52] (m) Three-dimensional rendering of the growing coccolith crystals within vesicles based on cryo-TEM tomography data sets.[53] (n) Analyses of the distances from points on the crystal surface to the closest membranes. EM, electron microscopy; FIB, focused ion beam; SEI, solid electrolyte interface.

6. Equitable and inclusive access to instrumentation and infrastructure

In the following sections, we abstract key findings from these discussions.

Integrating infrastructure and instrumentation in materials laboratories of the future: Embedding AI/ML in closed-loop make, measure, and model cycles

Advancements that synergize experimental science, theoretical models, AI-driven data analytics, and high-performance computing infrastructure possess substantial potential to redefine future laboratories. Although the replication of human-like ingenuity and creative reasoning remains an unsolved challenge in AI, computational methodologies offer unparalleled capabilities for data analysis at scales and speeds that are beyond human cognitive limits. The laboratory of the future will strategically integrate these diverse competencies with the greatest opportunities arising from the ability to augment human intellect and intuition.

Emerging avenues where AI stands poised to significantly influence scientific research include

1. *Autonomous and directed experimentation.* Utilizing active learning strategies for balancing exploratory and exploitative actions, autonomous experimental setups can intelligently focus on rare yet critical events, thereby liberating researchers from laborious tasks. This paradigm represents an advanced form of compressed sensing with cognitive capabilities.
2. *Large-scale multimodal data mining.* With the increasing prevalence of *in situ* and *operando* experiments, AI algorithms furnish computational pipelines for isolating and identifying statistical features in heterogeneous data. This enables rapid scientific insights and informs subsequent

experimental designs with low latency. Moreover, semantic relationships can be constructed across large, structured data repositories—whether computational, bibliographic, or curated—to break down traditional data silos.

3. *Real-time data reduction.* The escalating capabilities of sensors, characterized by reduced cost and enhanced spatial–temporal resolutions, have resulted in data generation rates that exceed the computational capacities of individual academic institutions. Emerging research in embedded systems aims to mitigate these challenges by employing custom hardware architectures such as field-programmable gate arrays (FPGAs) and application-specific integrated circuits (ASICs) to reduce data velocities and storage requirements.
4. *Real-time analytical and operational control.* In fields such as materials science, where synthesis and characterization processes are inherently dynamic, artificial intelligence algorithms can serve as rapid approximators for complex control systems. This enables real-time, autonomous adjustments and course corrections. Such capabilities are particularly pertinent for autonomous discovery in far-from-equilibrium processes, extending to various domains including electrical energy storage, catalytic systems, metallic alloys, oxide glasses, co-amorphous molecular systems, and polymeric nanocomposites.

AI transcends the mere acceleration of scientific research; it fundamentally reconfigures the scientific methodology. Experimental paradigms previously intractable due to analytical complexities become feasible, facilitating a departure from reductionist approaches to engage multifaceted, multi-objective phenomena. Economically efficient AI-driven experiments enhance research scalability, encourage risk taking, and democratize access to otherwise cost-prohibitive systems. The declarative specification of experiments in both human- and machine-readable forms paves the way for unparalleled scalability and parallelization, deviating from traditional apprenticeship models focused on tactile skills—where PhD candidates and researchers can focus on creativity, innovation, and expert analytics.

To fully integrate AI and ML into future materials discovery laboratories, several challenges and categories warrant attention:

1. *Computing infrastructure.* Existing high-performance computing (HPC) architectures are suboptimal for experimental data analytics, necessitating high availability, deterministic networking, and computing resources. The prevalent centralized, scheduler-based model impinges upon automated workflows due to network congestion and resource availability. A bespoke computational infrastructure, tailored for scientific workloads, should be developed, incorporating high-availability, self-healing, and load-balancing functionalities via Kubernetes or similar orchestrators, thereby facilitating continuous deployment and AI/ML-based control over data flows.
2. *Storage infrastructure.* Achieving FAIR scientific data is a pressing issue. Developing open-source, rigorously documented file formats and metadata schemas is crucial.[32] Community-wide standardization, or at least interoperability standards, are essential, along with platforms for secure data sharing and hosting.
3. *Skill development and science education.* The skill set of the contemporary experimental scientist is increasingly computation-centric. Thus, curricula must be restructured to include core computational tools like data analytics and AI/ML techniques pertinent to data collection and analysis across scientific disciplines.[12,18,36]
4. *Interdisciplinary collaboration.* The facile adaptability of AI methods to scientific questions raises concerns, especially given the propensity for overfitting in machine learning models that can masquerade as genuine understanding. A concerted effort to break disciplinary silos is imperative for the codesign of machine learning techniques and validation methodologies that respect both the foundational principles of ML and parsimony required for materials science.
5. *Open science and hardware.* The proprietary nature of scientific instrumentation hinders technique innovation. A shift toward an open-source community development model, compliant with standards such as IEEE and ISO for data transfer and curation as well as experimental protocols (i.e., ASTM-like), is necessary. Purchasing power should be leveraged to demand Software Development Kits (SDKs) and Application Programming Interfaces (APIs) from manufacturers, thereby lowering barriers to automation and interoperability. Moreover, codebases should be well documented and architecturally sound to be accessible to scientists with limited coding expertise.

Integrating AI and ML into scientific research is poised to redefine traditional methodologies, enabling unprecedented scale, speed, and complexity in experimental designs. This paradigm shift cannot only accelerate data analytics, but it can also democratize access to advanced research, facilitating interdisciplinary collaborations and risk taking. However, realizing this transformation requires overcoming substantial challenges, including the development of specialized computing infrastructure, standardized data storage solutions, and modernized educational curricula. Addressing these hurdles through strategic planning and interdisciplinary collaboration will be instrumental in unlocking the full potential of AI-driven laboratories for future materials discovery and broader scientific endeavors.

Bridging length and time scales in modeling and measurement

Capturing the structure, composition, and chemical state of materials at various length scales is a complex challenge that cannot be effectively accomplished using a single technique. Being able to dissect a complex composite material or device and map out the structural details with atomic precision in 3D, and then correlate this to its property or performance in a device in a state that best reflects the intrinsic starting material and fundamental operating mechanism represents a grand challenge. Instead, it necessitates the integration of multiple methods bridging length, time, and energy scales. X-ray, optical probes, electron microscopy, and time-of-flight measurements are the most commonly used across alloys, amorphous, and composite materials.[56] By fusing data from these various sources, we can circumvent and surpass the inherent limitations of each individual technique. Multimodal characterization enables a comprehensive view of materials properties and behavior, going (far) beyond the capabilities and purview of a single method.[57]

Multimodal characterization is typically performed on unique samples, often necessitating specialized hardware development that facilitates the transfer of samples from one instrument to another. This approach allows analyzing targeted microstructural and interface features, such as surface structure, grain boundaries, and defects. In the realm of materials science, there is an inherent correlation between length and time scales. Smaller systems evolve over much shorter time scales compared to larger systems. Capturing the entire dynamical response of a material across all relevant length and time scales as it couples to external fields (i.e., stress, electric current, ion flux, and temperature) represents a formidable and unsolved computational challenge.[58] New tools and techniques are imperative to select the appropriate method for study based on the specific application and requirements. For example, *in situ* techniques allow for the study of transient states.[59] Understanding the mechanisms involved in these states requires the ability to resolve metastable conditions that sometimes occur on picosecond time scales but can nevertheless be critical to eventual synthetic outcomes or functional properties. Here, we discuss key challenges and opportunities in bridging length and time scales.

Challenges in bridging scales

Measuring over large length and time scales. One significant challenge is measuring across a vast range—indeed, a terra incognita that spans multiple decades of length and time scales. Preparing samples for large-scale experiments with uniformity is challenging, as is translating laboratory-scale research to functional large-scale systems. The relevant time scales span from picoseconds to years. Access to advanced probes such as free-electron lasers provides access to picosecond time scales and can help decipher ultrafast phenomena. However, very long time scales that are imperative for assessing material failure can also be challenging to interrogate. Understanding material behavior at longer time scales requires accelerated aging protocols or long-term *ex situ* experimentation, which incurs a substantial resource burden.

Breaking the shackles of proprietary data formats. Integrating data from various multimodal characterization tools is often performed manually on proprietary software with limited transparency and often even less interoperability, which oftentimes results in errors and leaves much to user interpretation. Automated processing of multimodal data in an interoperable format across different platforms is essential to initiate a new paradigm of crowd-sourced tool development that will democratize access and accelerate materials design loops.

Instrumentation development. Much of instrument development has historically been the focus of national laboratories. However, neutron, x-ray, electron, and other national user facilities are stretched to the hilt. Establishing regional shared facilities at academic institutions is challenging but an urgent imperative. Such hubs will require innovative access, operation, maintenance, upgrade, and replacement models, which are not possible to run in an effective and world-leading manner when solely reliant on user fees.

Opportunities in bridging scales

Multifidelity experiments. Instead of fixating on "perfect" experiments with high precision, an alternative philosophy would emphasize lower fidelity, high-throughput experiments. These can potentially enable the broad survey of design spaces, even if primarily to provide initial qualitative insights. Such preliminary models can help researchers identify promising regions of the design space where more detailed, high-fidelity experiments are necessary to refine models and obtain precise quantitative predictions. Multifidelity experiment design linking to AI/ML models can be crucial in designing such experimental protocols and navigating complex design spaces.[60]

Multiscale modeling. Developing synergistic computational models to study mechanistic interactions at appropriate length and time scales is critical for developing a holistic understanding of the associated limiting phenomena and underlying tradeoffs. In addition, such computational models should be integrated with hierarchical characterization techniques to derive comprehensive insight into the scale-bridging mechanisms. The key challenge, but also an opportunity for future development, lies in bridging the appropriate scales between characterization and mesoscale modeling and analytics (e.g., see **Figure 6**).[61,62] Mesoscale physics along with advancements in machine learning can serve as an interpretive and predictive vehicle for data/imaging from hierarchical characterization techniques. This framework highlights the concurrent need for synergistic advancement in image-based analytics and digital simulations with embedded scale hierarchy such as for multifunctional porous architectures and to connect to advancements in disordered materials.[63,64]

Robotic experiments and automated anomaly detection. Advancements in computer vision and imaging open the door to conducting experiments with robotic platforms, ensuring greater reproducibility as compared to human

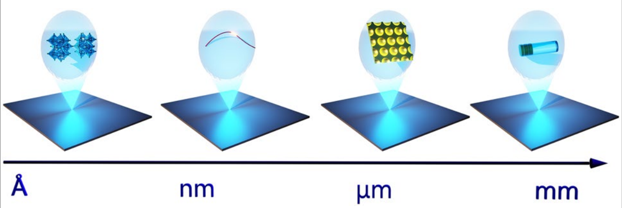

Figure 6. Spatiotemporal scale hierarchy in multiscale material systems.

interventions. Additionally, automated anomaly detection can identify unexpected patterns or data anomalies, which can then be flagged for human analysis to obtain deeper insights. The synergy between automation and human intuition holds the potential to significantly enhance our understanding of materials behavior.

Interrogating dynamical transformations of materials in functional environments and far from equilibrium

The field of materials science and electron microscopy has witnessed remarkable advancements in recent years, enabling in-depth investigations into dynamic transformations in alloys, amorphous materials, and composites within functional environments. *In situ* scanning and transmission electron microscopy (S/TEM) has emerged as powerful tools for studying the behavior and degradation of these materials during active operation. Various *in situ* methods have been developed, including environmental cells for gases and liquids, mechanical testing setups such as compression and tension stages, and heating and cooling devices. These techniques empower researchers to explore materials functionality and mechanisms of degradation under operational conditions. For example, *in situ* liquid cells facilitate the investigation of crystal synthesis and electrochemistry,[65–73] whereas *in situ* gas cell microscopy could significantly enhance our comprehension of corrosion resistance in high-entropy alloys and composites within specific gas environments.[65] Despite these advancements, several challenges remain that must be resolved in materials laboratories of the future.

Higher time resolution in STEM. While temporal resolution below the millisecond level has been attained in TEM through the use of direct detection electron cameras, STEM imaging, although offering the advantage of chemical contrast and simultaneous chemical analysis, often lags in temporal resolution. Materials laboratories of the future require the development of fast scan systems for STEM imaging and the implementation of machine-learning-based, electron-efficient, fast acquisition, and signal enhancement techniques in data analysis to significantly enhance the time resolution of *in situ* STEM imaging, potentially by orders of magnitude.

Materials in extreme environments. Materials at extremely high and low temperatures, temperature gradients, pressures, and/or loading rates are particularly challenging to observe at high resolution.[74] Materials that can perform satisfactorily in such environments are critically important to key industries, including aerospace, power generation, and mining among others. Therefore, advances in both instrumentation and high-throughput data and experimental modalities, coupled with an AI-driven design processes for materials in extreme conditions, are sorely needed.

Big data analysis microscopy. Currently, a fast camera in a TEM can achieve 10–100 K frames of images in a second, resulting in massive data outputs. Leveraging AI/ML for rapid data processing is essential. ML methods allow for the processing of hundreds of images within minutes. Researchers have already begun implementing ML with *ex situ* microscopy to track reaction dynamics and atomic displacement.[66,67] For instance, the U-Net convolutional neural network (CNN) has been utilized for particle boundary segmentation, enabling the extraction of the evolution of particle number, size, and shape changes. Fast detection of atom spatial distributions can be effectively achieved by employing a CNN-based algorithm.[68,69] Moreover, the Automatic Target Generation Process (ATGP) preconditioned joint nonnegative matrix factorization (NMF) has been developed to reveal trace signals in electron energy-loss spectroscopy (EELS) that could otherwise be overlooked.[75] Materials laboratories of the future have the opportunity to affect a paradigm change by implementing relevant analysis algorithms during *in situ* S/TEM experiments, allowing for real-time feedback to optimize experimental parameters. Additionally, new data acquisition algorithms, such as real-time adaptive sparse sensing,[76] should be devised to minimize the electrons required in experiments, thereby enhancing temporal resolution and detectability.

Integration of advanced techniques. Many innovative characterization techniques provide access to previously elusive information for electron microscopy, promising new insights into materials functionality and degradation when performed in tandem or in *in situ* environments. Examples include correlative microscopy between atom probe tomography (APT) and electron microscopy,[77] the integration of APT with *in situ* reactor chambers for the analysis of compositional changes during oxidation, which then could be correlated to STEM-based structural analysis,[78–80] or the integration of new STEM and EELS techniques, such as 4D-STEM and monochromated EELS, with *in situ* capabilities. Integration of electron microscopy approaches with other complementary characterization techniques permits overcoming the inherent limitation of electron microscopy methods, while enhancing scientific understanding.

We next outline the challenges and potential contributions of four-dimensional (4D)-STEM and monochromated EELS in understanding the functionality of composites, alloys, and amorphous materials in materials laboratories of the future.

1. *Four-dimensional-STEM.* Recent advancements in direct electron cameras and data analysis algorithms have enabled 4D-STEM, which simultaneously provides both real and reciprocal space information.[81–83] This advancement supports phase retrieval for specimen information recovery and has recently demonstrated its ability to acquire information challenging to obtain with conventional STEM imaging, including super-resolution,[84] sub-nm scale electric-field mapping,[85,86] chemical bonding imaging,[87] and imaging of beam-sensitive soft[81,87,88] and biological materials.[89] The potential of 4D-STEM significantly extends to the study of alloys, amorphous materials, and composites. For instance, it can effectively monitor grain orientation, size, and grain-boundary evolution in alloys during *in situ* microscopy. It also analyzes short- and intermediate-range ordering in amorphous phases and reveals space-charge effects at phase boundaries in polymer-ceramic composites, such as solid electrolytes for batteries. As an illustrative example, Zachman et al. demonstrated 4D-STEM-based DPC imaging, extracting long-range electric field data and enabling simultaneous imaging of atomic structures and interfacial charge distribution.[90] Integrating 4D-STEM with *in situ* microscopy is crucial for monitoring dynamic structural and charge distribution changes under simulated working conditions. To achieve this, a rapid scanning system with sparse sampling for real-time data acquisition is needed for fast *in situ* 4D-STEM imaging.
2. *Low-loss EELS.* Recent advances in monochromators have significantly enhanced the energy resolution in EELS, enabling the detection of phonons, excitations, and electronic band structures that were previously inaccessible with conventional EELS techniques.[91,92] While monochromated EELS has traditionally been applied to the study of low-dimensional materials and nanostructures, it also provides valuable insights into alloys, amorphous materials, and composites, including their interfaces and boundaries. For example, monochromated EELS has been demonstrated to map electronic structures at grain boundaries in polycrystalline solid electrolytes, revealing narrowed bandgaps in these regions.[93] This finding, coupled with results from *in situ* biasing TEM and macroscopic studies, suggests that grain boundaries contribute to dendritic growth in garnet solid electrolytes. Recent advancements in vibrational EELS spectroscopy enable the investigation of phonon signals related to ion transport in solid-state ionics, offering a novel approach to quantify ion transport behavior at interfaces. These techniques are applicable to various boundaries and interfaces, irrespective of their crystallinity. Additionally, low-loss EELS requires a small beam current and can be acquired in aloof mode, resulting in significantly reduced electron-beam damage. This makes it suitable for analyzing beam-sensitive materials, such as certain amorphous materials or composites involving soft materials. However, the integration of monochromated EELS with *in situ* capabilities is often constrained by hardware limitations. Materials laboratories of the future will need five-axis stages enabling high-energy-resolution EELS spectroscopy under *in situ* conditions.

In summary, recent advancements in materials science and electron microscopy and other correlative advanced microscopy methods, such as atom probe tomography, have provided powerful tools and techniques for studying dynamic transformations in alloys, amorphous materials, and composites under functional environments. Overcoming challenges in time resolution, data analysis, and integration of advanced techniques is essential for continued progress in the field, ultimately leading to a more comprehensive understanding of material behavior and performance.

Atom-precise assembly across length scales

Throughout history, the synthesis of new materials has been largely Edisonian, with as much success from chemical intuition as from serendipity. Mechanistic insights into the dynamic processes through which ions and molecules organize into large-scale architectures have been accumulated indirectly from years of compiled successes and failures, without direct evaluation and understanding of how simple chemical bonding interactions and geometric considerations can lead to atomically precise assembly over macroscale products. This approach can lead to a metric-driven mindset to achieving materials performance, without harnessing the fundamental science tools that can ultimately help us to understand, control, and scale up the production of new materials.

The materials laboratory of the future will be capable of efficient, on-demand synthesis of atomically precise materials to address society's rapidly evolving needs. To accomplish this grand challenge, a new approach to synthesis science must be fostered[94] that focuses on developing deeper insights into the nature of solvated species in solution, pathways for nucleation and crystal growth, and how metastable intermediates affect the final products.[95–100] Only then will there be sufficient understanding of how atoms and molecules assemble, so that synthetic pathways for materials can be designed *a priori* in ways that mimic retrosynthetic analysis for organic molecules.

Central to achieving this insight will be an investment in and development of methods that provide *in situ* insights into the mechanisms that govern chemical synthesis starting from the very earliest stages of nucleation. New sample environments such as continuous flow reactors that couple time and length scales will be imperative for interrogating and ultimately achieving deterministic control over reaction trajectories.[98,101] More specifically, the following experimental capabilities would lead to substantial steps forward:

1. *Interrogation of solution species and oxidation states.* The local coordination environment of ionic precursors in solution-phase reactions and how these evolve in the lead up to assembly, can be evaluated using local structure probes such as x-ray absorption spectroscopy (XAS) and pair distribution function (PDF) analysis. Additionally, XAS is sensitive to the oxidation state and medium-to-long-range electronic effects.
2. *Elucidate nucleation and growth pathways.* The selection of the ultimate product and eventual phase can be set at the earliest stages of synthesis with the formation of the earliest nuclei that subsequently grow into the bulk product. The crystallographic diffraction tools (e.g., x-ray [XRD] or neutron diffraction [ND]) that are used to evaluate the bulk structure of the final materials are blind to these critical nucleation processes. These require local structure probes such as small-angle scattering and total scattering with PDF analysis that are sensitive to the atomic structure of the earliest clusters that form, and how these evolve and grow into larger-scale architectures. Once nucleated, the growth of different phases can also be followed using small-angle scattering or dynamic light scattering, which are sensitive to the particle size, shape, and distributions thereof.
3. *Monitoring kinetics and thermodynamics.* In principle, any probe that can quantify a reagent, intermediate, or product state can be used to evaluate the apparent kinetics of the synthesis reaction, including XAS, PDF, XRD, SAXS, and neutron-scattering counterparts. For reactions that involve transformations in the solid state, a conventional treatment of reaction kinetics based on the concentration of different species needs to be reconsidered because the concentration and rate will have different meanings at different length scales.[102,103] NMR (nuclear magnetic resonance) and neutron spectroscopies can be used to quantify ion dynamics and diffusion/transport phenomena directly.
4. *Morphological evolution* can be probed in two- or three dimensions using x-ray/neutron/electron microscopies and tomographies, with possible coupling to measurements at x-ray absorption edges to extract element-specific or oxidation-state distributions.

Interpreting the reaction data, which, at an intermediate point in the reaction, can be multicomponent mixtures, a distribution of different states/species, is challenging and will benefit from improved data analytics and machine learning approaches. As these techniques mature and become more widely used, the information they reveal will provide valuable input to theoretical modeling.[104–106] For example, constrained molecular dynamics reactive force field models have the potential to guide the design of materials that are far from equilibrium, but require extensive training from experimental data sets to be effective.[58,107] This will require highly precise modeling that eventually evolves beyond what *ab initio* methods can achieve, and finite element analysis methods will have an important role to play in bridging time and length scales. Realizing atomically precise synthetic methods will require an open dialog between experimentalists, theorists, and modelers that is tightly integrated to understand how each variable influences the reaction pathway. This is particularly challenging as reactions are scaled up because many of the fundamental steps that precede nucleation and growth of new phases are still not understood (**Figure 7**). By understanding mechanisms of self-assembly, researchers can leverage that knowledge to develop new materials at larger scales.

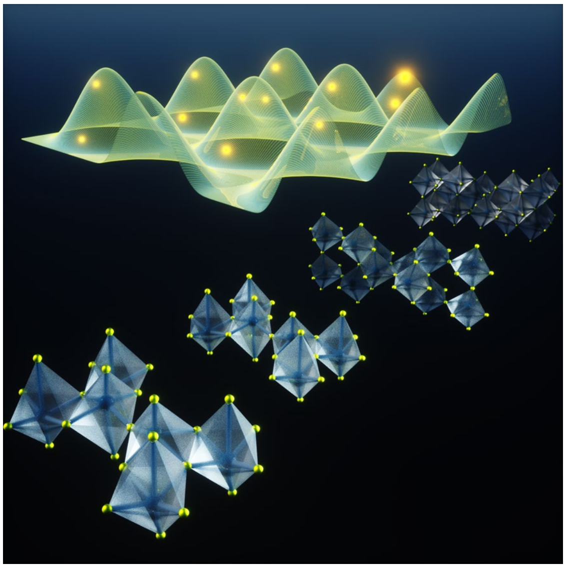

Figure 7. Materials laboratories of the future will encode the ability to navigate complex free-energy landscapes to stabilize specific metastable configurations of matter, shown here for different V_2O_5 polymorphs.

Workforce development

Effective utilization of new toolsets, AI/ML workflows, and integrated active-control synthesis methods will require not just resolving technical impediments and integration across disciplines, abstractions, and traditionally siloed workflows, but also the training of a next-generation workforce with the interdisciplinary skills to address the challenges and take advantage of the opportunities afforded by generational changes in automation, artificial intelligence, scale-bridging modeling, and instrument development.[2,18] The recent revolution in the resolution of materials characterization has resulted in more advanced, dedicated instrumentation and requires training of the next generation of instrumentation users and developers. Yet, there must be more capacity to support the required workforce development at all levels. For example, at university and national laboratory facilities, new instrumentation and increased access to innovative equipment are needed to train specialists ranging from undergraduate students to postdoctoral researchers. Without a significant increase in access to instrument time, both for academia and to support industry, US research leadership is endangered and US industrial productivity and innovation are severely constrained.

A similar situation exists in the area of computational materials science and data science. Recruiting and retaining STEM students and postdocs with computational expertise (coding and data) in building the US scientific infrastructure is extremely difficult due to the overwhelming demands for such skill sets in the commercial sector. Consequently, additional well-compensated career pathways for software developers and data scientists within materials science need to be developed. Establishing and nurturing this data-empowered workforce is a key driver to ensuring truly FAIR access to data and to achieving interoperable APIs and data registries.

The ideas discussed next must be explored to mitigate the declining number of domestic students attending graduate school and even fewer interested in joining academia at US institutions. There is a need for industries and national laboratories to partner with universities in implementing workforce development to enable the materials laboratories of the future.

Instrumentation infrastructure and workforce development

Developing the next generation of scientists to be the workforce of the materials laboratories of the future requires one to address first, how to compensate for the wave of retirement of experts, and second, how to equip a new generation of scientists with skills that have not previously been relevant, such as advanced data analysis and AI/ML techniques.[108,109] Of crucial importance is the recruitment and retention of students into STEM programs.

To achieve this, there must be a value proposition for students to go into research, such as access to state-of-the-art equipment in university or national laboratories combined with salaries that are competitive with the industrial sector. Possible pathways for recruiting undergraduate students into graduate programs include reimagined "research experience for undergraduate (REU)"-type programs to get students excited about pursuing doctoral degrees in measurement science and integrated materials design aspects of materials science or related fields, higher, more attractive, stipends for research assistants (RAs) in graduate school, as well as additional doctoral research positions in alloys, amorphous, and composite materials and manufacturing at academic institutions.

Accessibility of instrumentation must also play a crucial role moving forward. In particular, the democratization of access to basic and cutting-edge instrumentation must be enabled by eliminating barriers including affordability for users from underserved communities. Finally, it is important to guard against the depth and breadth of educational efforts working in opposition. A nationwide drive could be pursued, perhaps in concert with accreditation agencies, to balance curricula such that students are educated to become experts in a specialized field of materials science while having intellectual breadth in STEM.

Career paths in instrument and measurement science

Career paths for newly trained instrument scientists exist in many fields, including materials synthesis, data science, and advanced materials characterization. Materials research in the United States is at the forefront of novel materials synthesis, from advanced metallic alloys to polymers to semiconductors, thin-film ceramics glasses and composites, strengthened by strong thrusts in synthesis at the national nanoscience user facilities, including those supported by DOE and NSF. Trained instrumentation scientists and engineers, including in vacuum and novel deposition systems, are in high demand.

The opportunities in the materials characterization area are also numerous, ranging from individual R&D laboratories to large-scale facilities. For example, the United States has a portfolio of world-leading national neutron and x-ray light sources where the next generation of coherent x-ray sources are poised to image mesoscale volumes. However, beamlines and national user facilities are stretched thin and often unable to keep pace with increasing demands for more sophisticated measurements. Similarly, advances in state-of-the-art electron microscopy infrastructures require highly trained engineers and scientists to continue pioneering developments in materials characterization.

Opportunities also exist in the computational and data science fields. While strengths in these areas exist mostly in individual groups, there is an opportunity to build a larger community, streamline education, and bridge the current gap in materials and data science across length and time scales. All of these areas rely on a constant supply of engineers, scientists, or users to maintain and grow the current US leadership role in the world. A key challenge is to nurture and grow well-compensated and intellectually fulfilling career tracks in instrument science with mobility and collaboration across national laboratories, academic research centers, and instrument companies.

Most effective mechanisms for disseminating emerging data analytics tools

Throughout the discussions on workforce development, a common theme that emerged was access. With access to instrumentation for the multiple purposes of data collection, expertise development, and the inception of new techniques and instruments comes a need for access to data, data storage, and data analysis. Increased availability of data repositories and data analytics tools would satisfy the scientific need to integrate computation and theory with experimental work, apply AI/ML to materials challenges, and perform multiscale studies of materials. One could envision a future laboratory funded by multi-principal investigator awards to support data storage and computing appropriate to the data produced by the instrumentation, the open-source production of appropriate software, and online open access training in using this software and best practices in scientific software development. Such training could furthermore enable the creation of autonomous laboratories with closed-loop control between synthesis and characterization.

The most effective mechanisms for the training of data analysis experts and the dissemination of emerging data analytics tools are likely a combination of the summer school model in concert with the development of online educational communities for distance learning. Remote instrumentation operation will enable operators to be trained in almost all aspects of instrument operation without being physically present in the laboratory, and enhance the ability to re-train working engineers and scientists to meet the challenges of the industries of the future.

Training the next generation of materials researchers

These expanded opportunities for training and workforce development can only be realized through investments in additional instrument capacity specifically designed for state-of-the-art research while supporting access to in-depth training. As investment shifts to large, specialized facilities, the need for local instrumentation for training and preliminary experiments only increases. Another great opportunity to regain some of the lost expertise in instrument design or maintenance can be realized by providing student internship opportunities with instrumentation developers, such as microscope manufacturers, and by offering user support that passes on a meaningful understanding of instrumentation.

Finally, education in instrumentation design, in particular electron optics or vacuum design, needs to start early and be focused. College courses in such topics should be developed for specific science and engineering majors, while coding literacy and proficiency should become a core requirement for all engineering and science majors. This combined with open APIs and data registries can help turn the clock back on "black box" science and yield a new generation of empowered and aware researchers that can push the frontiers of measurement science while adapting instrumentation and infrastructure to address core science questions.

Equitable and inclusive access to instrumentation and infrastructure

Routine and state-of-the-art instrumentation and infrastructure are critical to maintaining US competitiveness in materials research. The current location and accessibility of such facilities have implications related to participation and inclusivity. Providing access to state-of-the-art facilities is seen as integral for the "democratization" of science and the training of the workforce of the future. Several successful characterization user facilities exist, including the DOE BES user facilities,[110] NSF Materials Innovation Platforms,[111] the Nuclear Science User Facility, and regional microscopy facilities that warrant examination to determine best practices. The potential for remote access and operation of instruments (e.g., DOE 2000 project and CEMAS at The Ohio State University) lowers barriers to use and decreases institutional costs. Similarly, the provision of remote or online scientific and instrumentation expertise will increase equitable and inclusive participation and will increase the development of a diverse workforce.

A principal weakness of equitable and inclusive access is the cost of major instrumentation facilities. The current economic model employed at most universities is not sustainable because user fees do not cover the costs of operating the facility, providing trained scientific staff, supporting maintenance contracts, teaching and training new users, and repairing the equipment. For example, facilities in the United States typically recoup only ~43% of operating costs from internal and external user fees.[112] The balance of the operating costs is covered by internal subsidies. The user fee and local subsidy model is a barrier to equity and inclusivity; external user fees can be prohibitively expensive even when matched to internal rates; external users have the added burden of travel costs; and facilities tend to operate tight instrument schedules and staff to minimize costs. Hence, there is a need for resources or programs to obtain funding for local instrumentation and staffing to train and to provide user time for resource-limited users such as those from primarily undergraduate, non-R1 or very-high research activity universities, Historically Black College and Universities (HBCUs), and Minority Serving Institutions (MSIs). Other weaknesses include that for remote operation, the data typically cannot be shared with the user in real time; thus, data storage and associated transfer costs can be problematic for the facility.

Other opportunities for inclusive access to instrumentation have been identified. In particular, the lessons learned from state-of-the-art major equipment facilities have the potential to be applied to make a broader range of equipment accessible in an equitable fashion. There is a need to build user facilities for materials synthesis and processing, and potentially specialized instrument facilities. New models for equipment sharing and expertise are needed to share routine instrumentation with under-resourced institutions (e.g., undergraduate, non-R1, HBCU, and MSIs), as well as to avoid duplication of underutilized equipment.

Another opportunity to lower barriers could be to make affordable instruments, for example, by using 3D printers or open-source instrumentation, and developing open-source software for data analysis. A successful user facility also requires dedicated instrumentation scientists and staff who have independent career paths and stable long-term (multi-year) funding; unfortunately, funding for such positions is uncommon at many academic institutions. There are emerging opportunities to build instrumentation infrastructure for autonomous experimentation/self-driving laboratories for the United States that would focus on integrating synthesis tools with characterization and testing tools to create closed-loop research capabilities, but these would require remote access and the regional/national networks previously identified.

Another opportunity to increase equitable and inclusive access is to reduce the cost of research tools. Just as Moore's Law made compute power affordable to the point where supercomputers are carried as phones, Moore's Law for research, and the movement to democratize science by building affordable research tools can lower barriers for those to whom large instrumentation centers are hard to access. Specific investments in low-cost instrumentation and development should be supported, with long-term funding for instrumentation science.

A final identified opportunity is to more inclusively involve undergraduate, non-R1, HBCUs, MSIs, and other institutions as partners to form regional and national centers. A key element is to enable modes of access that do not necessarily require funding or burdensome justification in order to encourage creativity and innovation. The latter is critical to democratize access, providing opportunities for creative minds in all institutions to contribute fully to the challenges and opportunities facing science and engineering in years to come.

Current models of shared resources are not sustainable, given the prohibitive cost of acquiring and maintaining state-of-the-art equipment, software licenses, and supporting dedicated research scientists. Although regional models exist to provide centers of excellence, they are inadequate to support inclusive access across all levels of research and the ubiquitous training needed for the future workforce. Investments are needed to support long-term instrumentation science, remote access, and technical support for regional centers and universities. Without meaningful investment in outreach, education, and direct connections to underrepresented and underserved communities, the threat is that the status quo of a lack of diversity, equity, and inclusion in science will continue. In the end, access to routine and state-of-the-art instrumentation and infrastructure can enable disruptive science by increasing equity and inclusion.

Looking to the future

Envisioning, designing, and realizing the full promise of materials laboratories of the future as sketched in the preceding sections will require a continuing national conversation to ensure that advancements in multimodality, integrated AI/ML workflows, automation, and pushing beyond current frontiers of spatial, temporal, and energy resolution occur in concert with democratized access. Several open questions require further consideration.

First, materials laboratories of the future will need to integrate large volumes of data and different data formats, encompassing different length- and time scales, which will arrive at different time points and need to be processed and digested "on the fly" to inform further experimentation. It remains to be determined what sorts of standards (e.g., IEEE or ISO) for data transfer, data curation, domain-specific transparent file formats as well as experimental protocols (i.e., ASTM-like) need to be developed. It furthermore remains to be seen which entities will facilitate, coordinate, or even just "nudge" such development, and how they will channel the disparate needs and aspirations of different stakeholders. As alluded to in previous sections, data-sharing and user-accessible interfaces are a key imperative to seamlessly integrate data analytics and AI. Several examples of data registries have now emerged, which are crucial for larger-scale analyses across multiple laboratories. This will require addressing important questions about how best to enable and empower a FAIR framework while respecting and protecting intellectual property in an age with increasing emphasis on public–private partnerships and a greater engagement of industry across the materials development continuum.

Automated experimentation with active learning holds promise for focusing on rare and important functionality, enabling acceleration, and relieving the burden of repetitive and time-consuming tasks. A second major set of open questions pertains to how experimentalists will be trained and empowered to formulate designs in a manner that intelligent computational agents can enact and adapt the systems to complete the tasks. In autonomous human–robot interactions, a key question is how will the most effective division of labor, communication, collaboration, and trust be achieved?

From the perspective of democratized access, mail-in beamlines and facilities such as the electron microscopy center at The Ohio State University show exceptional promise as exemplars of remote access. A third major set of questions pertains to the set of opportunities that can be enabled by a combination of automation and remote operation. Can remote operation transform student training and democratize access or does it concentrate needed capabilities and promote "one-size-fits-all" bland homogeneity?

A clear consensus that emerged from the workshop is the acute need for a "Hub and Spoke" model for regional user facilities that emulate some aspects but advance beyond current synchrotron, semiconductor foundry, and DOE Nanocenter models. Such facilities would encode student training and instrument development in their core mission and further pilot open API and data-sharing models. The concepts of "integration" and "codesign" can serve as a key organizing principle for future research, involving various groups, including national laboratories scientists and academic researchers. Midscale infrastructure investments have promise to advance integrated models that go beyond the scope of Major Research Instrumentation "e.g.: https://new.nsf.gov/funding/opportunities/mri-major-research-instrumentation-program" initiatives. There is furthermore a need for targeted investments that are strategic and timely but that are also nimble and agile and evolve with time to address new research needs and provide democratized access across a broad range of institutions. In tandem, there is an urgent need for a concerted and cohesive effort focused on instrumentation development, which must have as its cornerstone a way to define career tracks for instrumentation development scientists, scientific AI/ML engineers, and software designers. Additionally, there is a need for greater coordination, cohesion, and scaling of current training programs, strengthening but also threading together the current patchwork of summer schools, remote courses, workshops, and hackathons as part of a comprehensive workforce development strategy.

Conclusion

In summary, "materials laboratories of the future" are critical to accelerating the pace of materials discovery and for maintaining leadership in manufacturing innovation. Such laboratories can entirely reimagine materials science by enabling real-time atom-by-atom manipulation of matter and "on-the-fly" modification of reaction trajectories to arrive at desired structural or microstructural outcomes; establish deterministic control of nonequilibrium pathways to *a priori* design schemes to access metastable phases of matter; provide a multimodal 3D atom-precise understanding of the evolution of structure of matter in response to coupling to external fields under realistic operational conditions; embedding AI in nontrivial tasks to decode physics and chemistry design principles, efficiently navigate multidimensional design spaces using clear scientific hypotheses, and effectively interface with human intelligence; and "zoom-in/zoom-out" as required to understand phenomena at different length scales.

While there remain many open questions about how best to realize the potential of such laboratories while ensuring democratized and equitable access, the community consensus is to define and establish "Hub and Spoke" regional shared facilities that can simultaneously advance technical limits of instrumentation while also providing scalable models for training, nurturing an instrumentation workforce, and enabling accelerated scaling of materials along the materials development continuum.

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Conflict of interest

On behalf of all authors, the corresponding authors state that there are no conflicts of interest.

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