OPINION

MATERIAL MATTERS

A successful strategy for MGI-inspired research

By **Gregory M. Odegard, Zhiyong Liang, Emilie J. Siochi, and James A. Warren**

The Materials Genome Initiative (MGI) was announced in 2011 as a US Government multiagency effort to accelerate the discovery, design, development, and deployment of new materials twice as fast as before, at a fraction of the cost.[1] The MGI seeks to overcome the time for insertion of a new material (from the current decades time frame reduced to a few years) by aligning the product design process with the materials design process, so that they can proceed hand-in-glove. This goal was to be accomplished through the creation of a materials innovation infrastructure that, through the fusion of computational and experimental methods mediated by well-managed data, could substantially lower the barriers to state-of-the-art material characterization, simulation, and testing techniques in materials R&D. This reduction in barriers is the hallmark of MGI, as the ideas themselves are not especially new, but the impediments to their implementation can be substantial, requiring significant investments that are often the sole provenance of multibillion-dollar revenue corporations or, in a few cases, small ventures that specialize in such techniques.

It is thus unsurprising that MGI research often requires larger research teams, as single-investigator endeavors are unlikely to have the broad portfolio of methods required for such an undertaking, and research grants supporting these types of efforts are commensurately larger. There are a number of MGI-specific programs that have been initiated over the past decade,[2] some with specific callouts to the initiative, while others have been tasked by their agencies to support the initiative in a more synergistic manner, as pursuit of MGI goals allows for the rapid development of new materials that allow agencies, at least in principle, to meet specific mission objectives far more quickly. The US Department of Defense (DoD), Department of Energy, the National Institute of Standards and Technology (NIST), the National Science Foundation (NSF), and the National Aeronautics and Space Administration (NASA) have all established substantial efforts in support of the MGI, including the formation of Centers of Excellence where academic and industrial partnerships can flourish, and allow the best-in-class methods to see adoption by manufacturers.

A major interest for NASA is the development of the next generation of structural materials for crewed deep-space exploration. While we have enjoyed the success of sending rovers to Mars, robots are not nearly as demanding as people. Deep-space exploration crews will require a significantly higher payload of food, water, air, vehicles, and habitats to be taken on the journey, all of which add significant mass, thus requiring more fuel. More fuel adds more mass, which, in turn, requires more fuel. Thus, the fuel cost associated with crewed deep travel is significantly higher than that of rover exploration and requires significantly lighter structural materials than state-of-the-art materials to reduce overall rocket mass and fuel costs.

Composite materials made of carbon nanotubes (CNTs) instead of carbon fibers are promising for providing higher-performance composites with a reduced mass. CNTs are a much newer technology than carbon fibers and have received significant attention since the inception of the US National Nanotechnology Initiative (NNI) in 2000. Because of their significantly higher stiffness and strength relative to carbon fibers, they should, in theory, provide composite materials with higher-performance metrics. However, the development of structural CNT composites has been greatly hindered by challenges in retaining nanoscale high CNT properties when manufactured at scales required for structural applications and difficulty in creating efficient load-transfer mechanisms between CNTs and the polymer matrix. Despite early evidence of the successful use of CNTs in composite materials,[3,4] these two factors have remained roadblocks to the successful development and implementation of CNT composites for two decades after the start of NNI.

To address the need for lighter structural composite materials for crewed deep-space exploration, and the roadblocks associated with manufacturable and effective CNT composites, NASA funded the Space Technology Research Institute (STRI) for Ultra-Strong Composites by Computational Design (US-COMP) in 2017 as a five-year project with a USD$15 million investment to develop the next generation of CNT

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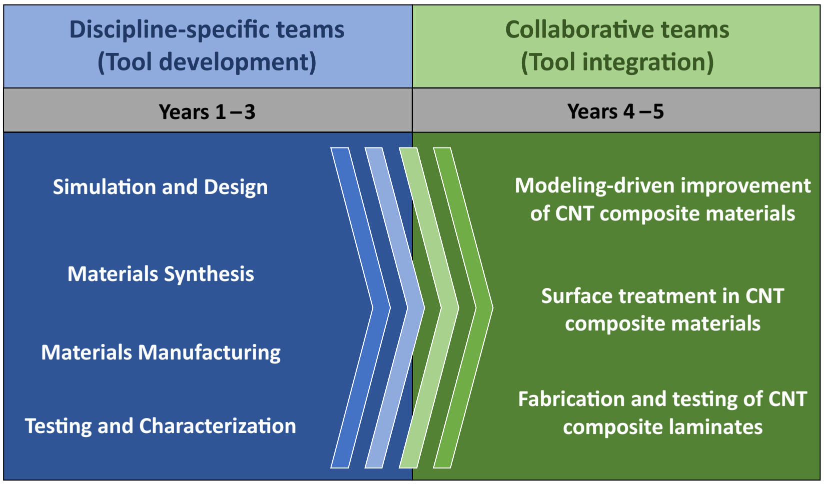

Figure 1. Evolution of Ultra-Strong Composites by Computational Design team structure. CNT is carbon nanotube.

composites that had properties exceeding state-of-the-art carbon fiber composites (see https://us-comp.com). The large US-COMP team consists of 11 universities, two commercial materials suppliers, the US Air Force Research Laboratory, and NASA collaborators. Mechanical performance targets were specified by NASA, including improvements in specific stiffness (stiffness per unit mass density) and specific strength (strength per unit mass density) relative to state-of-the-art carbon fiber composites. Because of the size of US-COMP and the difficult requirements of the project, NASA and US-COMP recognized that a MGI-style approach would need to be adopted for the project to succeed.

Ideally, US-COMP could have adopted a previously established approach to implementing MGI principles into a large-scale materials development effort as there have been multiple efforts to develop large-scale collaborations to facilitate MGI-style research since the 2010s time frame. The NanoMine project[5–7] was developed to provide a database of curated nanocomposites data to facilitate future materials design development. In 2014, DoD and NIST sponsored a workshop to lay the groundwork for establishing a materials innovation infrastructure.[8] This collaboration ultimately involved many different US Government agencies and researchers in a wide range of materials development sectors. The Designing Materials to Revolutionize and Engineer our Future program of NSF supported numerous interdisciplinary, team-based projects to provide access to materials data for the materials research community.[9] Multiple efforts have also focused on Integrated Computational Materials Engineering (ICME) solutions,[10–12] which heavily use multiscale modeling with continuous design feedback loops.

Despite these efforts, large, multiscale efforts with defined common objectives remain rare,[13] and have had largely bespoke collaboration models, although some ideas on how to systematize the procedure have been proposed.[14] US-COMP leadership had to navigate this new landscape and established a model for success to develop a novel CNT composite that met the mechanical performance requirements. The first three years were focused on tool development and initial materials exploration, and the final two years were focused on integrating the tools and knowledge to achieve the project goals. This article describes the evolution of US-COMP over five years and its ultimate success. This case study should serve as a potential model for future large-scale MGI projects.

Effective teaming

The original MGI strategic plan envisioned the need for broad team collaboration to achieve materials design goals.[15] The initial structure of US-COMP was based on four discipline-specific teams: (1) Simulation and Design, (2) Materials Synthesis, (3) Materials Manufacturing, and (4) Testing and Characterization (see **Figure 1**, left). Each team was composed of US-COMP researchers with a primary expertise focused on one of these areas. The original purpose of the discipline-specific teams was to develop the necessary tools that would eventually be needed in the final stages of the project. For example, the Simulation and Design team developed computational tools at multiple length scales to enable accurate and efficient predictability of materials behavior based on materials nano/microstructure. The Materials Synthesis team explored unique synthesis methods to enable materials development. The Materials Manufacturing team established manufacturing methods to scale up production of composites for eventual composite panel-level production and testing. The Testing and Characterization team established novel testing methods that were scaled-down versions of standard methods, especially designed for the smaller proof-of-concept panels that would eventually be produced by US-COMP.

While the discipline-specific team structure was necessary and effective in establishing the fundamental tools that would be relied upon later in the project, US-COMP needed to transform itself after three years to effectively use the developed tools to reach the institute goals. This was envisioned in the original MGI strategic plan: “Further, advances in fundamental scientific knowledge and tools must be transitioned and integrated into engineering practice and application.”[15]

The structure of US-COMP evolved toward a collaborative team structure (see Figure 1, right). Instead of teams based on traditional areas of expertise, each team was now composed of all stakeholders (academic, industrial, and national laboratory) with common goals, regardless of discipline. Thus, each collaborative team had experts related to materials modeling, testing, synthesis, and manufacturing all working toward addressing an identified problem, but each focused on a particular facet of the challenge. For example, the collaborative team focused on modeling-driven improvement of CNT composite materials included multiscale modelers, composite manufacturing experts, the CNT yarn manufacturer, and NASA researchers who worked together toward a better understanding of the mechanical failure characteristics of the composite and to provide suggestions for improving manufacturing techniques to yield improved composite toughness. With this new diverse environment, interdisciplinary communication and collaboration were accelerated, the fundamental tools were effectively integrated, and the higher-level mechanical performance targets could be addressed directly.

The shift in team structure highlights two important lessons of large-team MGI research. First, the team/interaction model needs to be flexible, so that it can be adapted as teams transition from tool development to tool integration modes. Second, a large MGI team needs to eventually transition to a collaboration-based mode to encourage interdisciplinary interaction and enable attainment of higher-level goals.

Effective collaboration

Being composed of researchers from universities, federal research laboratories, and industry, US-COMP was challenged with the mixed priorities and goals associated with these different research sectors. The standard mode for universities is to publish research as quickly as possible to mutually benefit faculty (merit, promotion, and tenure) and students (building their resume). It is tempting for faculty to push their students to conduct high payoff Technical Readiness Level* (TRL) 1 basic research that leads to multiple journal papers, whereas companies and national laboratories are more willing to forgo low-hanging fundamental research fruit for more use-driven research that leads to commercializable products (intellectual property) supporting mission needs.

For US-COMP, the first three years were focused on fundamental research (tool development) that yielded numerous journal articles. Following the third year of the project, US-COMP shifted the research and team structure to prioritize manufacturing-level improvements with the understanding that some critical aspects of the research touch on areas considered sensitive by the industry team members. This move brought the industry and government laboratory partners more deeply into the project, as the work was more directly tied with higher TRL products. A major benefit of this change was the more direct participation of industry and government laboratory researchers that was underutilized in US-COMP during the tool development stage. Thus, a balance was struck between publishing research in the first few years and engaging the broader partner base while pushing the TRL up in the last couple of years of the project.

Because of the direct collaboration with industry and government laboratories, and the shift to more use-driven research, US-COMP also had to establish nondisclosure agreements (NDAs) and a protocol for publishing research that included potential intellectual property (IP) and export control (EC) considerations. A committee that included representatives from NASA and the industry partners was assembled to approve all manuscripts, posters, and presentations before public dissemination for IP and EC considerations. The NDAs and the dissemination committee were thus a blanket of protection for all of the US-COMP stakeholders and provided an environment of open communication and trust within the institute.

US-COMP was fortunate to have industrial partners that were eager to adopt the emerging technology and willing to engage in detailed discussions about model tool-building in years 1–3 and model integration in years 4 and 5. With their direct involvement in the modeling discussions, the industry partners were able to use the physical insights gained from simulation predictions to make manufacturing parameter changes on the fly. These changes saved the companies from pursuing synthesis pathways in a purely and costly empirical manner. In turn, the industrial partners provided the academic partners with guidance in modeling parameters (e.g., materials selection, environmental conditions) that were highly relevant to materials manufacturing. Such guidance is rarely provided to academic researchers, who usually choose modeling parameters based on intuition only. Most importantly, this industry/academic collaboration was all performed without the release of IP (CNT synthesis details, polymer formulations) due to the NDAs.

During the course of the project, another important lesson of large-team MGI research was learned: regular and consistent communication is essential for success. For example, most of the collaborative teams met on a weekly or biweekly basis. Each meeting was a combination of research updates (students, faculty), sharing of information (between academic, industry, and government laboratory researchers), strategic planning, and troubleshooting discussions. The proliferation of virtual meetings during the COVID-19 pandemic accelerated this transformation. Many US-COMP researchers were involved in multiple collaborative team meetings on a regular basis, thus providing a broader perspective on the efforts of US-COMP than before. In the final two years, the shift to application-level discussions brought a new wave of enthusiasm to the teams.

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[*] https://en.wikipedia.org/wiki/Technology_readiness_level.

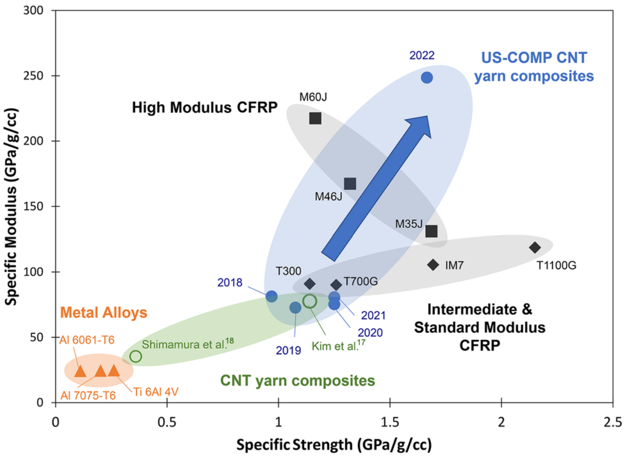

Figure 2. Specific property map for aerospace materials, including carbon nanotube (CNT) yarn unidirectional composites from Ultra-Strong Composites by Computational Design (US-COMP) (denoted by year); see References 17 and 18. The graph also includes state-of-the-art unidirectional carbon fiber-reinforced polymer (CFRP) composites (denoted by carbon fiber used) and engineering metal alloys.

Effective leadership

Multiple levels of leadership were required for the success of US-COMP. At the top, the US-COMP Leadership Team (composed of the director and a representative from each discipline-specific team) was charged with the general day-to-day management of the institute, including coordination of resources, planning annual review meetings, forward planning, and all other general administrative issues. The NASA technical monitor also participated in meetings for post-award monitoring purposes and to engage with the team for potential collaborations with NASA researchers. Perhaps the most important element, however, was facilitating conversation at all levels of the institute. In nearly all of the discipline-specific and collaborative team meetings, at least one member of the Leadership Team was present to facilitate the conversation, provide higher-level project guidance, and fully understand the progress and needs of each of the projects. The Leadership Team did not want any lapses in communication to affect the progress of the multiple teams.

Although the Leadership Team and the senior researchers participating in US-COMP played an important role in guiding the project and facilitating collaboration, there is little doubt that the participating students were a critical driver in the success of US-COMP. A large, multi-university project is a prime opportunity for students to work closely with researchers and students from different disciplines, research culture environments, and physical locations. Thus, they are exposed to a diversity of team cultures that they would not necessarily gain from working with only students in their own research group. The demands of such collaborations required the US-COMP students to learn new communication skills that were further enabled by the growth of virtual collaboration tools. Perhaps the most transformative collaborations were with students and researchers on opposite sides of the computational/experimental divide, particularly under the collaborative team model.

Results and moving forward

At the end of the fifth year of the project, US-COMP had succeeded in developing a scalable polymer matrix composite that had tensile stiffness and strength properties that exceeded the state-of-the-art carbon fiber composite.[16] **Figure 2** shows the evolution of the US-COMP CNT yarn composite tensile properties spanning 2018–2022, as well as properties from other aerospace-grade materials systems for comparison. Perhaps the most striking feature of the US-COMP data in Figure 2 is the sudden rise in the mechanical properties shortly after the transition to the collaborative team structure. Thus, it is clear that the final push to achieve the goals required a collaborative team mindset to integrate and utilize the tools that were developed in the early phase of the project.

The success of this large MGI-style project is attributed to the flexible and evolving team structure, balancing of university–industry–national laboratory priorities, consistent and frequent communication, active leadership involvement, and a diverse student collaboration environment. Without any of these factors, it is unlikely that a polymer composite material with the properties shown in Figure 2 could have been developed in only five years. Such a large-scale, university-based, MGI-style project could not have happened without a significantly large investment from the federal government, in this case a NASA STRI, focused on quantified metrics that provided a means of measuring advances toward the common goal.

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