Structural Materials Data Demonstration Project: Resource for Thermal Process Modeling

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Abstract

Integrated Computational Materials Engineering requires the availability of supporting data for modeling across multiple length scales. It also requires robust data schema and input-output protocols. To address these needs, a team working under a grant from the National Institute of Standards and Technology has launched the Structural Materials Data Demonstration Project, a collaborative effort led by ASM International to establish best practices for materials database development and application. In its initial phase, the project is focusing on the heat treatable aluminum 6061 alloy and ternary subsystem of Al-Mg-Si, incorporating experimental diffusion, phase equilibria, microstructural, and mechanical property data. This paper outlines the purpose and scope of the project and discusses challenges in materials data management and organization. It also describes a test problem in which demonstration data can be used to model the effects of composition and heat treatment on various properties of aluminum 6061-T6.

Introduction

The field of materials science and engineering is changing dramatically, driven by increasing computational capability, more efficient experimental approaches, and an explosion of data through enhanced sensor and acquisition technologies. In recognition of this transformation and to help speed it along, the Materials Genome Initiative (MGI) was launched in 2011 with the goal of discovering, developing, and deploying advanced materials in half the time and at a fraction of the cost typically required today.[1]

Figure 1 provides a graphical overview of the Materials Genome Initiative. The foundational element is the materials innovation infrastructure, consisting of computational tools, experimental tools, and digital data. These resources are being developed and employed in support of national goals in such areas as clean energy, national security, human welfare, and equipping the next generation workforce for prosperity and success.

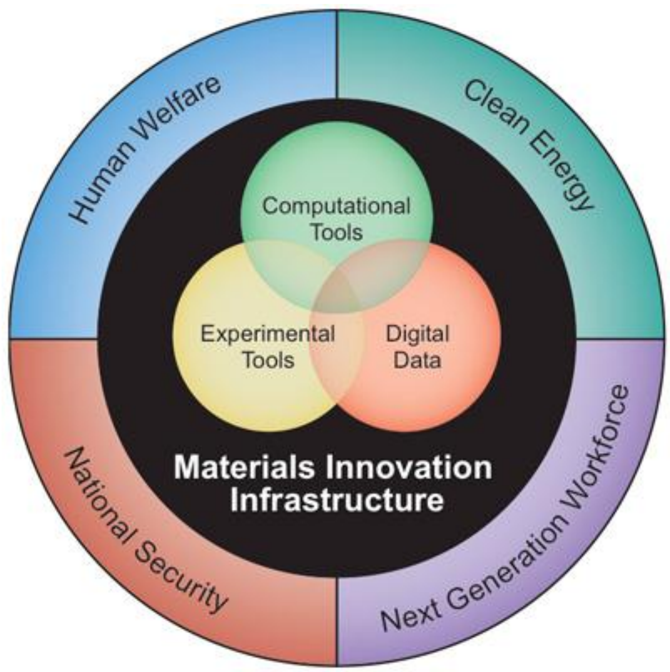


Figure 1: The Materials Genome Initiative, a large-scale public-private endeavor, seeks to accelerate the discovery and commercialization of new materials through mass collaboration, data sharing, and the development of advanced experimental and computational tools. As envisioned by the National Science and Technology Council, the goal of the MGI is to increase national competitiveness, particularly in the area of manufacturing, while addressing some of the nation's most pressing concerns. (Source: Ref. 1)

Achieving the ambitious goals of the Materials Genome Initiative demands a new way of thinking about materials science and engineering. One important aspect of this is Integrated Computational Materials Engineering (ICME), which is defined in a National Academies report as "the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing process simulation,"[2] ICME is regarded as a transformational discipline that can improve national competitiveness and security. One significant obstacle standing in the way, however, is a lack of adequate standards, data, and integration tools – especially in manufacturing supply chains – as a recent study points out.[3] The authors specifically cite the need to develop open-source tools for sharing pre-competitive data as being of primary importance.

The National Institute for Standards and Technology (NIST) has a strategic role in advancing the objectives of the MGI, particularly in the area of digital data, consistent with its overall mission. Through efforts in the Materials Measurement Laboratory and Information Technology Laboratory groups, NIST is providing both technical leadership and support in areas critical to meeting the materials information needs of the scientific and engineering community.

A case in point is a workshop that was held in 2012 called the "Materials Genome Initiative Workshop – Building the Materials Innovation Infrastructure: Data and Standards." This session brought together over 125 experts to address questions regarding data representation and interoperability, data management, data quality, and data usability in the context of various length scales and application domains. The findings from the workshop, which were published in a NIST report[4], also highlighted key cross-cutting challenges including the need for strong community leadership, open data sharing, and a federated data repository system.

In response to these needs and to meet the broader objectives of the MGI, especially in the area of digital data, ASM International has established the Computational Materials Data (CMD) Network, which aims to advance materials development and deployment by facilitating information sharing across the materials community. The CMD Network is working with the materials community to support projects and initiatives that will build and sustain the materials innovation infrastructure. A summary of these efforts can be found at www.cmdnetwork.org.

One specific project already underway is the development of an open data repository and database for metallic structural materials. The Structural Materials Data Demonstration Project (SMDDP) Repository and Database is intended for use by the materials data community as a means of accelerating progress toward the digital data goals of the MGI as described in the NIST report. The development of the database and its utilization in the area of thermal process modeling is the main focus of this paper.

SMDDP Project Overview

The Structural Materials Data Demonstration Project is a cooperative effort between ASM International, NIST, Granta Design Ltd. and its affiliate Materials Data Management Inc., Kent State University (KSU), and Nexight Group. The project has the following objectives:

- Establish well-pedigreed and curated **demonstration datasets** for non-proprietary metallic structural materials data over all relevant length scales.
- Work with NIST and the materials data community to develop materials **data schema and ontologies** for the demonstration datasets, cognizant of broader interests and datasets.
- Develop and carry out a series of **test problems** that represent relevant use cases for the repository.
- Make the datasets **open** to the materials data community for use in data analytics, modeling, and educational purposes.
- Actively engage the materials data community and widely disseminate the findings from the project.
- Develop and implement **data capture and curation procedures** that can serve as models for other data repositories.
- Develop and implement **data access procedures** that can serve as models for other data repositories.
- Establish the framework for the utilization of the demonstration datasets for **educational purposes.**

Handling multi-scale material data, as required for ICME, is a particularly important element in any MGI-related data management project. Examples of such data environments are found in the works of Marsden *et al*.[5] and Arnold *et al*.[6,7]. These references provide practical solutions – including schema, protocols, and configurations – for managing dynamic materials databases, putting them to the test on composite materials and a model superalloy, ME3. In addition, the works of Campbell *et al*.[8,9,10] and Bartolo *et al*.[11] lay out examples and rationale for the development of materials data and file repositories, their role in materials design, and the need for a federated system of materials data repositories and materials-specific data informatics. All these works shed light on the interplay between experimental and computed data at various length scales, how to acquire and maintain material pedigree information, and key data issues regarding import, export, and access control. In summary, they are excellent starting points for developing a federated system of open access data repositories within the materials community that can meet the needs of researchers engaged in MGI work.

Building on this prior knowledge, and as shown in Figure 2, is a schematic representation of the framework in which the SMDDP Repository and Database exists. Designed for flexibility, the system accepts input from a variety of sources and in a variety of formats. Among the sources currently being used are public and commercial databases as well as data from industry, government, and academia. Multiple interfaces facilitate data transfer, accepting data in various formats, including Excel-based templates and direct input from testing equipment.

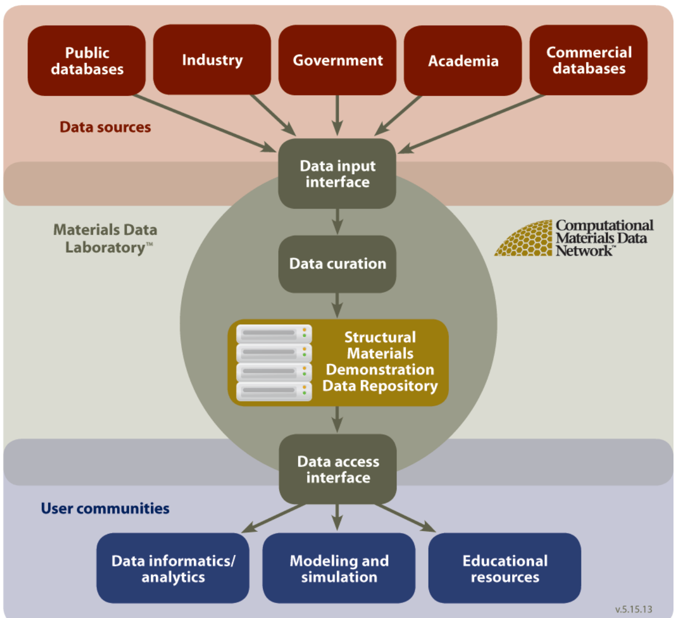


Figure 2: The Structural Materials Data Demonstration Project is a collaborative effort involving industry, academia, and government agencies working together to develop and validate the type of data management infrastructure necessary to support the Materials Genome Initiative. The central element, the SMDDP Data Repository, is a dynamic database configured on the Granta MI platform.

Before any data can be placed in the repository, they must undergo curation, not only to improve data quality but also to adapt the input interfaces to evolving materials data needs. Once the process is complete, the curated data can then be stored, accessed, and manipulated as needed. The database constructed for the project is based on Granta MI software, a data platform that maintains a dynamic environment that can be accessed for data analytics, modeling and simulation, and educational purposes. The repository is built upon the DSpace repository platform customized by NIST and Kent State University for materials data (NIST DSpace) as part of a federated data repository system.[12,13]

One of the needs for the Structural Materials Data Demonstration Project is to establish a practical, low-maintenance, open-access data storage system that has exceptional long-term reliability and the potential to meet current and anticipated compliance requirements for federated data repositories.[14] This is achieved, in part, by using existing standards and technologies, an important of element of which is the Open Archives Initiative Object Reuse and Exchange (OAI-ORE) specification. Adhering to OAI-ORE standards helps remove obstacles to data interoperability, ensuring wide data dissemination capability while minimizing information loss. It also addresses potential longevity concerns, especially those associated with metadata – the other key to the success of the project – as shown in Figure 3.

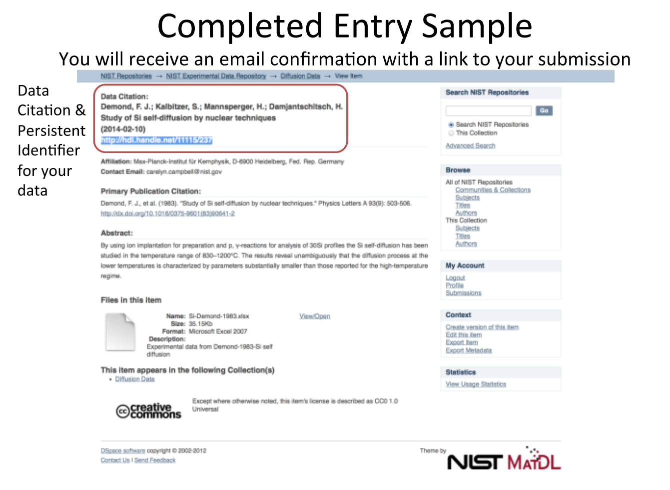


Figure 3: As illustrated in this data entry record from the NIST DSpace Repository, the Structural Materials Data Demonstration Project Repository and Database follows OAI-ORE and metadata standards to enable and foster a federation of materials data repositories.

By recording essential semantic information to describe research data and by verifying that the information is faithfully represented in future encodings, the Structural Materials Data Repository guarantees valid and reliable operation to support long-term digital data discovery, access, and storage. Furthermore, as part of the NIST federated data repository system, the SMDDP Repository stands to be a valuable resource for the ICME community, providing common, standards-based data storage with efficient metadata and data import-export, while simultaneously protecting proprietary database interests. How this general framework is being developed is discussed in the next section.

SMDDP Project Execution

The Structural Materials Data Demonstration Project is being conducted in three phases marked by the progressive development of key data repository elements along with exposure to increasingly larger segments of the materials digital data community. This escalated plan is structured over an approximately 18 month period as illustrated in Figure 4.

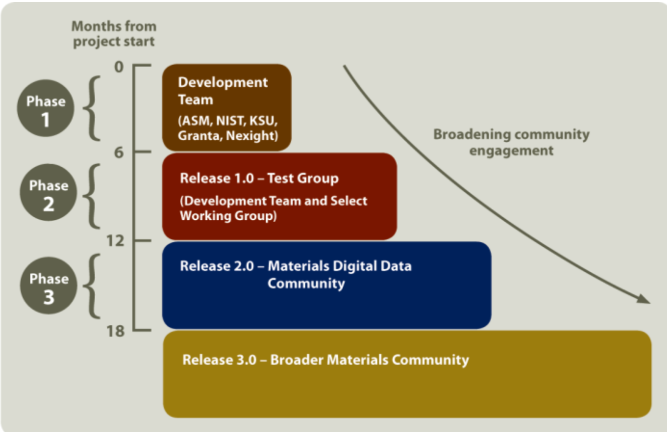


Figure 4: The Structural Materials Data Demonstration Project is following a phased rollout plan. With each phase, the data repository is becoming progressively larger as is the community being given access to it. Release 1.0 contains diffusion and mechanical property data for Aluminum 6061, and is being evaluated by a select test group. Release 2.0 will include phase diagram and microstructural data, and will be available to the broader materials digital data community.

A strategic decision made in the Structural Materials Data Demonstration Project is the selection of a model structural material. Recognizing the challenges that can result from building databases for proprietary or export-controlled materials, the team sought out a "post-proprietary" material. Based on the breadth of application experience and availability of relevant data from a variety of sources, they selected aluminum 6061, a heat treatable alloy of the Al-Mg-Si family.

The project has recently completed Phase 1, and Release 1.0 of the data repository and database is currently being evaluated by a small test group. The initial phase of the project focuses on the development of the data schema for two important data types: diffusion data and mechanical property data. Limiting the data types in the initial release has allowed project members to concentrate on developing the overall data structure in the Granta software environment as well as the related data import and export interfaces.

Figure 5 is the main navigational page for the Structural Materials Data Demonstration Repository and Database. Information on this page includes general guidance on how to use the interface, details on the SMDDP project, and additional project references. An interactive database map is also included on the main navigational page, and is shown in greater detail in Figure 6.

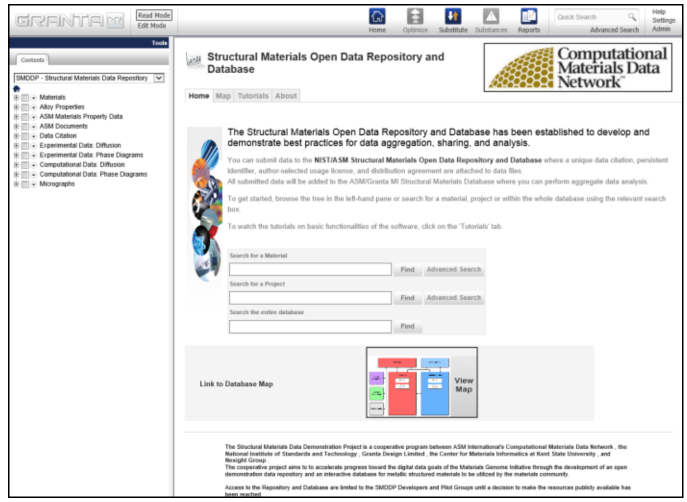


Figure 5: The main navigational home page for the Structural Materials Data Demonstration Repository and Database lets users submit data to the repository and find and access data of interest. It also offers access to tutorials, a site map, and background information, including how to submit data along with related identifiers, citations, and usage intent.

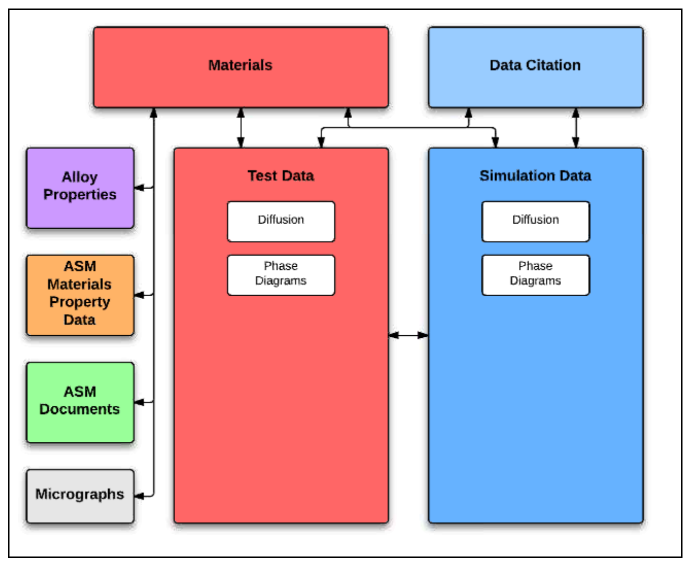
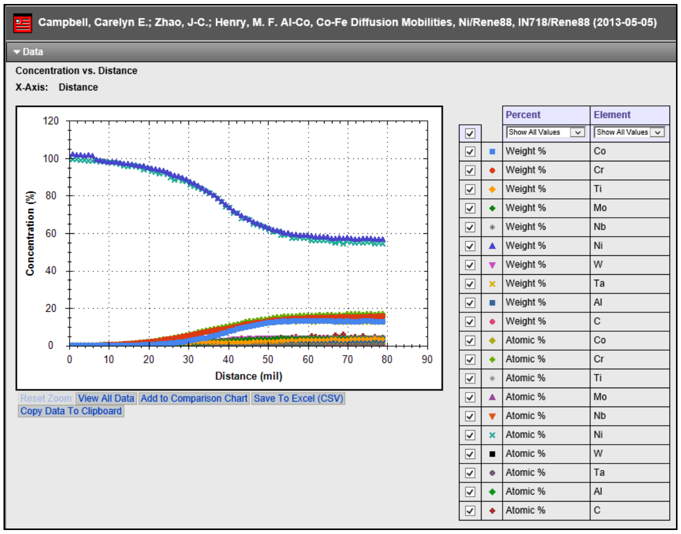
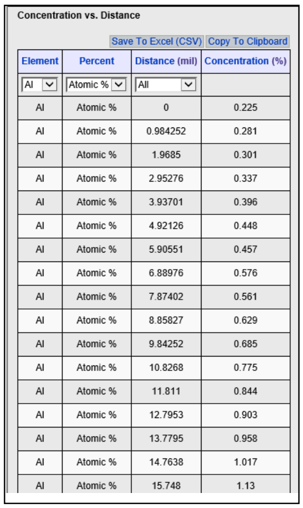


Figure 6: The Structural Materials Data Demonstration Repository and Database home page has a database map that serves as a search tool as well as a schematic representation of the repository. The map is cross-linked with the folder tree and also provides access to videos under the Tutorials tab.

Looking more closely at the data schema for each of the two data types, Figure 7 represents a portion of the schema for diffusion data displayed graphically alongside the associated data pairs. Likewise, Figure 8 shows a portion of the schema for the mechanical property data.





Concentration vs. Distance

Save To Excel (CSV) Copy To Clipboard

Element	Percent	Distance (mil)	Concentration (%)
Al	Atomic %	All	
Al	Atomic %	0	0.225
Al	Atomic %	0.984252	0.281
Al	Atomic %	1.9685	0.301
Al	Atomic %	2.95276	0.337
Al	Atomic %	3.93701	0.396
Al	Atomic %	4.92126	0.448
Al	Atomic %	5.90551	0.457
Al	Atomic %	6.88976	0.576
Al	Atomic %	7.87402	0.561
Al	Atomic %	8.85827	0.629
Al	Atomic %	9.84252	0.685
Al	Atomic %	10.8268	0.775
Al	Atomic %	11.811	0.844
Al	Atomic %	12.7953	0.903
Al	Atomic %	13.7795	0.958
Al	Atomic %	14.7638	1.017
Al	Atomic %	15.748	1.13

Figure 7: The Structural Materials Data Demonstration Repository and Database includes diffusion data in both graphic and tabular form. Multi-dimensional data can be displayed and compared. Graphical representations and data sets can be visualized and extracted.

As the project progresses into Phase 2, two parallel efforts are underway. The first expands the database with additional diffusion and mechanical property data. More than augmenting the breadth of data included, this effort is contributing to an important process, the evaluation and adaptation of the data input interfaces. Concurrent with that, the SMDDP project team is adding other types of data to the repository, including phase diagram data and microstructural data.

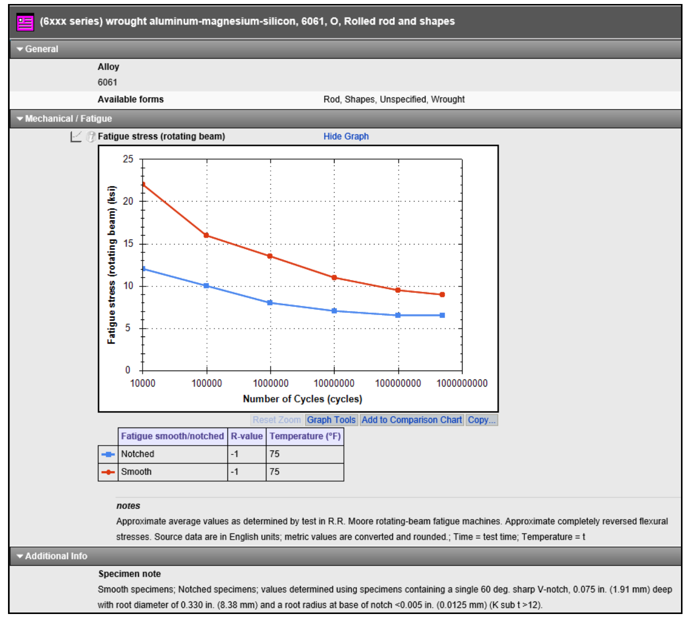


Figure 8: The Structural Materials Data Demonstration Repository and Database includes mechanical property data such as fatigue strength versus number of cycles to failure.

Applications to Thermal Process Modeling

Another important objective for the materials data demonstration team is to identify and solve selected "test problems" using the data captured in the SMDDP Repository. These problems will allow team members to assess not only the quality of the data, but also the ease with which the data can be accessed for modeling and simulation. The results of the modeling exercises can then be added to the repository as envisioned in a number of materials information systems developed previously[5-7].

The initial test problem will focus on thermal process modeling – specifically, modeling the effect of artificial aging treatments on the mechanical properties of aluminum 6061. Aluminum 6061 was chosen for the project because its properties along with the manufacturing and heat treating processes typically employed are well documented and widely available.

Heat treatment is critical for achieving maximum strength levels in aluminum 6061, and there are many important applications in the peak aged or T6 temper. Aluminum 6061 is a precipitation hardening alloy and its primary strengthening mechanism derives from the nucleation and growth of needle-shaped β" precipitates. The size, volume fraction, and spacing of the precipitates are determined by the original composition of the alloy along with artificial aging time and temperature and a variety of other processing details such as natural aging time and quenching rate.

Prior efforts to model the formation and evolution of β" precipitates in aluminum 6061 – based on size and size distribution – include *ab initio modeling* of phase coherency and structure[14] as well as phase field[15] and Lifshitz-Slyozov-Wagner modeling[16] using CALPHAD (Calculation of Phase Diagrams) data for precipitate coarsening. Modeling the effect of precipitate characteristics on mechanical properties, particularly tensile and yield strength, has also been pursued[17]. In addition, several authors, including Rometsh[18] and Hirsch[19], have described how to incorporate these fundamental mechanisms and relationships into an ICME framework for Al-Mg-Si alloys.

In the test case selected for the Structural Materials Data Demonstration Project, data sets captured in the database will be used to analyze these various models and compare calculated results with measured values previously loaded into the database. In subsequent phases of the project, diffusion property data and phase diagram data will likewise be incorporated into the models in order to predict size and volume fraction of the β" precipitates. This, in turn, will be used to predict the yield strength of the 6061 alloy. Although this type of modeling is by no means groundbreaking, the open availability of the data presents a great value to the materials community for modeling work and will remain a focus of continuing development throughout the project.

Next Steps

The Structural Materials Data Demonstration Project team will continue to add to the depth and breadth of the data contained in the demonstration database, keeping it open, in the near term, to a small test group for modeling and verification. To facilitate further input and use, the database will be made available to the materials community at large in the latter phases of the project. Achieving the longer-term goal requires keeping the SMDDP database on a development path that follows best practices for federated data repositories.

Another equally important long-term objective of the Structural Materials Data Demonstration Project is to provide an educational resource for the materials digital data community as well as graduate and undergraduate instruction.

Conclusion

The Structural Materials Data Demonstration Project has been established to provide an open access database borrowing upon and developing best practices for data capture, structuring, and sharing. By focusing on a post-proprietary structural material with broad application interest, the project allows diverse data sets to be collected and included across the range of length scales necessary for modeling with ICME tools. The initial work has focused on capturing and structuring data for diffusion and mechanical properties. Additions of data sets for phase relationships and microstructural properties are being made and provide the basis for modeling of thermal processes for the subject alloy. An initial test case to illustrate the effect of artificial aging on the strength properties of 6061-T6 is underway.

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