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Schema Elements for Granta Annual Report: FY2023

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1 Executive Summary

Granta: Materials Intelligence (Granta: MI) is a commercial database software distributed by Ansys, Inc. that is utilized by the Nuclear Security Enterprise (NSE) to organize and store relevant materials data. Lack of standard and well-documented database schema is the primary obstacle to an NSE additive manufacturing (AM) database, so the objective of this project is to create and document such a schema.

In FY21, an approach for designing, documenting, and managing a standard database schema was described based on the creation of *schema elements* to be used as building blocks for creating various database tables without duplication. In FY22, these methods were applied through a multi-site collaboration to create and document the schema elements necessary to build a thermogravimetric analysis (TGA) testing table.

In FY23 the following progress was made, again through multi-site collaboration:

- The existing schema elements were modified to accommodate differential scanning calorimetry (DSC) data, and a table, Test Data: DSC, was created for managing DSC data.
- The following schema elements were created or significantly appended:
    - Instrument Parameters
    - Test Data and Results
    - Equipment Information
    - Calibration Information
    - Testing Series Information
    - Project Information
    - Document Information
- The following new tables were created using the above new/revised schema elements:
    - Projects
    - Testing Series
    - Instruments
    - Documents
- The existing Test Data: TGA table, along with the tables described above, were released on an unclassified development enterprise instance of Granta: MI and on the classified enterprise instance.
- A decision was made to store AM build information in two separate tables: one table for data corresponding to a specific instance of a build, and one table to store process parameters that may be used in multiple build instances. A draft of the schema elements needed for these tables was created.
- A process for change control of database schema was proposed.

In FY24 the schema elements necessary to complete a working AM database for at least one AM technology will be completed. Further support from programs benefitting from enterprise AM and materials data management would enable significant speedup of the schema development process due to its innate parallelizability.

2 Introduction

Granta: Materials Intelligence, also known as Granta: MI or Granta, is a commercial database software distributed by Ansys, Inc. that is utilized by the Nuclear Security Enterprise (NSE) to organize and store relevant materials data. For a complete discussion of the use of Granta: MI at NSE sites, see the FY21 annual report[1]. Granta: MI is used by five NSE sites locally, and all NSE sites have access to an enterprise instance on the Enterprise Secure Network (ESN) as well as an unclassified development instance. It has been recognized by NNSA management that a shared repository for additive manufacturing (AM) data would not only ensure data and knowledge is not lost but would provide a pool of information relating AM inputs (build parameters, raw materials properties, post-processing information) to the as-built properties of AM parts. Such a dataset would enable optimization of AM build design and promote the shortening of fielding times for new AM components.

The lack of standard and well-documented database schema is an obstacle to an NSE AM database, so the objective of this project is to create and document such a schema. A schema consists of a set of attributes (a.k.a. 'data fields') for each type of data (e.g., build process, post-process information, raw materials information, specimen test information, etc.) as well as documentation of the definitions of each attribute so each site can use the schema consistently.

In FY21, an approach for designing, documenting, and managing a standard database schema was described, along with a set of standards and best practices to encourage consistency. The approach centers on the concept of a *schema element*, which is a collection of attributes used to describe a particular aspect of the data and used, in whole or part, and combined with other schema elements, to construct database tables. The same schema element may be used in multiple tables, which promotes consistency and avoids unnecessary duplication.

In FY22[2], these methods were applied to create and document the schema elements necessary to build a thermogravimetric analysis (TGA) testing table. These activities involved close collaboration with Granta: MI points of contact (POCs), shown in Table 1, at several NSE sites through regular biweekly teleconferences.

In FY23, the TGA testing table was made available, as described in Section 2, to all sites for evaluation on both the unclassified development Granta: MI instance and on the ESN instance. The schema elements process was then applied by the Granta: MI team at the Pantex site to modify the existing schema to accommodate differential scanning calorimetry (DSC) data. Similarly, the LANL team appended existing schema elements sufficiently to create new tables for data related to test data, including Testing Series, Projects, Documents, and Instruments. The updated schema elements are presented in Section 3, and the layouts for these new tables are shown in Section 4. Progress was made in FY23, led by the KCNSC Granta: MI team, on the standardization of schema for storing AM build and process information, as described in Section 5. Also, several additions and modifications were made to the previously established standards and best practices, as summarized in Section 6. Work planned for FY24 is described in Section 7.

[1] LA-UR-21-29682
[2] LA-UR-22-30313

Table 1. List of regular participants in cross-site Schema Elements project discussions. Bolded names represent primary points of contact from each site.

LANL	SNL	LLNL	KCNSC	PX
• **Jillian O'Neel** • Jack Brett • Philip Schembri • Rachel Martin • Robin Pacheco • Alison Ticknor	• **Samuel Moran** • Inkiad Ahmed • Richard Karnesky • Matthew Witman	• Ryan Whitmore • **Daniel Gardner**	• **Leslie Embrey** • Juanita Stephen • Brooke Shaffer	• **Frank Cordova** • Timothy Sanchez
NNSS	**PNNL**	**SRNL**	**Y-12**	**AWE**
• **Michele Arcade** • **Travis Bame**	• **Kriste Henson**	• **Paul Korinko** • Christopher Rasmussen • Camden Chatham	• **Lloyd Arrowood**	• **Craig Lowe** • Fred Moran

3 Releasing the Test Data:TGA table

In FY22 the 10 schema elements[3] necessary to create a TGA testing table, called 'Test Data: TGA', were created, and in FY23 the table was released on both the unclassified development Granta: MI instance and on the classified ESN instance.

There has been extensive discussion among the NSE Granta POCs about which database the materials characterization testing tables, such as Test Data: TGA, should reside in. There already exists an NSE Weapons Materials Database (WMD), which contains material specification metadata, material properties, and materials availability risk information[4]. The objective of the Schema Elements project is to create schema for an NSE Additive Manufacturing Database (AMD), which will presumably be separate from the NSE WMD. But materials characterization test data is generated for both AM and 'traditional' materials (i.e., those in the NSE WMD), so it was not obvious which database the Test Data: TGA table should be added to.

Four data architecture scenarios for the location of materials characterization data were discussed among the POCs:

1. In the NSE WMD, with cross-database links between the characterization tables and the NSE AMD when characterization data is generated on AM materials.
2. In both the NSE WMD and the NSE AMD (i.e. duplicating schema)

[3] Record Information, Project Information, Data Files, Instrument Parameters, Test Conditions, Test Information, Specimen Information, Test Data & Results, Testing Series Information, and Material Pedigree Information

[4] For more detail see "FY22 At-Risk Materials Annual Report", LA-CP-22-20818.

3. In a separate database, with cross-database links to both the NSE WMD and the NSE AMD when characterization data is generated on traditional and AM materials, respectively.
4. In a single database in which all data (including AM and WMD data) resides.

Considerations affecting which scenario to choose include:

- Combining too much data in a single database may create performance issues. For example, LANL has experienced slow performance of the indexing used by the Granta: MI Elastic Search when large datasets and/or attachments are included in records.
- Duplication of database objects, such as the 'Sites' discrete type list, should probably be avoided because it will take effort to keep them synchronized. Duplicating/synchronizing schema across multiple databases can be done using the Data Updater tool in MI: Admin[5], but this is a semi-manual process and is thus subject to human error.
- It might be preferable to split the task of database administration, including setting permissions, across multiple databases because:
    - These tasks may be more easily delegated to multiple people.
    - Some users may need access (or want to view) only certain types of data (e.g., only AM data or only availability risk data), and permissions are easiest to control at the database level.

  It is possible to manage access to (and/or views of) certain data using access controls, profiles, and layouts, but this adds a maintenance burden.
- Linking across databases is currently possible but limited (e.g., linked tabular data and smart links across databases is not possible as of v2022R1). However, Ansys has showed plans to improve cross-database links.
- Tracking properties, specification metadata, and availability risk of AM materials would require some duplication if the NSE WMD and NSE AMD are separate.
- Some schema in the NSE WMD needs to remain unchanged so data in that database can be updated/synchronized with availability risk information provided regularly by Ansys.

Based on these considerations, none of the data architecture scenarios are without risk. However, the LANL team has gained some experience with the Data Updater tool, and we judge it to be generally sufficient for synchronizing at least database-level schema objects across multiple databases. In addition, we assign weight to the value of the modular nature of separate databases. Thus, we have proposed and implemented, at least for evaluation purposes, scenario 3. I.e., there will be three separate databases: the NSE WMD, the NSE AMD, and the NSE Materials Characterization Database (MCD). The latter of these will house materials characterization test data and related records. Success will strongly depend on whether Ansys adequately implements cross-database linking.

Currently, the Test Data: TGA table has been copied (using Data Updater) from the Schema Elements database to a new NSE MCD. It is this NSE MCD that sites are using to evaluate the TGA schema, and it is there that production data will be uploaded on the ESN. Figure 1 shows an example Test Data: TGA record, along with records created by different sites for the purposes of testing the schema.

[5] See the MI:Admin help menu for documentation of the tool's capabilities.

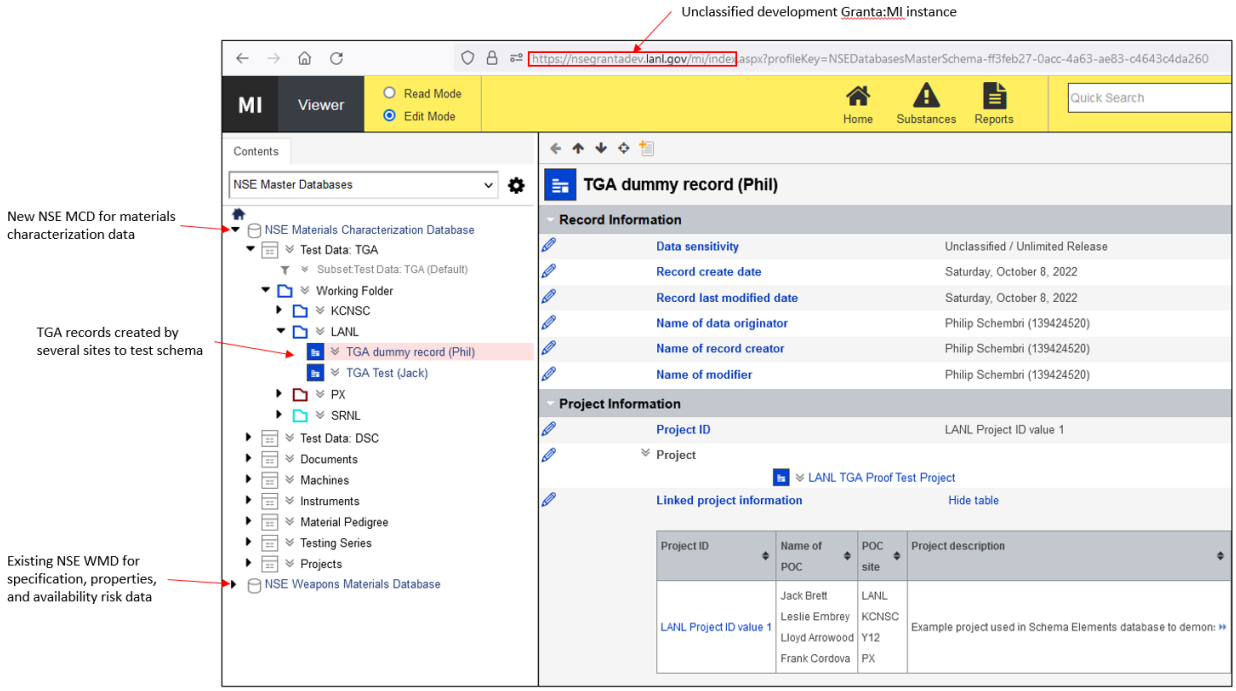

Figure 1. Screenshot of the new NSE MCD on the unclassified Granta: MI development instance, accessible by all NSE sites.

Even with three separate databases, a single *primary* schema development database is sufficient in which to perform the development of the schema elements because the three databases will share all schema elements. However, to maintain primary instances of record link groups and tabular linking attributes across databases, each database may require its own primary schema-only instance in which to maintain the tables constructed from the schema elements. The mechanics of this will need to be formalized and documented in FY24.

4 Schema Elements

This section contains a complete list of the released schema elements as of the end of FY23. These include attributes necessary for managing TGA data as well as those (underlined) added to accommodate DSC data. Each subsection presents the definition of the schema element, the attributes (including their types, as defined in Table 2, and value sets if applicable), and notable changes to the schema element made in FY23.

Table 2. Definition of attribute types referenced in this section.

Abbreviation	Attribute Type
PNT	Floating point value
RNG	Two floating point values; one for minimum and one for maximum

STXT	Short text (<256 characters)
LTXT	Long text
DCT	Discrete type, a.k.a. 'drop down menu' with pre-defined choices
DAT	Date
FIL	File
TABL	Table with rows and columns consisting of other attribute types. Data could be linked from other tables.
HYP	Hyperlink
FDA	Series float functional data, a.k.a. curve data with a primary 'x-axis' parameter and other parameters possible.
IMG	Image file

4.1 Record Information

4.1.1 *Definition*

This schema element contains information about the record itself, including when it was created, modified, and reviewed, and who did those things. It does not contain any information about materials or data. As such, it is likely to be used in the same way (all attributes in the same order) in all tables (maybe even all databases). Some information in this schema element, such as *Record create date*, should be available in the (automatically populated) Record Properties Granta object; however, we are duplicating in these attributes because not all users have access to record property information.

4.1.2 *Notable changes for FY23*

The value set for Data sensitivity was modified to be more systematic and to make OUO[6] marking consistent with DOE policy documents, including DOE M 471.3-1.

4.1.3 *Attributes*

Table 3. Record Information Schema Element Attributes.

Attribute Name	Attribute Type	Value Set

[6] The NNSA sites are migrating from 'OUO' to Controlled Unclassified Information (CUI) at different rates. This value set will eventually be modified to reflect this change.

Data sensitivity	DCT w/ meta LTXT (for notes)	Unclassified / Unlimited Release Unclassified / OUO / Exemption 3 Unclassified / OUO / Exemption 3 / CRADA Unclassified / OUO / Exemption 3 / ECI / EAR Unclassified / OUO / Exemption 3 / ECI / ITAR Unclassified / OUO / Exemption 3 / Patent Caution Unclassified / OUO / Exemption 4 / Third-party Proprietary Unclassified / UCNI Classified / Confidential / FRD Classified / Confidential / RD Classified / Secret / FRD Classified / Secret / RD
Record create date	DAT	
Record last modified date	DAT	
Name of data originator	STXT	
Name of record creator	STXT	
Name of modifier	STXT	
Record owner	DCT	KCNSC, LANL, LLNL, NNSA, NNSS, PNNL, PX, SNL/CA, SNL/NM, SRNL, SRS, Y12, Non-NSE site
Record review	LTXT	
Record information notes	LTXT	

4.2 Project Information

4.2.1 *Definition*

This schema element contains information about the project that the record is a part of. It contains both attributes about the project that will reside in the Projects table, as well as links that can be used in other tables (ex: Test Data: TGA or other testing tables) to provide a traceable link back to the project record.

4.2.2 *Notable changes for FY23*

This schema element was appended with attributes intended to reside within a Projects table; i.e. to describe a project record. Previously it contained attributes that would primarily be used to link another record (e.g., a TGA test record) to a project record.

4.2.3 *Attributes*

Table 4. Project Information Schema Elements Attributes.

Attribute Name	Attribute Type	Value Set
Project ID	STXT	Unique in *Projects* table
Project	Static link to *Projects* table	
Project	Smart link to *Projects* table	
Linked project information	Linked TABL	Linking Value = Project ID
Names of project points-of-contact	STXT	
Project description	LTXT	
Funding organization	STXT	
Participating sites	DCT	KCNSC, LANL, LLNL, NNSA, NNSS, PNNL, PX, SNL/CA, SNL/NM, SRNL, SRS, Y12, Non-NSE site
Project start date	DAT	
Project finish date	DAT	
Project information notes	LTXT	

4.3 Data Files

4.3.1 *Definition*

This schema element contains data files and information about them for the purpose of traceability.

4.3.2 *Notable changes for FY23*

No major changes made in FY23 for this schema element.

4.3.3 *Attributes*

Table 5. Data Files Schema Element Attributes.

Attribute Name	Attribute Type	Value Set
Raw data file	FIL	
Final data file	FIL	

Other data file	FIL	
Raw data file link	HYP	
Final data file link	HYP	
Other data file link	HYP	
Data files notes	LTXT	

4.4 Instrument Parameters

4.4.1 *Definition*

This schema element contains attributes that describe the instrument setup and test program sufficiently for an operator to reproduce the test. This includes hardware and accessory information, as well as instrument/software settings such as gas flow rate, signal gain, etc. Finally, it includes test program information such that a test operator can replicate the test on their own instrument (ex: Step 1 – Ramp from 30°C to 150°C at 5°C/min, Step 2 – Isothermal hold for 5 mins, etc.).

4.4.2 *Notable changes for FY23*

An Equipment Information schema element has been created to store information about identification of hardware, namely: Instrument ID, Instrument, and linked instrument information. Thus, these attributes were removed from Instrument Parameters. The Test method description attribute was added to capture a free-form description of the test method since this is not practical to capture in structured attributes. By doing this, we enable the use-case of reproducing a test but not the use-case of searching/reporting on that information. The fact this kind of search is expected to be uncommon and this information is unlikely to be used as an independent variable in a study of DSC data helps to justify this decision.

Attributes (those underlined in Table 6) were added to accommodate parameter settings for DSC instruments. There was significant discussion of the Pan type attribute. Originally it was created as a discrete type attribute, but it was not possible to identify a list of possible values in such a way that they could be entered precisely. For example, both 'Aluminum' and 'Aluminum Hermetic' were necessary to include as options, and a user could then enter the former (more general) option when the latter (more specific) option was more appropriate. The issue was resolved by making the Pan type a short text attribute, forgoing the ability to control the input and thus the ability to make accurate searches and reports using the attribute. The fact that Pan type is unlikely to be used as an independent variable in a study of DSC data helps to justify this decision.

4.4.3 *Attributes*

Table 6. Instrument Parameters Schema Element Attributes. Underlined attributes are those added for DSC data.

Attribute Name	Attribute Type	Value Set
Test method file	FIL	
Test method description	LTXT	

Balance gas	DCT, multi-value	Air, Argon, Helium, Nitrogen
Balance gas flow rate	PNT, multi-value	
Specimen gas	DCT, multi-value	Air, Argon, Helium, Nitrogen
Specimen gas flow rate	PNT, multi-value	
Pan material	DCT	Aluminum, Ceramic, Platinum
Pan volume	DCT	50µL, 80µL, 100µL, 250µL
Furnace type	DCT	Evolved Gas Analysis (EGA) Furnace, Infrared (IR) Furnace, Wire Wound (Pt/Rh) Furnace
Exotherm	DCT	Down, Up
Purge gas	DCT	Air, Argon, Helium, Nitrogen
Purge gas flow rate	PNT	
Heat flow selection	DCT	Heat Flow TP1, Heat Flow TP4, Heat Flow T4P
Pan type	STXT	
Lid type	DCT	Standard Temperature Lid, High Temperature Lid, Mettler Toledo Aluminum Lid
Pan mass (reference pan)	PNT	
Pan mass (sample pan)	PNT	
Absolute thermal resistance	STXT	
Instrument configuration	LTXT	
Pre-test instrument verification file	FIL	
Pre-test instrument verification notes	LTXT	
Instrument parameters notes	LTXT	

4.5 Test Conditions

4.5.1 *Definition*

This schema element contains attributes that specifically describe the state of the specimen material during the test. These are variables such as test temperature, strain rate, etc. that impact the response of the material. They are intended to describe the test data for data consumers. It is acknowledged that

these attributes may partially duplicate some of the information in the Instrument Parameters schema element, which may describe the test in more detail but are not as useful for data consumers.

4.5.2 *Notable changes for FY23*

No major changes made in FY23 for this schema element.

4.5.3 *Attributes*

Table 7. Test Conditions Schema Element Attributes.

Attribute Name	Attribute Type	Value Set
Test atmosphere	DCT, multi-value	Air, Argon, Helium, Nitrogen
Test temperature	RNG	
Test temperature ramp rate	PNT, multi-value	
Test conditions notes	LTXT	

4.6 Test Information

4.6.1 *Definition*

This schema element contains non-instrument-specific meta-data attributes related to the test data stored in the record. This includes personnel, organizations, and documents associated with the test, as well as the time and date of the test.

4.6.2 *Notable changes for FY23*

The documents static link was removed because this was moved to the Document Information schema element in accordance with the convention that links *to* information will reside in the schema element *for* that information (See Section 7 point 3). Static links to the Test Data: TGA table and to the Test Data: DSC tables were added for the same reason, and links to other testing tables will be added as those tables are created. Because the Test group attribute is short text, consistency throughout the sites is crucial and, as documented in the help file for this attribute, we have agreed to maintain a list of valid test groups that will be validated before the release of the record.

4.6.3 *Attributes*

Table 8. Test Information Schema Elements Attributes.

Attribute Name	Attribute Type	Value Set
Test ID	STXT	Unique in *Test Data* table

Test site	DCT	KCNSC, LANL, LLNL, NNSA, NNSS, PNNL, PX, SNL/CA, SNL/NM, SRNL, SRS, Y12, Non-NSE site
Test group	STXT	"Valid" options provided in help file
Name of requester	STXT	
Name of test contact	STXT	
Name of operator	STXT	
Date test performed	DAT	
Time test performed	STXT	
Test type	DCT	Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC)
Document number of work order	STXT	
Document number of test standard	STXT	
Document number of test plan	STXT	
Document number of test report	STXT	
Document numbers of other documents	STXT	
Test Data: TGA	Static link to *Test Data: TGA* table	
Test Data: DSC	Static link to *Test Data: DSC* table	
Test information notes	LTXT	

4.7 Specimen Information

4.7.1 *Definition*

This schema element contains information about the specimen that was tested. For example, attributes may describe specimen size, geometry, manufacturing information, etc.

4.7.2 *Notable changes for FY23*

Specimen manufacturing description was a LTXT attribute and has been replaced by the discreet multi-valued Specimen manufacturing technique attribute to satisfy the use case of searching and test reproducibility among the sites.

4.7.3 *Attributes*

Table 9. Specimen Information Schema Elements Attributes.

Attribute Name	Attribute Type	Value Set
Specimen ID	STXT	
Specimen description	LTXT	
Specimen location	STXT	
Name of specimen preparer	STXT	
Specimen manufacturing description	DCT, multi-value with LTXT meta	Additive Manufacturing, Cored, Cut Off, Drilled, Electrical Discharge Machining (EDM), End Milled, Ground, Laser Cut, Milled, Polished, Pressed, Stamped, Turned, Water Jet
Specimen form	DCT	Liquid, Powder, Solid
Specimen geometry	DCT	Cubic, Cylindrical, Rectangular, Irregular
Specimen length	PNT w/ LTXT meta (for measurement method description)	
Specimen width	PNT w/ LTXT meta (for measurement method description)	

Specimen height	PNT w/ LTXT meta (for measurement method description)	
Specimen diameter	PNT w/ LTXT meta (for measurement method description)	
Specimen mass	PNT w/ LTXT meta (for measurement method description)	
Specimen density	PNT w/ LTXT meta (for measurement method description)	
Specimen information notes	LTXT	

4.8 Test Data & Results

4.8.1 *Definition*

This schema element contains attributes used to hold the data and results from a test. Generally, this schema element consists of functional data attributes that hold X-Y curve data as well as point, range, or tabular attributes that hold specific values. Data may be uploaded directly from test instrument sensors (e.g., load) or may be calculated (e.g. stress). Results are usually, but not always, determined by analyzing curve data.

4.8.2 *Notable changes for FY23*

The link to Analysis documents was removed in favor of the link that resides in the Document Information schema element. The Document number of analysis document attribute was retained, even though it may not be useful for linking.

Attributes (underlined) were added to accommodate DSC test results. Tabular attributes are used to store point values that may occur at multiple discrete temperatures in the functional data, allowing both the data and the temperature at which it occurred.

4.8.3 *Attributes*

Table 10. Test Data & Results Schema Element Attributes. Underlined attributes are those added for DSC data.

Attribute Name	Attribute Type	Value Set
Weight percent vs. time	FDA	Parameter = Time

Weight percent vs. temperature	FDA	Parameter = Temperature
Derivative of weight percent vs. temperature	FDA	Parameter = Temperature
Weight changes	TABL	
Temperatures at onsets of weight change	TABL	
Temperatures at maximum rates of weight change	TABL	
Residual weight	PNT	
Heat flow vs. time	FDA	Parameter = Time
Heat flow vs. temperature	FDA	Parameter = Temperature
Reversing heat flow vs. temperature	FDA	Parameter = Temperature
Nonreversing heat flow vs. temperature	FDA	Parameter = Temperature
Total heat capacity vs. temperature	FDA	Parameter = Temperature
Reversing heat capacity vs. temperature	FDA	Parameter = Temperature
Derivative of heat flow vs. temperature	FDA	Parameter = Temperature
Enthalpies	TABL	
Temperature at onsets	TABL	
Temperatures at peak maxima/minima	TABL	
Glass transition temperatures	TABL	

Analysis method	LTXT	
Name of analyzer	STXT	
Document number of analysis document	STXT	
Test data & results notes	LTXT	

4.9 Testing Series Information

4.9.1 *Definition*

This schema element contains information about the testing series that the record is a part of. It contains both attributes about the Testing Series that will reside in the Testing Series table, as well as links that can be used in other tables (ex: Test Data: TGA or other testing tables) to provide a traceable link back to the Testing Series record.

4.9.2 *Notable changes for FY23*

This schema element was released in FY23; previous versions were placeholders.

4.9.3 *Attributes*

Table 11. Testing Series Information Schema Element Attributes.

Attribute Name	Attribute Type	Value Set
Testing series ID	STXT	Unique in *Testing Series* table
Testing series status	DCT	Unknown, To Be Started, In Progress, Completed Pending Documentation and Report, Completed with Documentation and Report
Testing series sites	DCT	KCNSC, LANL, LLNL, NNSA, NNSS, PNNL, PX, SNL/CA, SNL/NM, SRNL, SRS, Y12, Non-NSE site
Testing series groups	STXT	"Valid" options provided in help file
Testing series principal investigators	TBL	
Testing series start date	DATE	
Testing series finish date	DATE	

Testing series purpose	DCT	Acceptance, Surveillance, Qualification (including aging/compatibility studies), Research & development, Material model development/calibration, Design data generation
Testing series description	LTXT	
Testing series images	TBL	
TGA tests	Linked TABL	Linking value = Testing series ID
DSC Tests	Linked TABL	Linking value = Testing series ID
Testing series	Static link	
Testing series	Smart link	
Linked testing series information	Linked TABL	Linking value = Testing Series ID
Testing series information notes	LTXT	

4.10 Material Pedigree Information

4.10.1 *Definition*

This schema element contains information about the material pedigree that the record is a part of. Most of the attributes are links since the information about material pedigree is contained natively in the Material Pedigree table, and we want to avoid duplication.

4.10.2 *Notable changes for FY23.*

No changes were made to this schema element in FY23. This schema element remains a placeholder to enable links from other schema elements.

4.10.3 *Attributes*

Table 12. Material Pedigree Information Schema Element Attributes.

Attribute Name	Attribute Type	Value Set
Material pedigree ID	STXT	Unique in *Material Pedigree* table
Material pedigree	Static link to *Material Pedigree* table	

Material pedigree	Smart link to *Material Pedigree* table	
Linked material pedigree information	Linked TABL	Linking value = Material Pedigree ID
Material pedigree information notes	LTXT	

4.11 Calibration Information

4.11.1 *Definition*

This schema element contains information about the calibration of instruments that are used in testing records. This schema element will mainly serve as a user log of calibration events that can be manually examined by data consumers, as needed. It is not intended to allow users to search or sort easily based on calibration information or to automatically relate test results to calibration information. Satisfying that use case would have required a more complex structure and it was determined that test results will rarely be studied as a function of calibration information.

4.11.2 *Notable Changes for FY23*

The initial version of this schema element contained multiple attributes that tracked the calibration standards, temperatures, constants, and raw data files uploaded by the user. This left some ambiguity between the definitions of calibration vs. verification and introduced too much unnecessary information. The solution was to condense the information into one tabular attribute which will track users and dates of calibrations performed as well as store relevant files. This satisfies the use-case of tracking who did the calibrations and when, as well as the use-case of inspection of calibration details by examining the files.

4.11.3 *Attributes*

Table 13. Calibration Information Schema Element Attributes.

Attribute Name	Attribute Type	Value Set
Calibration	TABL	
Calibration information notes	LTXT	

4.12 Equipment Information

4.12.1 *Definition*

This schema element contains attributes that describe equipment (i.e., hardware). Primarily these are attributes used to identify and describe the equipment in general, not as it was used for a specific application (which is captured in other schema elements; for example, Instrument Parameters). This

schema element includes attributes and link groups that would be used to link *to* an equipment record *from* another record, for example a test record (per the convention described in point 3 in Section 7). 'ID' attributes used for linking are specific to the type of equipment (e.g., Instrument, Machine, etc.) to allow multiple types of equipment to be linked from a test record.

4.12.2 *Notable changes for FY23*

This schema element was created in FY23.

4.12.3 *Attributes*

Table 14. Equipment Information Schema Element Attributes.

Attribute Name	Attribute Type	Value Set
Instrument ID	STXT	Unique in Instruments table
Machine ID	STXT	Unique in Machines table
Linked instrument information	Linked TABL	Linking Value = Instrument ID
Linked machine information	Linked TABL	Linking Value = Machine ID
Instrument	Static link to *Instruments* table	
Instrument	Smart link to *Instruments* table	
Machine	Static link to *Machines* table	
Machine	Smart link to *Machines* table	
Manufacturer	STXT	
Model	STXT	
Serial number	STXT	
Site-specific identification	STXT	
Link to equipment in external database	HYP	
Name of equipment point of contact	STXT	
Owning site	DCT	KCNSC, LANL, LLNL, NNSA, NNSS, PNNL, PX, SNL/CA, SNL/NM, SRNL, SRS, Y12, Non-NSE site
Owning group	STXT	
Equipment description	LTXT	
Equipment image	IMG	

Equipment information notes	LTXT	

5 Layouts for new tables added in FY23

The table layouts in this section are those that were created in the NSE Materials Characterization Database. They use attributes from the schema elements described in Section 4, and in most cases the layout section title matches the name of the schema element from which the attributes come. Link groups are differentiated from attributes by the italicized description in brackets.

5.1 Layout for DSC table

Table 15. Layout for DSC table.

Section	Attribute or link group
Record Information	Data sensitivity
	Notes
	Record owner
	Record create date
	Record last modified date
	Name of data originator
	Name of record creator
	Name of modifier
	Record review
	Record information notes
Project Information	Project ID
	Project *[smart link group]*
	Linked project information
	Project information notes
Testing Series Information	Testing series ID
	Testing Series *[smart link group]*
	Linked testing series information
	Testing series information notes
Data Files	Raw data file
	Final data file
	Other data file
	Raw data file link
	Final data file link
	Other data file link
	Data files notes
Document Information	Documents *[static link group]*
Test Information	Test ID

	Test site
	Test group
	Name of requester
	Name of test contact
	Name of operator
	Date test performed
	Time test performed
	Test type
	Document number of work order
	Document number of test standard
	Document number of test plan
	Document number of test report
	Document numbers of other documents
	Test information notes
Test Conditions	Test atmosphere
	Test temperature
	Test temperature ramp rate
	Test conditions notes
Material Pedigree Information	Material pedigree ID
	Material Pedigree *[smart link group]*
	Linked material pedigree information
	Material pedigree information notes
Specimen Information	Specimen ID
	Specimen description
	Specimen location
	Name of specimen preparer
	Specimen manufacturing description
	Specimen form
	Specimen geometry
	Specimen length
	Measurement method description
	Specimen width
	Measurement method description
	Specimen height
	Measurement method description
	Specimen diameter
	Measurement method description
	Specimen mass
	Measurement method description
	Specimen density
	Measurement method description

	Specimen information notes
Equipment Information	Instrument ID
	Instrument *[smart link group]*
	Linked instrument information
Instrument Parameters	Test method file
	Test method description
	Exotherm
	Purge gas
	Purge gas flow rate
	Heat flow selection
	Pan type
	Lid type
	Pan mass (reference pan)
	Pan mass (sample pan)
	Absolute thermal resistance
	Instrument configuration
	Pre-test instrument verification file
	Pre-test instrument verification notes
	Instrument parameters notes
Test Data & Results	Heat flow vs. time
	Heat flow vs. temperature
	Reversing heat flow vs. temperature
	Nonreversing heat flow vs. temperature
	Total heat capacity vs. temperature
	Reversing heat capacity vs. temperature
	Derivative of heat flow vs. temperature
	Enthalpies
	Temperature at onsets
	Temperatures at peak maxima/minima
	Glass transition temperatures
	Analysis method
	Name of analyzer
	Document number of analysis document
	Test data & results notes

5.2 Layout for Projects table

Table 16. Layout for Projects table.

Section	Attribute or link group
Record Information	Data sensitivity

	Notes
	Record owner
	Record create date
	Record last modified date
	Name of data originator
	Name of record creator
	Name of modifier
	Record review
	Record information notes
Project Information	Project ID
	Project description
	Names of project points-of-contact
	Funding organization
	Participating sites
	Project start date
	Project finish date
	Project information notes
Testing Series Information	Linked testing series information
Test Information	Test Data: TGA *[smart link group]*
	Test Data: DSC *[smart link group]*
Equipment Information	Instruments *[smart link group]*
	Linked instrument information
	Machines *[smart link group]*
	Linked machine information

5.3 Layout for Testing Series table

Table 17. Layout for Testing Series table.

Section	Attribute or link group
Record Information	Data sensitivity
	Notes
	Record owner
	Record create date
	Record last modified date
	Name of data originator
	Name of record creator
	Name of modifier
	Record review
	Record information notes
Project Information	Project ID

	Linked project information
	Project *[smart link group]*
Testing Series Information	Testing series ID
	Testing series status
	Testing series sites
	Testing series groups
	Testing series principal investigators
	Testing series start date
	Testing series finish date
	Testing series purpose
	Testing series description
	Testing series images
	TGA tests
	Testing series information notes
Material Pedigree Information	Linked material pedigree information
	Material Pedigree [s*tatic link group]*
Document Information	Documents *[static link group]*
Test Information	Test Data: TGA *[smart link group]*
	Test Data: DSC *[smart link group]*

5.4 Layout for Documents table

Table 18. Layout for Documents table.

Section	Attribute or link group
Record Information	Data sensitivity
	Notes
	Record owner
	Record create date
	Record last modified date
	Name of data originator
	Name of record creator
	Name of modifier
	Record review
	Record information notes
Document Information	Document ID
	Title
	Author(s)
	Editor(s)
	Publisher
	Publisher (non-NSE)

	Publication date
	Document type
	Keywords
	Link to document file
	Document file
	Document information notes
Testing Series Information	Testing Series *[static link group]*
Test Information	Test Data: TGA *[static link group]*
	Test Data: DSC *[static link group]*

5.5 Layout for Instruments table

Table 19. Layout for Instruments table.

Section	Attribute or link group
Record Information	Data sensitivity
	Notes
	Record owner
	Record create date
	Record last modified date
	Name of data originator
	Name of record creator
	Name of modifier
	Record review
	Record information notes
Project Information	Projects *[static link group]*
	Linked project information
Equipment Information	Instrument ID
	Manufacturer
	Model
	Serial number
	Site-specific identification
	Link to equipment in external database
	Name of equipment point of contact
	Owning site
	Owning group
	Equipment image
	Equipment information notes
Calibration Information	Calibration
	Calibration information notes
Document Information	Documents *[static link group]*

Testing Series Information	Testing Series *[static link group]*
Test Information	Test Data: TGA *[smart link group]*
	Test Data: DSC *[smart link group]*

6 Progress on AM build and process schema elements

In FY23 work began to create schema elements for storing AM build information and process parameters. The KCNSC team took the lead on this part of the project. Their approach was to collect from each site the attributes being used in their local AM databases for storing AM build and process information, to document the use-cases for each attribute, to precisely define each attribute, and to resolve any duplication of attributes. It was expected that not all AM technologies might be addressed initially (e.g., selective laser sintering (SLS) might be addressed first), but that the result would be a significant improvement over the stock 'AM Builds' table attributes provided by Granta, which is confusing, inconsistent, and poorly defined.

It was anticipated that these attributes would be sorted into schema elements for AM *Build* Information (including data, such as build date and name of operator, describing a specific instance of a build) and AM *Process* Information (including process parameters, like laser power and hatch spacing, that may be the same for multiple build instances). Originally it was expected that these two schema elements would be assembled, along with other schema elements, into an AM Builds table (as in the Granta stock schema). However, as discussed in Section 4 of the FY22 report[2], the new ASTM standard[7] for AM data management divides AM build data into two separate tables – Builds and Processes. This paradigm is in contrast to that used by the Granta stock AM schema, which stores both build and process parameters in a single table. This difference was discussed at length among the NSE site POCs, especially in the context of the following two use-cases that were difficult to satisfy when storing both build and process parameters in a single table:

- Sometimes, as in Figure 2, a single build instance contains multiple parts, and different sets of processing parameters are used for those different parts. In this case, there is a one-to-many relationship between build information and process information.
- Sometimes, as in Figure 3, multiple instances of the 'same' build are performed using the (nominally) same processing parameters. In this case, there is a many-to-one relationship between build information and process information.

The NSE sites have thus made the decision to deviate from the stock Granta AM schema by dividing AM build and AM process information into two tables, with links between them (and probably also to a table storing part information, whose records can be linked directly to both build and process records).

As of this writing, the KCNSC team has assembled input from all sites to create draft AM Build Information and AM Process Information schema elements addressing SLS technology. In FY24, these schema elements will be reviewed by all sites, revised, documented by the KCNSC team, and assembled into functioning AM Build and AM Process tables.

[7] ASTM F3490-21, Standard Practice for Additive Manufacturing - General Principles - Overview of Data Pedigree

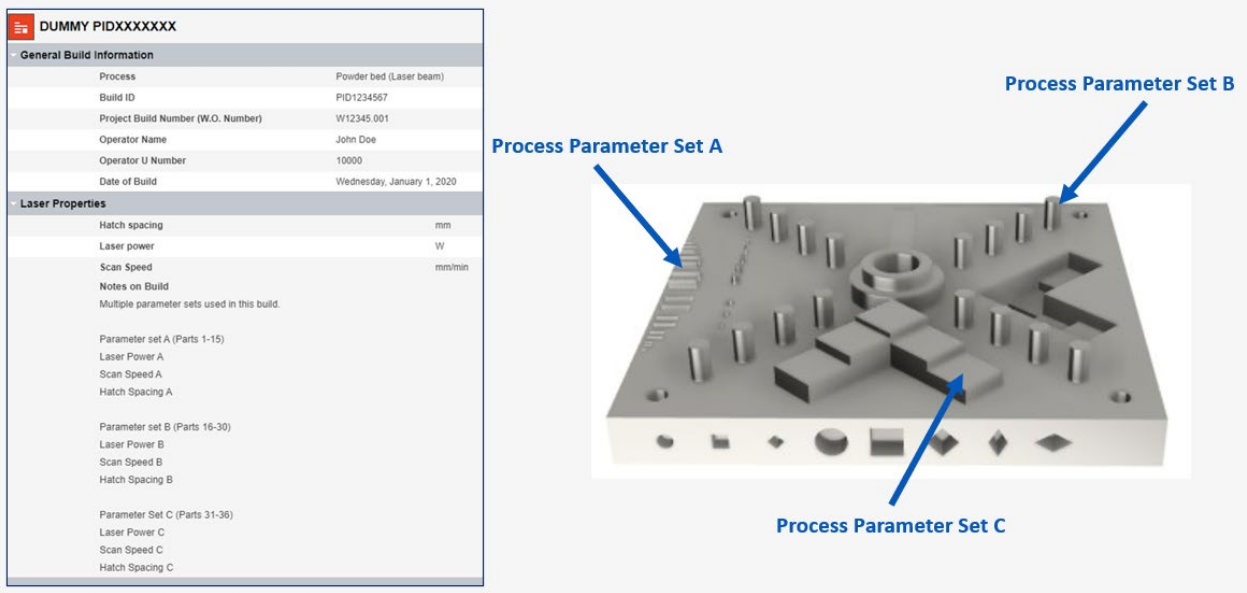

Figure 2. A notional example of a single build that uses three different parameters sets.

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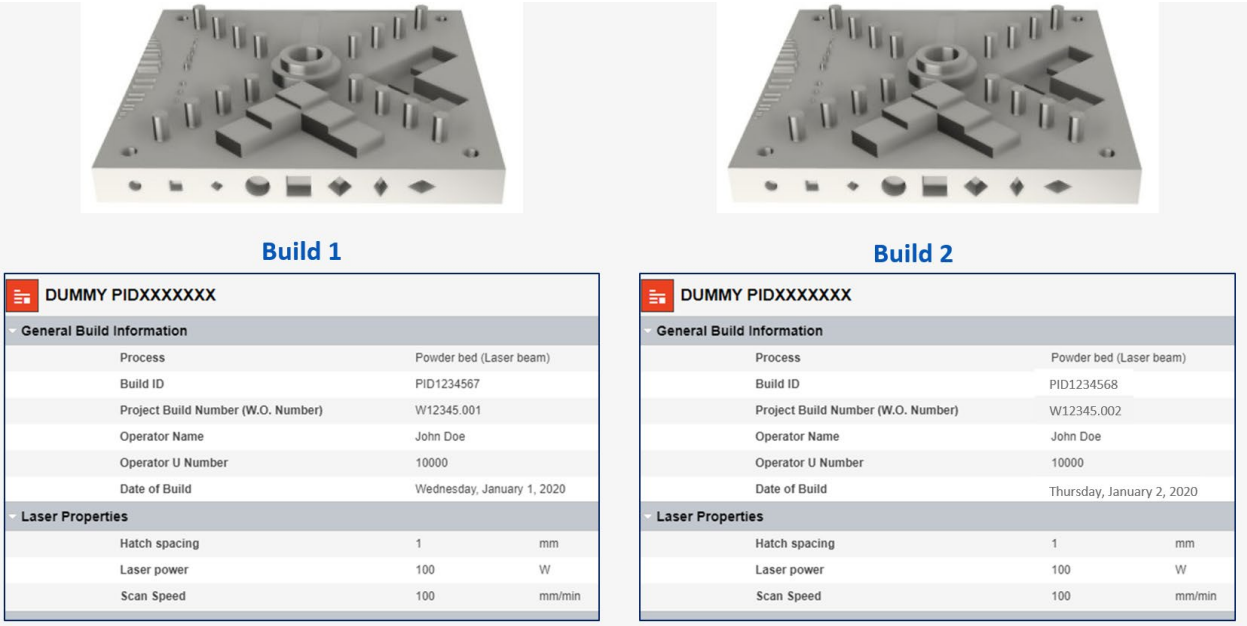

Figure 3. A notional example of multiple build instances (with different Build ID number and built on different dates) of nominally the same parts using the same process parameters.

7 Conventions, standards, and best practices (updated)

The following list of conventions, standards, and best practices for the NSE implementation of Granta: MI has been updated to include FY23 developments. These conventions and best practices are intended to be utilized across all schema elements, and they will be communicated to users through the *help files* available to users as a URL link on the attribute name.

1. **Attribute naming**:
    - Attributes will not have identical names if they are not intended to be used in a functionally identical way.
    - In a name with more than one word, the first word is capitalized, and the rest is lowercase.
    - Attributes containing people's names should be named "Name of xyz".
    - Functional attributes should be named 'y-axis quantity vs. x-axis quantity'.
    - Linked tabular attributes should be named 'Linked xyz information' where 'xyz' is the type of data linked from the linked table (which could, but is not required to be, the linked table name).
2. **Notes attributes:** Each schema element will contain a long text attribute called "*Schema element name" notes* (ex: Record information notes) that is intended to serve as a catch-all notes attribute for that section of the table.
3. **Linking conventions:** Links between records will, in general, consist of one or more of the following:
    - A short text attribute corresponding to the unique 'ID' in the table that is being linked to. For example, project records contain a unique, short text attribute called Project ID and testing series records contain a unique, short text attribute called Testing series ID. This is useful for automating static or smart link generation.
        - 'ID' attributes used for linking should be enforced to be unique in their native tables (i.e., Project ID should be unique in the Projects table), except in special cases.
    - A static record link.
    - A smart record link.
    - A tabular attribute with the previously mentioned short text ID attribute as the linking value and relevant linked columns defined.

    While the schema element may contain all the above objects, implementation into a database table may involve down-selecting objects. For example, either a static *or* a smart record link, but not both, should be implemented based on whether the links will be one-to-one or one-to-many.
    - For example:
        - A smart link can be used to link a test record to a Pedigree record by matching the Pedigree ID in both records since a test record can correspond to only a single Pedigree (although a Pedigree may correspond to many tests).
        - A static link would be used to link test records to a Documents record since a test may reference multiple documents and each document may be referenced by multiple tests, precluding the ability to create links by matching Document ID or Test ID in both records.

    In FY23, it was determined that these linking attributes (or link groups) should be part of the schema element describing the information being linked *to*. For example, links *to* the Documents table, and the Document ID attribute, should be part of the Document Information schema element. This ensures they are captured in exactly one schema element.

4. **Naming of people:** To aid in searching, people's names in short text attributes must be written consistently. The following convention is proposed.
    - First name and last name as they appear in the OneID phonebook.
    - For NSE personnel, the DUID from the OneID phonebook in parentheses following the name.
        - E.g., Jillian O'Neel (123456542)
5. **Reviewer convention:** Rather than using separate attributes for each different kind of record review, which isn't flexible enough, a long text attribute will be used with the format described below. Each reviewer will append with their own entry on a new line. Current review types include "Technical Review" for data accuracy, "Granta Review" for conformation to database conventions, and "Classification Review" for review by a Derivative Classifier. The format will be:
    - First name and last name (unique ID) - date - review type
        - E.g., Jack Brett (123456543) - 3/8/2021 - Granta Review
6. **Files in Data Files section:**
    - Files in this schema element will be stored in individual attributes rather than in a flexible, tabular 'Files' attribute. This facilitates ease of uploading.
    - Unless otherwise specified, files are understood to be retained for traceability purposes only. Data consumers should only take data from attributes.
    - Human readable (e.g., ASCI) files are preferred. If binary files must be used, they must be excluded from the Granta search engine by unchecking the 'allow file contents to be searched' option.
    - A data file is required if one exists and is not too big to upload.
    - If files are too big to be uploaded, they may be stored externally (for example, in an institutional large file store) and a hyperlink to the file's location may be uploaded to the file link attributes (ex: *Raw data file link*). It is understood that these links could break if directories on the external system change; therefore, it is recommended that data uploaders establish a directory structure on the external system that is as robust and standardized as possible.
    - If more than one "other data files" exist, they should be zipped together and the .zip folder should be uploaded to the *Other data file* attribute.
7. **Guidelines for discrete attributes**:
    - A discrete list can be 'ordered' (by checking the appropriate box in MI: Admin), meaning that Granta: MI assigns value to each choice. For example, the list consisting of the values 'red', 'yellow', and 'green' can be ordered so a user can search for values 'above' yellow. Care should be taken to order the choices in a way that would make the most sense to a data consumer. For example, is a user searching for all values 'above' yellow looking for records with yellow & green or yellow & red?
    - If a discrete list is not ordered (ex: a list of all NSE sites), the values in the discrete type should be sorted in alphabetical order ("Arrange by Name" in MI: Admin) and the "Ordered" box should not be checked.
8. **Guidelines for managing value domains**:
    - Discrete types are recommended when the list of choices is not too long and when the list doesn't change too much (since it must be managed by a database administrator).
    - A linked table (or linked database) is recommended when values can/should practically be added by users and/or when metadata about the value are useful to capture. Note that this option:
        - Requires effort from the database administrator to set up but not to maintain.

        - May require effort from the user to ensure data is entered into the correct table.
    - Text attributes are recommended when discrete types and linked tables are not practical. If possible, a value domain should be created by each site and documented to aid review process. Examples of attributes where this method is used include 'Organization' and 'Location', as well as attributes for people's names.
        - Note that Text attributes with no documented or enforced value domain should be considered of primary use for 'reproducibility' use-cases, not for searching/reporting use-cases since data may be entered differently by different users. This applies to long text attributes like 'Test method description' that describe how a test is performed (for reproducibility) but doesn't support searching or sorting based on the data.
        - More specifically, data stored in text attributes with no documented or enforced value domain should be assumed *not* to be consumed as independent variable. E.g., it will not be possible to study the DSC behavior of records in a testing series as a function of the data in the (short text) Pan type attribute.

9. **Unit systems**
    - Attributes that have units should be assigned the applicable unit in the mm-N-s consistent unit system as the default unit.
    - As units are assigned to attributes, admins should verify that the selected unit is consistently and correctly set-up in MI: Admin. This includes using "Derived from other units" whenever possible and correctly inputted "Unit System Equivalents".
    - When reviewing schema elements, units and equivalent units will also be reviewed for consistency.
10. **Help files:** A help file is required for each attribute and must be in the standardized format, which consists of the four sections below. If any of these sections do not apply, they will contain 'N/A'.
    - Definition: the definition of the attribute
    - Standards: conventions that must be adhered to
    - Best Practices: recommended conventions
    - Image: an image to clarify any of the above
11. **Required attributes**: The Granta: MI software can force an attribute to be required, based on the layout. Since the decision to require attribute data may depend on the project uploading the data, it is proposed that a layout only require data if omission of that attribute data would significantly diminish the value of the record data. Required attributes are noted as such in the Standards section of the help file.
12. **Conventions for 'ID" values**: Attributes such as Specimen ID and Project ID are used to identify linked records. There is no required format for the short text in these attributes since sites may have existing conventions. However, help files should recommend a format to help when an existing convention does not exist.
13. **External data management standards & practices**: Integration with other established data management standards and practices is preferred; however, the team has noted instances where deviation is necessary due to the database use cases and/or Granta: MI software limitations. These standards include ASTM F3490-21 for Additive Manufacturing Data as well as internal practices such as documentation for the treatment of Official Use Only / Controlled Unclassified Information. Specific deviations are noted in the PowerPoint slides for the schema element which are available on the project SharePoint. Any deviations that require action from a data

uploader or are helpful for interpretation for a data consumer are communicated via the specific attribute's html help file.

14. **Owner vs. point-of-contact**: It is often desired to have a name listed alongside data and metadata in Granta so that data consumers know who to contact for more information. Upon discussion, the term "owner" is often suggested for the attribute name that contains this information (e.g., Instrument owner, Data owner, Project owner, etc.). However, it was determined that "owner" implies a level of control over the data that does not reflect the paradigm of the database. Therefore, we often chose to use the term "point-of-contact" which better reflects the actual purpose of the metadata.

8 Schema element revision process

During FY23 it became necessary to revise existing schema elements. The process followed to document the changes was as follows:

1. The original PowerPoint file documenting the use-cases, attribute types, and discussion/decisions was edited to reflect changes and/or additions.
2. The revisions were presented to the cross-site team via teleconference using the edited PowerPoint slides.
3. Two weeks (the time between cross-site teleconferences) was allowed for each site to understand the changes, ask questions, and make suggestions.
4. Steps 2 and 3 were repeated as necessary until no further changes were needed.
5. The updated PowerPoint was added to the SharePoint (replacing the original), and changes to the schema in the Schema Elements database were made to reflect the revised schema element.

In FY23 it was primarily the LANL team following this process, and it is proposed that other sites either follow the same process when developing schema elements or propose changes to the process.

9 Summary and FY24 plans

In FY23 the cross-NSE-site Schema Elements team appended existing schema elements to create the following tables in a development instance of a new NSE Materials Characterization Database:

- Test Data: TGA
- Test Data: DSC
- Projects
- Testing Series
- Instruments
- Documents

In addition, significant progress has been made toward the creation of AM Build and AM Process tables, which should be usable in FY24.

Depending on available resources (funding and personnel) across the NSE team, work in FY24 will concentrate on the following, prioritized from highest to lowest:

- Copying existing schema to a production database on the ESN on which AM project data can be managed.

- Releasing working versions of AM Build and AM Process tables and creating the NSE AM Database for at least one AM technology (e.g., laser powder bed).
- Creating schema elements and tables for AM raw materials, machines, and part information.
- Appending the available materials characterization tables, possibly to include uniaxial quasi-static testing

In FY23 the LANL, Pantex, and KCNSC teams were very active in the creating of Granta: MI schema, demonstrating that tasks in this project are highly parallelizable. If more sites can identify resources, this project can be completed sooner, allowing Granta: MI to be used as an enterprise materials data management resource.