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Shape Memory Materials Database Tool—A Compendium of Functional Data for Shape Memory Materials

Othmane Benafan, Glen S. Bigelow, and Avery W. Young*

A database tool is developed for archiving and exploring shape memory materials including shape memory alloys (SMAs), superelastic alloys, magnetic SMAs, shape memory polymers, and shape memory ceramics. Over 750 000 data points and their pedigree metadata are extracted and stored into records. Data are handled via a graphical user interface running in a web application. The tool provides interactive menus for the selection of material types, properties, and filters, culminating with a visualization panel. Data are displayed in three forms, consisting of pie charts, 2D scatter plots, and ternary diagrams, all of which provide unique information pertinent to the materials and properties being explored. This database tool is a major stepping stone toward building an information system where an entire continuum of material novices to experts can have an infrastructure to explore and discover these multifunctional materials.

Since the first discovery of shape memory properties over eight decades ago,[1] there have been significant shape memory material (SMM) innovations spanning a variety of industry needs. SMMs are work-producing, functional materials where energy conversion occurs via a reversible, solid-state phase transformation activated by thermal, mechanical, magnetic, or chemical stimuli. Of these, thermally induced (shape memory effect), mechanically induced (superelasticity), or magnetically induced transformations are the most prevailing forms of transformations and have been observed in alloys, polymers, and ceramics. SMMs have been extensively used in the biomedical and space industry and sporadically in other areas such as aeronautics, automotive, and consumer goods.

Despite wide applicability in various practices, transitioning from designing "the" material to designing "with" the material still faces numerous challenges. Access to reliable SMM data and the ability to quickly view data summaries can help better define current material possibilities and define the focus of future experimental work. Moreover, SMMs possess additional functional properties, compared with conventional materials, such as transition temperatures, transformation strains, work output, blocking stresses, and percent reversibilities all of which are essential for a complete material understanding. Although avenues for obtaining such data are limited, for the most part, these properties can be measured and reported in a standardized format.[2,3] Documentation of such data, however, can only be found in disseminated literature (e.g., journal articles and conference proceedings), books, vendor datasheets, and many cases in laboratories' storage media. Up until now, it has been difficult to comprehensively find and compare existing experimental data to guide the design process, as is done with most conventional materials. This deficiency typically leads to information exchange loss, research duplication, or a general lack of understanding and inability to identify technical gaps.

Another challenge frequently encountered is the cultural paradigm shift when designing with these functional materials. The ultimate goal is to have designers and engineers use SMMs in new devices and applications and acquire the full benefits unattainable with other materials (at least not without some drawbacks). However, conveying data from journal articles or scientific reports to designers without a design-ready set of data could mean added time and resources to interpret such findings. For example, a simple question asking for the yield strength and ultimate tensile strength of these materials is frequently answered by more questions, graphs, and plots. As a result, the benefits of SMMs are often outweighed by prolonged product time and cost to market, hence resorting to design with conventional materials.

In the case of SMMs for actuator applications, it is routinely recognized that some level of training, which is a common technique used to stabilize and set the memory, is required to obtain the desired performance for a given actuator. This process is also highly dependent on the detailed understanding of pedigree such as processing parameters, chemistry and form, etc. A successful use of an actuator material shall consider the history, which, for most SMMs, is not properly documented, nor can it be unearthed with little effort.

It is these shortcomings that form the basis of this work to build a single SMM information system where users can quickly evaluate the current state-of-the-art SMMs and make an informed decision toward an SMM design (material or application design). The tool is a searchable database designed to provide a repository of SMMs where compositional, processing, and property data can be accessible in one place. Moreover, it is

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The ORCID identification number(s) for the author(s) of this article can be found under https://doi.org/10.1002/adem.201901370.

DOI: 10.1002/adem.201901370

the intent of the SMM database tool to identify trends and link elemental compositions to respective thermomechanical properties, enabling a more efficient material down-select to a composition with the desired properties for a given application. Unlike Review articles where significant data are compiled, this database tool is developed with user interfaces to quickly refine and compare substantial datasets based on material: 1) family (e.g., alloys, polymers), 2) elemental composition (NiTi-based, Fe-based, and NiMn-based), 3) test type (e.g., uniaxial constant-force thermal cycling, differential scanning calorimetry, bend-free recovery, and light exposure), 4) production method and processing (e.g., vacuum induction melting, powder metallurgy, and heat treatments), or 5) property's range of interest (e.g., filters). This metadata are linked to respective data points within the database along with reference information to guide the user back to the original work.

Surprisingly, to the best of the author's knowledge, there are no existing SMM databases. Early work by Tang et al.[4] reported on a property database for shape memory alloys (SMAs) mostly focused on the superelasticity of binary NiTi. Similarly, the Medical Materials Database[5] by the American Society for Metals (ASM) International offers some degree of data on nitinol, coatings, and other SMAs used in medical devices. Park and Washington[6] developed a polymers and smart materials database (PSMD) which contained limited SMAs and polymer datasets. Recently, Citrine Informatics[7] through various partnerships has also been working on SMA datasets combined with machine learning algorithms. Other sources such as material datasheets from material producers only offer limited information on commercially available materials but not on materials under research and development. The current work outlines a path to fill this gap by mining SMM properties starting with experimental data. The SMM database tool schema is sufficiently general to accommodate frequent SMM data for most material types, with the flexibility to define new attributes. The remainder of this article will focus on the building blocks of the database tool and methods used to construct each element of the database.

The database tool was designed to store, organize, display, and share experimental data (and associated metadata) for SMMs research dating back to the 1950s. The database tool was structured to accommodate diverse datasets, as shown in **Figure 1**. The following organization was utilized.

Data Capturing (01: Literature and 02: Database): Information such as processing, properties, and source data is collected and archived in a standardized format. These data are in the form of scalar quantities (e.g., temperature, strain, year, etc.) or strings (e.g., authors' names, processing history, etc.) and are captured from external sources such as journal/handbooks, existing databases (e.g., Granta Design, MatWeb, etc.), or internal test programs (e.g., NASA's proprietary data). The pointwise data are then formatted into simplified spreadsheet tables along with their pedigree, which in turn are queued to a multimodel Oracle database management system with records and fields.

Graphical Interface (03: Interface and 04: Selection): A graphical user interface (GUI) is used to access the database. The GUI provides a streamlined architecture to select the material of interest and the desired properties within the database. Given the anticipated large amounts of data, the GUI filters optimize usability by only displaying user-relevant data to quickly browse and perform searches. Python/Dash framework was used for building the GUI and the web applications for this database. The applications along with the database are hosted at the NASA Glenn Research Center to maintain version control and other security and maintenance requirements.

Data Visualization (05: Visualization): One of the main objectives of this database tool is the ability to visualize thousands of data points within seconds. The visual environment is currently presented in at least three forms including 1) 2D scatter plots, 2) ternary diagrams, and 3) pie/bar charts.

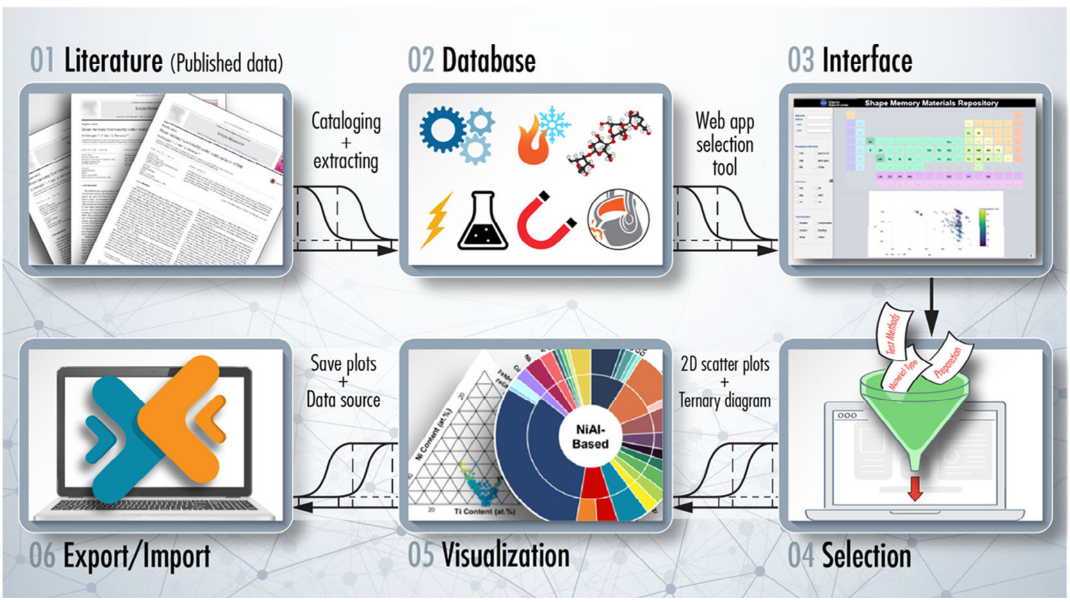

Figure 1. SMM database flowchart describing information flow from extraction, visualization, to data interchange.

In all cases, multiple data sets for a single material type or multialloy/multisystem data can be combined to provide insights and uncover new trends. The 2D scatter plots display any scalar data types with auxiliary dimensions using symbols and colors to clearly communicate large data sets. Similarly, ternary diagrams are used to overlay existing compositional data, with auxiliary colors and symbols to render correlations and trends. Finally, statistical plots in the form of pie, bar, or sunburst charts are displayed with statistical information relating to data sources, years in development, number of articles, etc. Common to all the visual environments, meta information is also displayed by hovering over any given data point within the graphing panels/frames.

Data Interchange (06: Export/Import): The database tool provides a data inflow and outflow using a standardized format. Users can export source data or save the visual plots when available, including the data source and any other relevant information. In cases where data cannot be disseminated

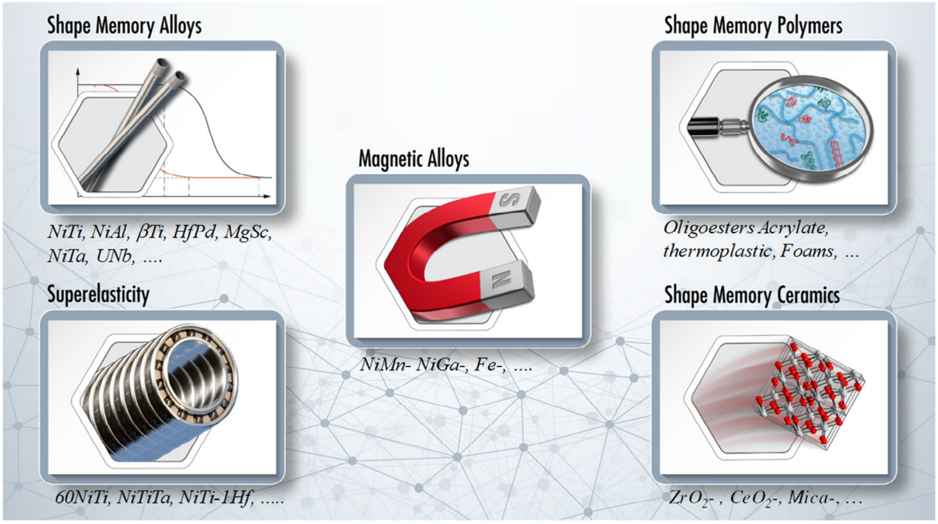

Figure 2. SMM database material types consisting of 1) shape memory alloys, 2) superelastic alloys, 3) magnetic shape memory alloys, 4) shape memory polymers, and 5) shape memory ceramics.

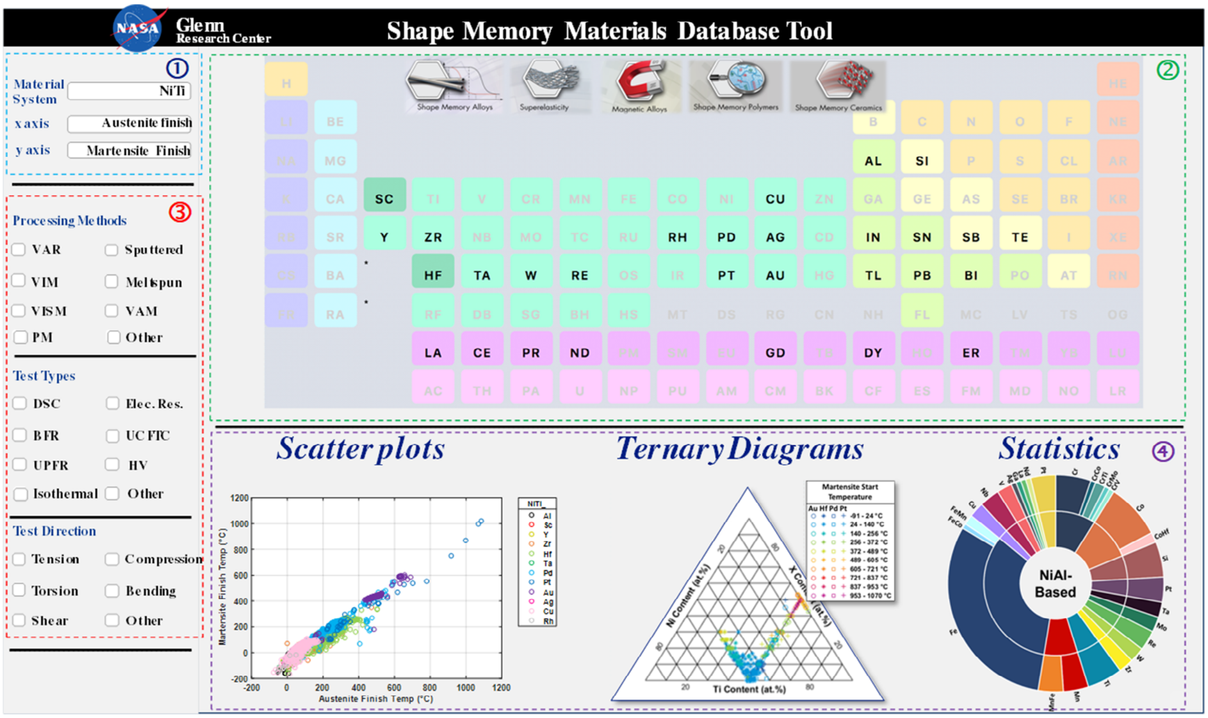

Figure 3. Web-based GUI used to select, filter, and display data. The tool consists of four main panels: ① property selector, ② element selection, ③ data filters, and ④ visualization and data exporting/importing panel.

Table 1. Property data content examples corresponding to SMA material type.

Properties		
Name	Symbol	Unit
Austenite start temperature	A_S	°C
Austenite finish temperature	A_F	°C
Martensite start temperature	M_S	°C
Martensite finish temperature	M_F	°C
Hysteresis ($A_F - M_S$)	ΔT_H	°C
Full width ($A_F - M_F$)	ΔT_{FW} (T_{span})	°C
Yield strength	σ_{YS}	MPa
Maximum strain/elongation	$\varepsilon_{Max}/\varepsilon_{Elong}$	%
Maximum stress/UTS	$\sigma_{Max}/\sigma_{UTS}$	MPa
Unloading strain	ε_{Unload}	%
Austenite start strain	ε_{AS}	%
Austenite finish strain	ε_{AF}	%
Martensite start strain	ε_{MS}	%
Martensite finish strain	ε_{MF}	%
Austenite slope	N/A	% °C^{-1}
Transformation slope	N/A	% °C^{-1}
Martensite slope	N/A	% °C^{-1}
Cooling trans. strain ($\varepsilon_{MF} - \varepsilon_{MS}$)	ε_T^{Cool}	%
Heating trans. strain ($\varepsilon_{AS} - \varepsilon_{AF}$)	ε_T^{Heat}	%
Lower-cycle temperature strain	ε_{LCT}	%
Upper-cycle temperature strain	ε_{UCT}	%
Residual martensite strain	ε_{MRes}^{M}	%
Residual austenite strain	ε_{Res}^{A}	%
Work [($\varepsilon_{AS} - \varepsilon_{AF}$) × σ_{App} × 100]	N/A	J cm^{-3}
Actuation strain ($\varepsilon_{LCT} - \varepsilon_{UCT}$)	ε_{Act}	%
Hardness	HV	HV

(e.g., data rights), the database tool still provides the source information for further inquiries. In addition, data can be imported into the database tool to promote growth and clarify the overall trends and correlations. At this point, only published data can be imported using the import tool.

Five material types are targeted as part of this effort consisting of 1) SMAs, 2) superelastic alloys (SEs), 3) magnetic SMAs (MSMAs), 4) shape memory polymers (SMPs), and 5) shape memory ceramics (SMCs). **Figure 2** shows the material types in the form of interactive push buttons used in the application environment, along with submenus associated with each category. Materials are classified by their base compositional systems or their specific elemental chemistry, allowing for a more systematic and refined search. For instance, SMAs are grouped in alloy bases of NiTi, Cu, βTi, U, etc.; MSMAs are grouped in bases of NiMn, NiGa, Fe, etc.; SMPs are grouped in oligoesters, acrylates, copolymers, foams, etc.; and finally, SMCs are grouped in ZrO_2, CeO_2, etc. Currently, the SE types are only focused on alloys with high nickel content (e.g., 60NiTi alloys) typically sought for tribology, hydrospace, and tool manufacturing usage, whereas medical-grade SE alloys will be addressed further along.

As a first step toward building this database, hundreds of thousands of data points pertinent to several material systems were extracted primarily from journal articles, conference proceedings, and handbooks. Starting with SMA and MSMA, approximately 750 000 entries have been archived covering 16 alloy bases. Emphasis was placed on NiTi-based formulations given the consistent nature of their research and development. Other limited data on SE and SMC also exist, and efforts are ongoing to populate the SMP category.

The application consists of four interactive panels designed to intuitively guide the users through the exploration process (**Figure 3**). On startup, the user is prompted to select the material type discussed previously, which in turn enables the subsequent panels. The first panel, the "property selection" panel (denoted by ① in Figure 3), provides a selection menu for the material system and axis control. For instance, if the SMA material type is selected, options pertinent to alloy bases will be populated in

Table 2. Data filters consisting of 1) processing methods, 2) test types, and 3) test directions.

Processing methods		Test types		Test directions	
Name	Symbol	Name	Symbol	Name	Symbol
Vacuum induction melting	VIM	Differential scanning calorimetry	DSC	Tension	T
Vacuum arc remelting	VAR	Uniaxial constant force thermal cycling	UCFTC	Compression	C
Vacuum arc melting	VAM	Uniaxial constant strain thermal cycling	UCSTC	Torsion	Tr
Plasma arc melting	PAM	Bend and free recovery	BFR	Bending	B
Powder metallurgy	PM	Uniaxial prestrain and thermal-free recovery	UPFR	Shear	S
Thin films	TF	Isothermal	Iso		
Coprecipitation process	CPP	Hardness (HV)	HV		
Sputtering	Sp	Electrical resistivity	Elec. res		
Physical vapor deposition	PVD	Magnetism	Mag		
Slurry casting	SC	Monotonic	M		
Melt spun	MS	Ultraviolet exposure	UV		
		Fatigue	Fat		

the drop-down menu along with any associated data that can be assigned to either the x- or y-axes. An example of property data content is shown in **Table 1**. The second panel is the "element selection" panel (denoted by ② in Figure 3) used to down select from the additional elements associated with a material system. This panel is presented in the form of a periodic table, and only those elements available in the database for the chosen subcategory are highlighted and accessible for use. This section also includes additional features to enable multielement selection such as quaternary or quinary alloys (e.g., NiTi + Hf + Zr) and/or multibase data comparison from different material systems (e.g., NiTi-based vs CuAl-based alloys). The third panel is the "data filters" panel (denoted by ③ in Figure 3) currently divided into three sections consisting of 1) processing methods, 2) test types, and 3) test direction. These filters essentially establish property constraints to streamline the material down-selection and exploration process. In addition, some of the meta-information is used in this panel to help provide additional insights. If the data were obtained using standardized practices such as the American Society for Testing and Materials (ASTM), a filter will be provided to only display data that conform to such practice. Examples of these filter parameters are shown in **Table 2**. Finally, the "visualization" panel (denoted by ④ in Figure 3) is where all the data records are displayed in 2D scatter plots, ternary diagrams, and pie/bar charts. Each plot is equipped with data navigation tools, color legends, and a tooltip that displays pedigree information and annotations when hovering over a data point. Once the exploration phase is satisfied, plots and formatted data files can be saved and exported.

The application also contains a formatted importer tool that allows any user to upload new records/pedigree to the database tool. The importer provides a preallocated header file to add new data points and new fields if necessary. The data importing process is not currently instantaneous; rather, the submission is reviewed by the application administrator and accepted after a quick assessment (e.g., verifying publication records, spurious data, etc.). Other supplementary features such as definitions, nomenclature, and standards will also be incorporated into the main application architecture.

Because SMAs were the initial focus of this project, it contains the most extensive data pool and will be used to provide preliminary examples. The sunburst diagrams shown in **Figure 4** offer a statistical overview of the number of research articles published in the NiTi-based and Cu-based SMA systems, 1290 and 2094 articles, respectively. The degree of study (i.e., articles published) for specific compositions within each base system is represented by the hierarchy moving outward, which corresponds to elemental additions of ternary, quaternary, and in some cases quinary alloys. Experimental data sets for the NiTi-based, Cu-based, and 14 other base SMA systems have been organized with this compositional hierarchy, which serves as a quick approach to visualize the available data records within the database tool.

In a similar approach, the timeline chart in **Figure 5** shows the number of publications per year studying each base in the SMA system. Although this timeline generalizes the compositional details shown in Figure 4, it offers a unique perspective into the history of the SMA research field, highlighting key breakthroughs and the shifting scope of compositional focus overtime.

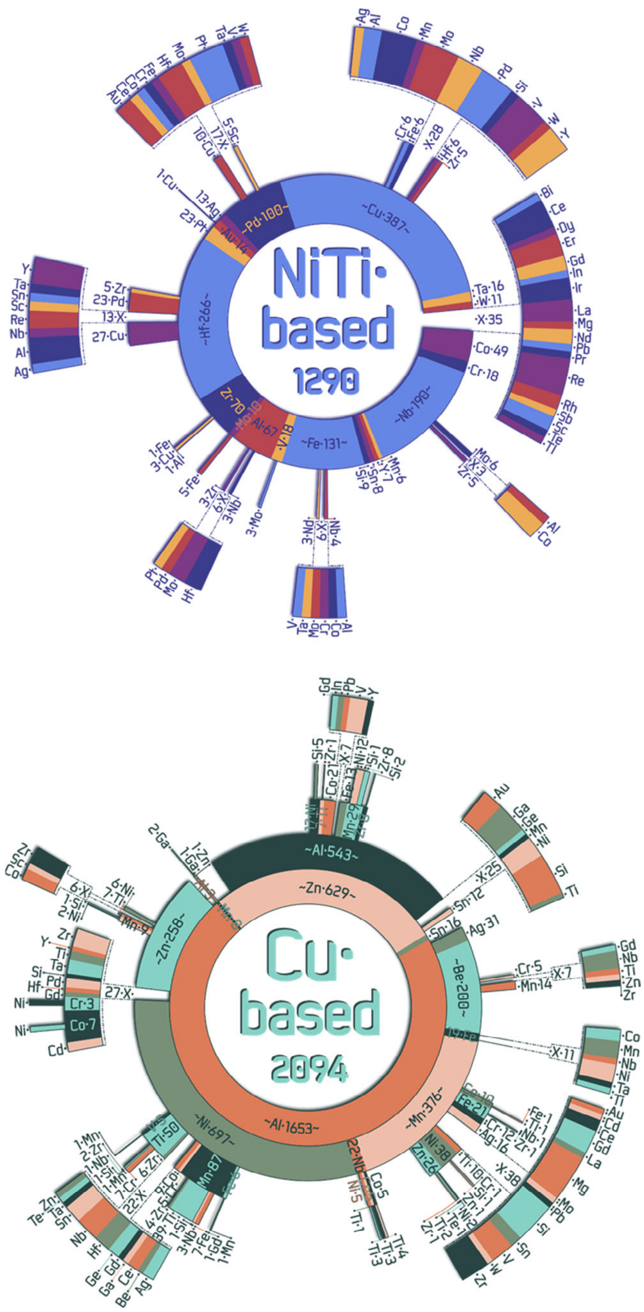

Figure 4. An example of multilevel sunburst diagram corresponding to the NiTi- and Cu-based alloy systems. The digits next to each element indicate the number of articles currently in the database tool. The elements in the innermost circle represent the base material. The next circle represents the first elemental addition (e.g., ternary NiTi + Hf). The outermost circle represents the last elemental addition (e.g., ternary NiTi + Hf + Pd). Where space was not available, an expanded wedge is displayed labeled by "X."

For example, it highlights how the Cu-based alloy was the primary focus in the 1980s and dominated the literature through the early 2000s, NiTi- and Fe-based alloys took off in the 1990s, and βTi research surged around the 2000s. These trends are generally associated with changing industrial demands as new products and requirements emerge.

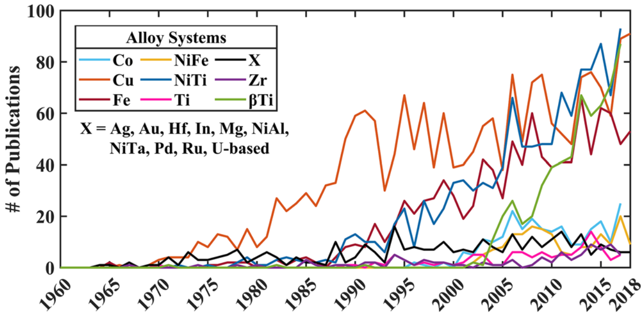

Figure 5. A timeline showing the number of articles published per year from 1960 to 2018 for various SMA systems.

The 2D scatter plots are the central tools used for data visualization. Any property can be plotted for hundreds of alloys to reveal trends and relationships in a matter of seconds. One example is mapping compositions to thermomechanical properties to not only validate known trends, but also quantitatively correlate transformational properties to elemental additions on an unprecedented scale. **Figure 6** shows a relationship between martensite finish (M_f) and austenite finish (A_f) for select NiTi-based alloys (Figure 6a) and CuAlMn alloys (Figure 6b). Although the effect of some elements is apparent in some cases, having a tool that can compare element to element, render overlaps, and provide a clear trend for these properties can prove to be indispensable from an alloy design perspective. This kind of plot

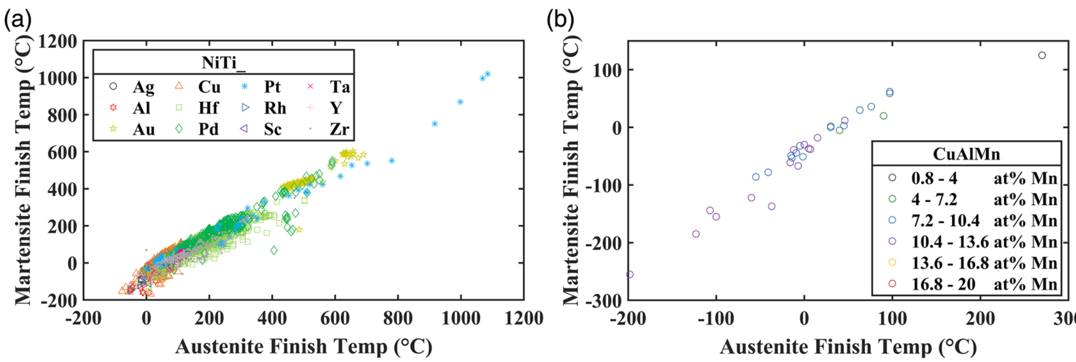

Figure 6. Scatter plots showing a relationship between martensite finish (M_f) and austenite finish (A_f) for a) NiTi alloys and b) CuAlMn alloys.

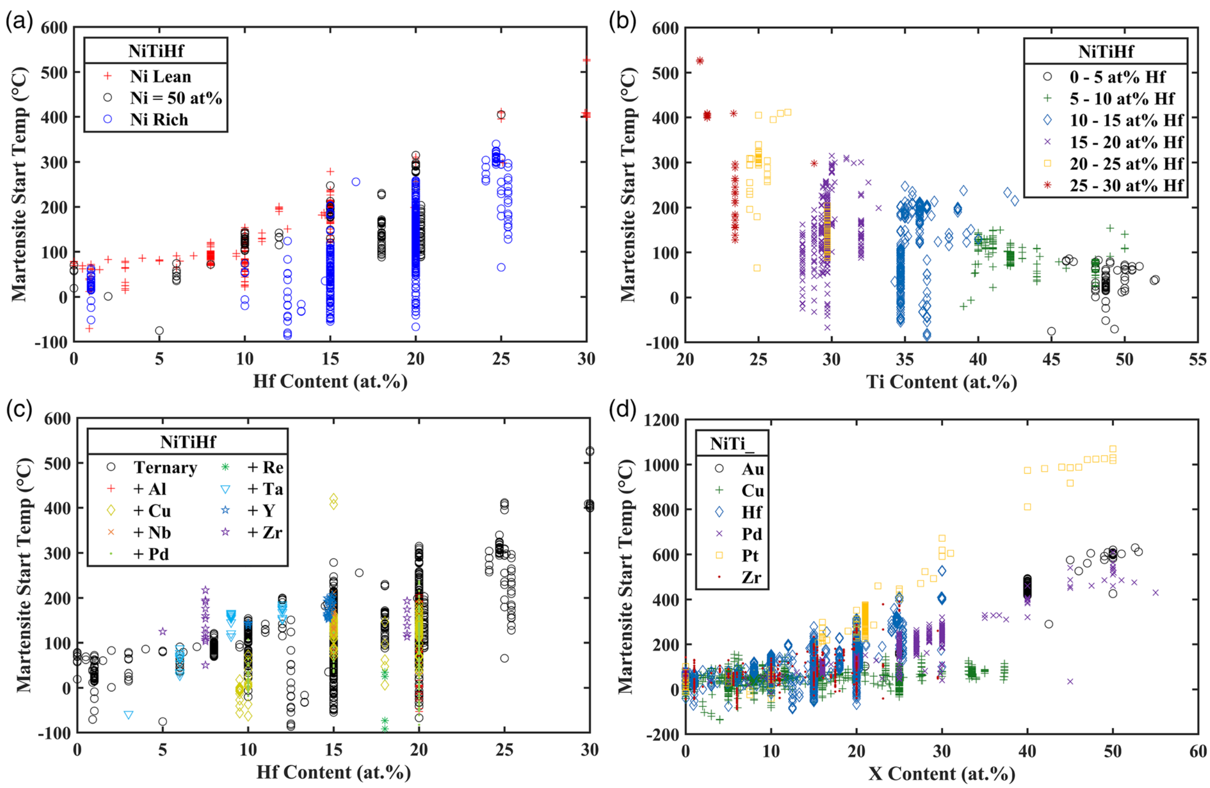

Figure 7. Examples of 2D scatter plots displaying the effect of a) Hf content, b) Ti content, c) quaternary elements on martensite start temperatures (M_S) in the NiTiHf alloy system, and d) the effect of ternary content on M_S in the NiTi + (Au, Cu, Hf, Pd, Pt, Zr) alloy systems.

also serves to identify key gap areas and guide researchers and explorers to embark on a new discovery with uncharted antecedence. In this particular example, if a user necessitates an alloy with the characteristic temperatures (M_f) and (A_f) in the range of 600 °C, the search can be quickly refined by ruling out any Cu-based alloy, and focusing on the NiTi-based system with Au and Pt additions.

Once a temperature range is identified, other example 2D plots can be used to assess the effects of chemical content (**Figure 7**a), ternary additions (Figure 7b), quaternary elements (Figure 7c), and multialloy data from multiple NiTiX systems (Figure 7d). An extension to these 2D plots can be used to create characteristic material functional or performance indices, as demonstrated by Arnold et al.[8] These material selection charts can be used to compare specific attributes across multiple alloy systems and bases. In these examples, if a multisolution exists for a given temperature range, other factors such as strains, forms, or cost can be evaluated and refined.

Finally, ternary diagrams pose additional benefits to data analytics by offering a more complete portrayal of each alloy's elemental composition, while coloring data points based on alloy properties. In the ternary diagrams shown in **Figure 8**a–d, colored data points are plotted to corresponding compositional coordinates, generating property "heat maps" that embody and validating known trends across several NiTi-based alloy systems. For example, Cu and Hf are known to decrease hysteresis (Figure 8a) and increase transformation temperatures (Figure 8b) when alloyed with binary NiTi, respectively; Figure 8a,b quantitatively links these property shifts to elemental compositions on an unprecedented scale and enables designers to easily pinpoint compositions that meet design constraints, before delving into empirical work. The plotting capabilities within the database also extend to ternary diagrams that include multiple ternary systems (Figure 8c) or quaternary alloying additions (Figure 8d). Additional data visualization tools will be implemented into the database as it develops further.

As the SMM field continues to grow, there is an unwavering need for efficient ways to archive, track, and explore the data produced from SMA research. The goal of the SMM database tool is to establish the infrastructure for building an information system where individuals on a continuum from experts to novices can explore, discover, and design with these multifunctional materials. The database tool provides an intuitive GUI experience encompassing five material types, approaching one million recorded data entries. The tool includes SMAs, SEs, magnetic alloys, SMPs, and SMCs. In this work, a description of this framework was provided along with examples and usage. A systematic guide on each module of this tool helps to introduce

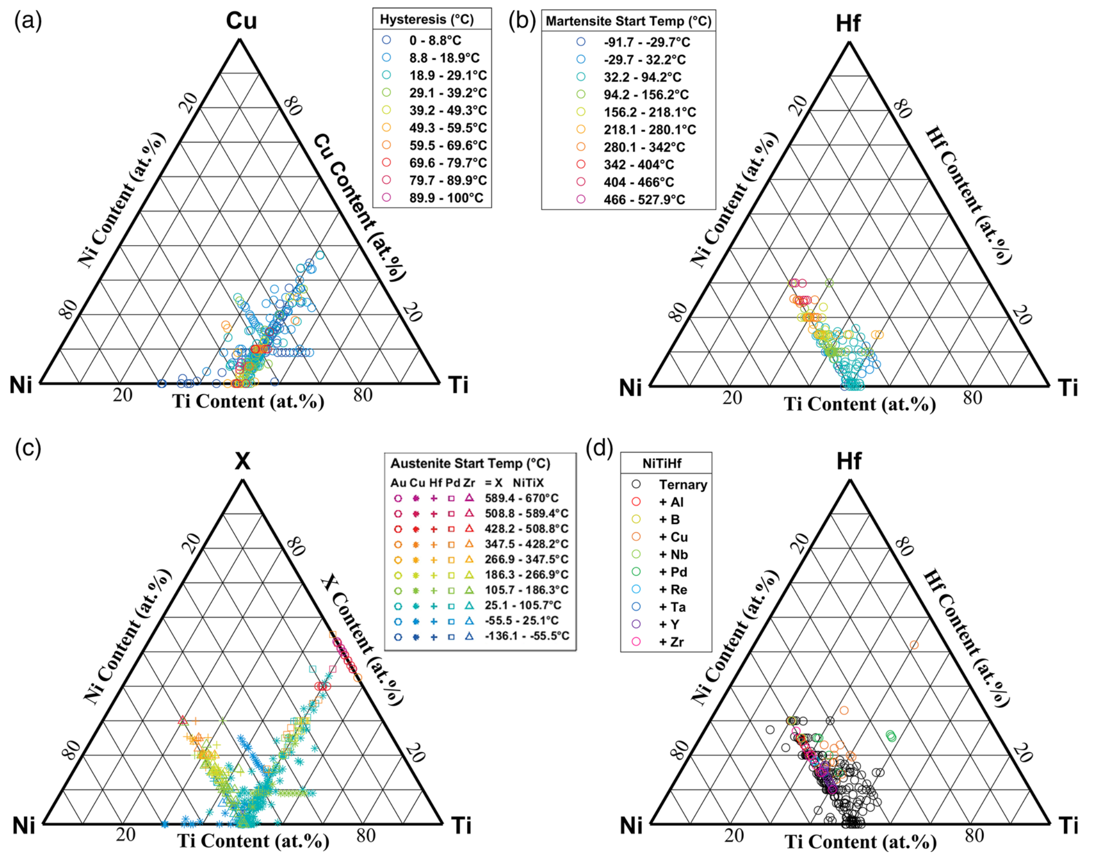

Figure 8. Ternary diagrams showing compositional representation along with color maps and symbols corresponding to a selected property. a) The effect of composition on hysteresis of a NiTiCu alloy, b) effect of composition on transformation temperatures of a NiTiHf alloy, c) effect of ternary additions on transformation temperatures, and d) effect of quaternary additions based on site preferences to base NiTiHf alloy.

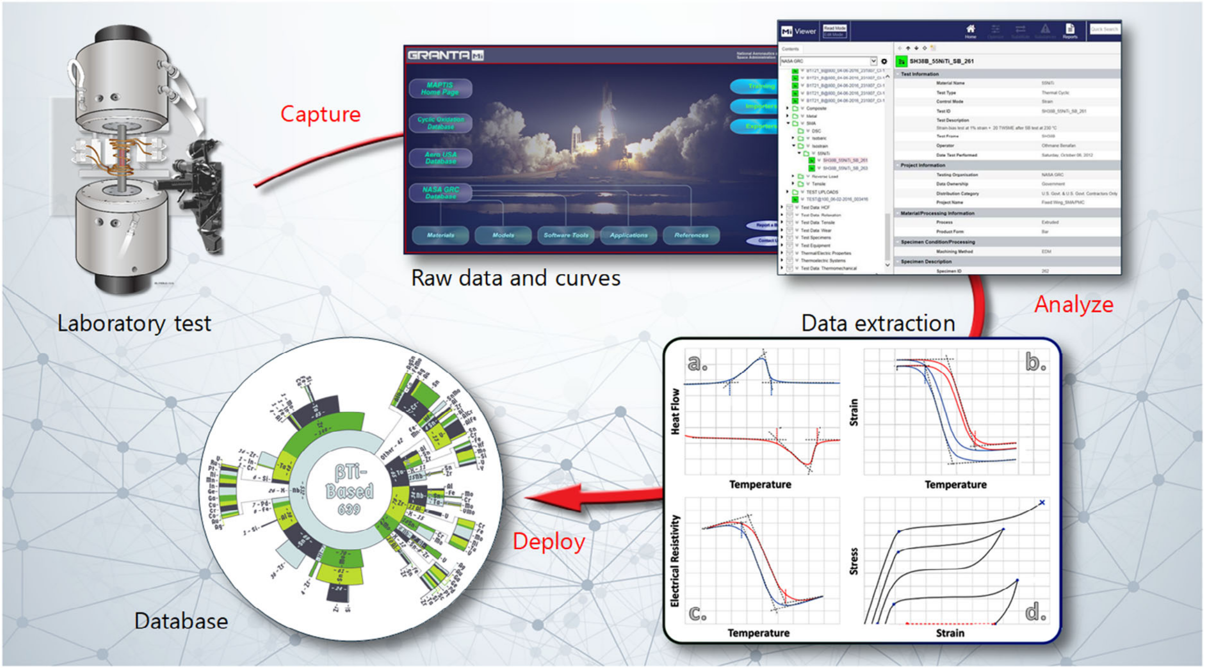

Figure 9. Process flow illustrating the SMM database vision that includes a bridge between laboratory tests, raw data archiving, standardized data parsing, and finally the work described here regarding the database tool.

interested users to this new framework and more importantly serves as an invitation to the shape memory community to join and contribute to this effort.

Although additional work is ongoing to advance this database tool, the ultimate vision aims toward a more comprehensive material management system. It is acknowledged that pointwise data and pedigrees alone will not suffice to fulfill the growing materials informatics needs such as the integrated computational materials engineering (ICME) and machine learning, among others. Consequently, plans are under way to expand the current tool into a SMM management system that captures the full response spectrum of the raw data (pointwise properties, curves, loading history, pedigree, etc.), standardized methods used to extract the data, and traceability for certification, through the process flow shown in **Figure 9**. This process is consistent with the four stages of the material data life cycle, as defined by the material data management consortium,[9] i.e., capture, analysis, disseminate, and maintain. Starting with raw data curves from laboratory test frames, there shall be a schema in which such data can be archived and classified based on test types or other decrees. Examples of such a structure is the NASA Glenn's customization of GRANTA MI Materials Information Management System,[9–11] where currently SMA attributes and tables have been developed and are ready for receiving data. Next, this raw data shall be parsed using standardized tools and methods, as described by the ASTM International or other established standards development organization. Unfortunately, as of today, there exists no such toolset to extract the data, resulting in each laboratory using their own methods to fit, extract, and report data values and accuracy. As a result, renewed efforts have commenced to develop shape memory modules targeted to uniformly and consistently extract SMM data from raw curves.

As is the case for most materials, SMM data analyses are often bound by subjectivity due to the nature of that data, in which case the users are the best intermediary to interpret the information. Only when such data are extracted and compiled, can the database tool be used to visualize and plot trends and relationships.

In addition, the authors have recognized the need to not only visualize the data, but also exploit the data. Machine learning is beginning to make enormous inroads within the SMMs arena, and it can serve as a powerful tool for research and discovery.[12–14] The current database tool can be a seed to such platforms with large amounts of data to accurately train the models and aid in improved predictions. This effort is currently being explored with external collaborators.

In closing, this database tool will be disseminated via NASA web applications to be deployed in 2020.

Acknowledgements

Funding from the NASA Aeronautics Research Mission Directorate (ARMD) Transformational Tools and Technologies (TTT) project is gratefully acknowledged. The authors thank several individuals who have contributed or are currently contributing to this effort including B.J. Ruffridge, C.R. Robinson, S.A. Bostic, and B.R. Weborg from the NASA Information and Applications Office. O.B. acknowledges useful database discussions with S.M. Arnold and F. A. Holland, and T.K. Condrich for graphical illustrious.

Conflict of Interest

The authors declare no conflict of interest.

Keywords

databases, data mining, machine learning, NiTi, shape memory alloys, shape memory materials

Received: November 7, 2019
Revised: February 10, 2020
Published online: March 1, 2020

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