

Communicating Materials Systems Knowledge through Processing-Structure-Properties-Performance (PSPP) Maps

A. N. Goulding^{a,b}, J. F. W. Leung^a and R. W. Neu^{a,b}

^a School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332

^b George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332

Keywords

Materials design, Processing-Structure-Properties-Performance relationships, Additive manufacturing, Ni-base superalloy

Abstract

Knowledge about the behavior of a specific materials system is concisely summarized in a Processing-Structure-Properties-Performance (PSPP) map. This is a useful tool that can effectively serve as a standard method of communication regarding the physical and chemical mechanisms that control the performance of a materials system, and gives guidance on the type of data required to accurately characterize that materials system in its entirety. This article describes a workflow to generate a map for any materials system, and then applies these steps to develop a map for Ni-base superalloy synthesized by additive manufacturing.

Introduction

In 2011, the White House announced the Materials Genome Initiative (MGI) to find ways to discover, develop, manufacture, and deploy advanced materials systems faster and more cost-effectively¹. It typically takes tens of millions of dollars over two decades to fully develop and qualify a new material for a critical application². This trend applies broadly to all materials systems, and implies that it is the materials design process itself that must change, if efficiency is going to be achieved. To decrease by half the time and cost of discovering, developing, and optimizing materials systems, the MGI calls on the materials community to embrace open innovation, and to change the process so that design steps can be done concurrently or in a more integrated way. To achieve this, the initiative further proposes that researchers integrate experimental test methods, computational tools such as inductive design exploration methods, and known knowledge databases to focus efforts on data driven approaches to materials design. As a result, the materials innovation ecosystem now involves computer scientists, data informatics, and system-design engineers who may have less knowledge and understanding of the complexities of a particular materials system than more seasoned materials experts.

Foundational materials science and engineering courses today still tend to emphasize "good science", as defined by "reductionism," rather than "good materials," which emerge when engineering, manufacturing, and economic factors are included in the mix. The science of materials has reached a level at which it now can radically change engineering practice. To be successful, a healthy mix of reductionist and systems viewpoints is needed. Much of this communication goes back to how materials science and engineering is traditionally taught, not as a systems-design problem, but as reductionism, a bottom-up scientific approach.

Students are invariably shown that the materials paradigm can be represented in a form of a tetrahedron, as that shown in Figure 1, with the corners representing the four-element paradigm of modern materials science and engineering. This representation is a highly ineffective way to impart the knowledge of how these entities of the materials system are logically linked. In a foundational course, pieces of these linkages are discussed from a reductionism point of view, but students often do not see the complete big picture, or "the system," that each material embodies. In 2008, the National Science Foundation (NSF) identified the reductionist tendencies in undergraduate materials science curriculum as a key limitation to integrated, systems based materials education³. The NSF found that core undergraduate materials education courses: thermodynamics, kinetics, and phase diagrams underpin the primary science of materials, while the supplemental courses in synthesis, structures, and properties form the corners of the materials paradigm. A limitation of this approach is that the supplemental courses are often approached from a "vertical" material application specific standpoint which limits student's ability to identify the relationships among process, structure, and properties within the materials system. As materials system become increasing complex and multidisciplinary, materials education should reflect this change with a "horizontal" approach highlighting fundamental drivers and multiscale linkages inherent in each materials system.

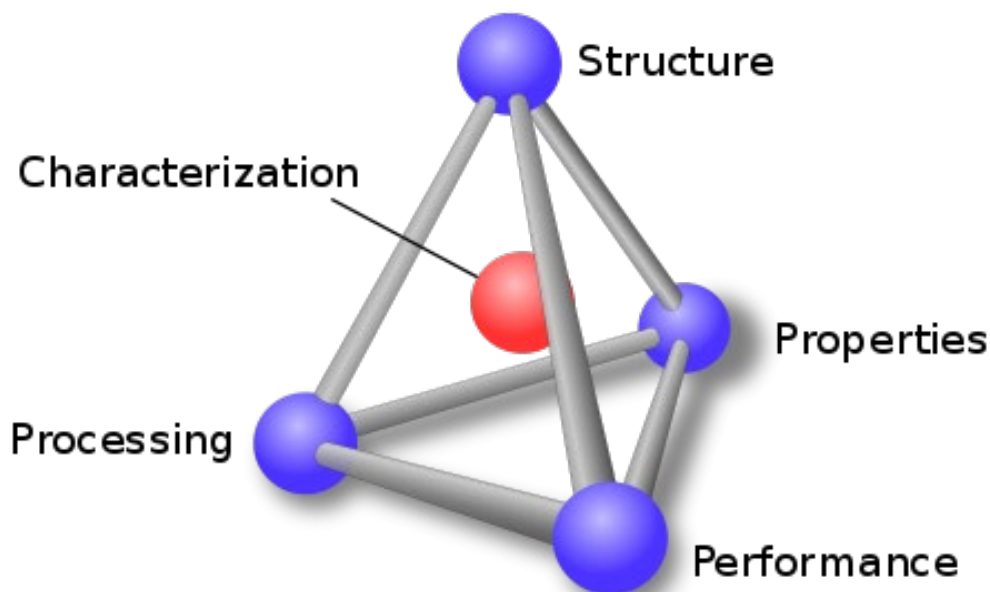


Figure 1: The materials paradigm represented in the form of a tetrahedron⁴

An example of an improved visual aid that carries vastly more information is shown in Figure 2. This "Systems Design Chart" was developed and used by Olson⁵ to successfully accelerate the development of new materials. This Processing-Structure-Properties-Performance map is a

critical exercise to understand the problem and the performance requirements. This is analogous to Quality Function Deployment (QFD) tools used to design engineering systems that are used to call attention to the customer needs. By bringing the needs of the consumer to the forefront of the engineering design process, QFD tools have created a structured approach to define consumer requirements and translate them into engineering attributes that meet the consumer needs. In a similar manner the “Systems Design Chart” brings the Processing-Structure-Properties-Performance linkages to the forefront of the material design process so the materials engineer can clearly see the key linkages that govern the materials system and use this knowledge to design and optimize the materials system by exploring the functional relationships between the processing attributes, structure, and properties. The value of such a tool is that it is a sensible framework for *efficient knowledge exchange* of a complex paradigm in a comprehensible way.

This framework can be effectively captured and expanded with Processing-Structure-Properties-Performance (PSPP) maps to guide materials design and materials education. Structure describes all scales of hierarchy from the atomic to macroscopic. Properties depend on this structure, while the multiple processing steps govern this structure. While design of materials today typically focuses on optimizing a few of the most important linkages, capturing the entire system provides engineers and scientists added insight, and perhaps inspires new ways to achieve the desired improved performance more efficiently and avoid missed opportunities. A PSPP map also has the important utility of identifying what pedigreed information must be captured in the metadata for materials data curation systems. Thus, the PSPP map is an important communication tool that should evolve as new knowledge is gained regarding a materials system.

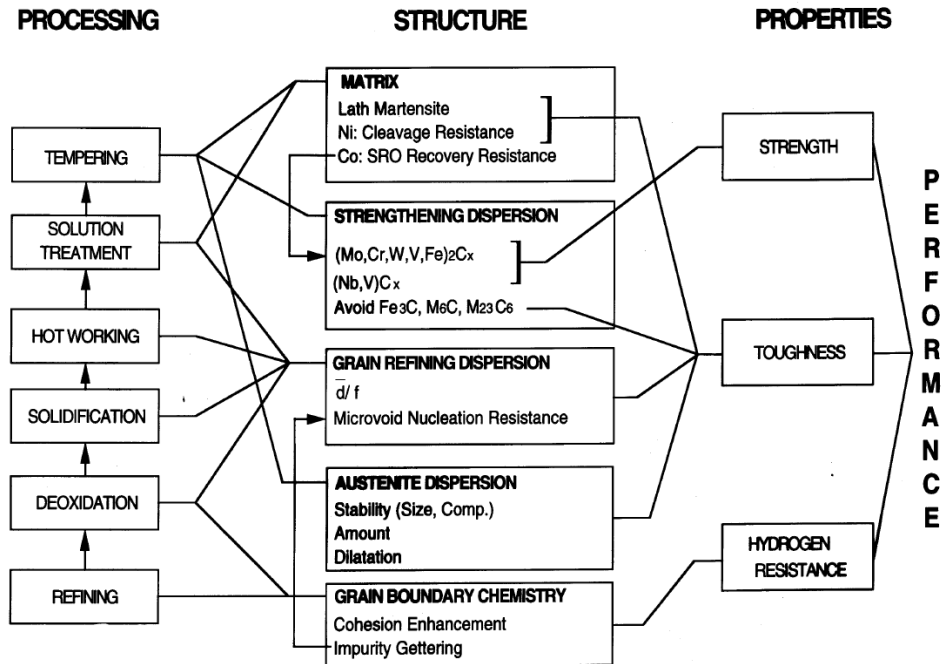


Figure 2: "Systems Design Chart" flow-block diagram generated by "Olson"⁵ to guide materials design

PSPP maps represent (1) key microstructural subsystems, (2) the primary links of these subsystems to the properties they control, and (3) the stages of processing that govern their dynamic evolution. Only after generating these maps, can systems analysis be applied to identify and prioritize key Processing-Structure (PS) and Structure-Properties (SP) relations. As suggested

by Olson⁵, "Often, part of this exercise involves some additional modeling or empirical data gathering to fill gaps in the knowledge required for making practical decisions about composition and processing details". In the same way, each confirmed linkage can be representative of a model that correlates the two blocks, where a multitude of linkages highlights the suite of models that are required to accurately predict the morphology of the materials system and the relationships between processing, structure, and properties.

This method has been successfully used by QuesTek Innovations to develop new alloys with unprecedented sets of properties, while this systematic procedure greatly reduces the amount of costly experimentation in traditional materials creation⁶. As an example, QuesTek materials designers reach their target metal using only a few actual melts to refine the computation-heavy design efforts. More recent efforts by QuesTek Innovations have shown the application of the system design chart in conjunction with computation modelling to reduce the qualification time of aerospace alloys⁷.

This paper advocates that the materials community more broadly use PSPP maps to convey this knowledge. This is similar to how Ashby's deformation mechanism maps in the 1980s helped students, engineers, and industrial clients graphically see the relationships among stress, temperature, deformation rate, and structure in a clear way⁸; and in the 1990s when property charts⁹ were used to graphically convey the relationship among properties to deal logically with conflicting objectives and accelerate the materials selection process⁹. With the adoption of Property Charts by software tools like CES EduPack by Granta Design¹⁰, these aforementioned tools empowered students to easily convey materials knowledge. Both are now ubiquitous tools used in the undergraduate curriculum worldwide. Now the materials design process needs to be addressed in a similar graphical way. Moreover, this communication of information is needed for establishing a "materials definition" that enables the designer of components to tailor the processing and structure to achieve spatially varying properties to improve performance. PSPP mapping provides the backbone for the materials definition and materials knowledge.

Generating a PSPP flow block system diagram (mapping) is the first step necessary in an effective and efficient design-based system approach to materials. Surprisingly, even after Olson demonstrated its utility in designing new alloys, the use of PSPP maps in materials design and instruction of future materials scientists and engineers is scarce in the literature and online instruction. We hypothesize that this can be overcome by clearly establishing the protocols for generating a PSPP map, which leverages the known knowledge database of the materials system to clearly and visually communicate the relevant variables and the various relationships.

This paper describes a workflow for creating PSPP maps to serve as a communication tool for both students and practitioners. Here we detail a generic workflow that a cartographer can follow to create a map for any materials system, and then illustrate the application of the workflow by creating a map for an age-hardened Ni-base superalloy fabricated by additive manufacturing targeting the performance required for high temperature applications. This paper is divided into three parts that synergistically address the need for effective and efficient material design, from developing the workflows to help students and engineers organize and communicate materials knowledge, to exercising the workflow for a current materials system, and then addressing how these strategies can enhance materials engineering education and the materials engineering community.

Workflow for Constructing a PSPP Map

A possible strategic workflow for creating a PSPP map has been defined by us recently¹¹. The building of the maps begins with identifying the required *Performance* of the targeted application, which dictates the *Properties* column. Under the *Properties* column, the cartographer should begin by listing the fundamental material properties required of the targeted application, which is derived from the performance profile of the materials. It is recommended that the properties initially be listed and enclosed individually. Following the *Properties* column, the *Processing* column is generated. The attributes of the *Properties* and *Processing* columns provide the boundary conditions constrained by the targeted application and known processing routes for the materials system, respectively. This workflow is graphically presented in Figure 3.

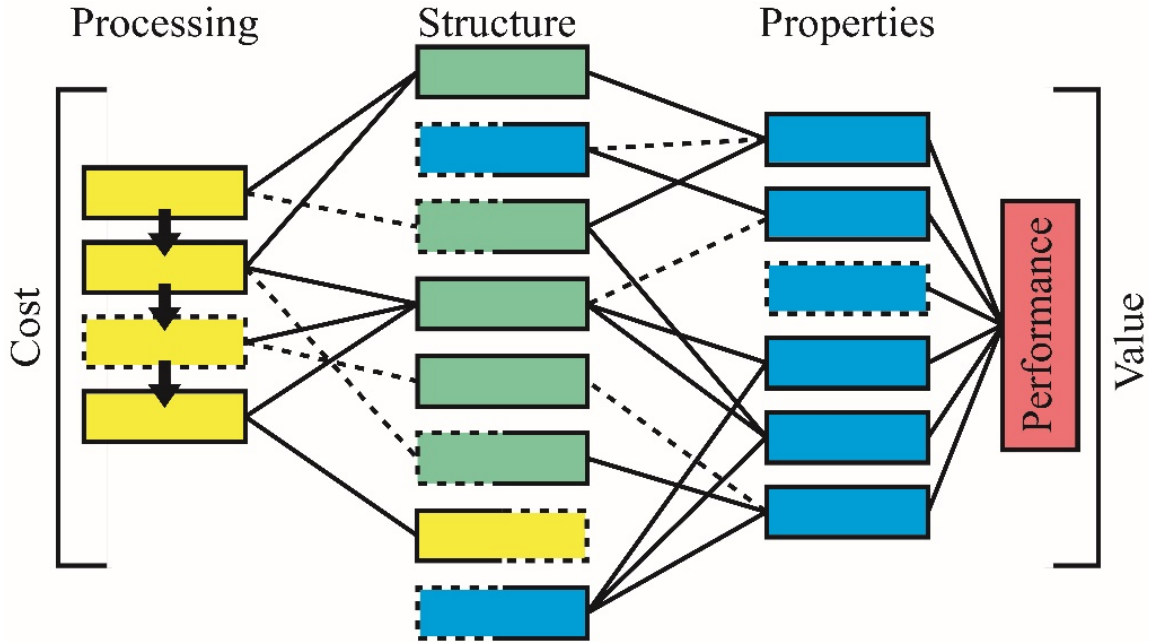


Figure 3: Generalized PSPP map exemplifying various conditions of the structure list

Under the *Processing* column, it is recommended that the cartographer begin by listing all the available or currently known processing steps involved in the production of the material defined by the system suitable for the targeted application. Each processing step should be blocked, and within each block the variable parameters involved with the step can be listed. When the processing route contains two possible steps that are mutually exclusive, they must either be redefined so that they can be included together in one block or streamlined to a specific processing route. The *Processing* column should consist of a set of sequential steps that constitute the entire desired processing route starting usually with the elemental composition or raw material stock. It is important for the *Processing* column to contain all directly controllable processing parameters involved in the making of the material being characterized. If there are overarching processing stages which involve interrelated steps, they can be grouped to highlight the key stages in the processing of the material, which is particularly important for complex systems.

After the *Properties* and *Processing* columns have been detailed, the various structural features of the material, which are controlled through the processing, can be listed, each in a separate block. The cartographer should begin by examining the elements listed in the *Processing* column and generate a list of structural features that are influenced by each processing step and their parameters. The structural features can be blocked either individually or in relevant

groupings depending on the level of detail that is desired. It is useful to categorize the structural components based on the scale of structural feature, from nanoscopic to mesoscopic length scales, to ensure that the structural hierarchy and associated physical and chemical mechanisms at each length scale are represented within the structure blocks. Additionally, the categorization of structural components allows the cartographer to understand the different microstructural characterization length scales that are required to accurately capture the microstructure features, thus guiding the scale of computational models and experimental tests that can be developed to fully define the structure space. Similarly, the *Properties* column, if the cartographer is unsure of which structural elements would be well suited to grouping, it is best to leave them blocked individually until the first iteration of the map has been detailed. Likewise, if the relevant structures are unknown at this time, the map can begin with general structures of the alloy system and refined in each subsequent mapping.

After the elements in the *Structure* column have been identified, the known and expected linkages between the blocks in the three columns are mapped, as shown in Figure 3 **Error! Reference source not found.** The primary linkages are between either *Processing-Structure* (PS) or *Structure-Properties* (SP). If a relationship between an element in one column and an element in an adjacent column is known, a solid line is used to connect the blocks. Known attributes and relationships, which may include knowledge from physical or mechanistic models, computational simulations, reduced-order models, and experimental or empirical knowledge can be used to verify the known linkages. If two blocks are known not to share a relationship, no line should connect them. If a relationship is expected, but not confirmed, a dashed line is used. The presence of a dashed line is useful to indicate that a relationship between these blocks is expected, but that further work must be done by either the cartographer to gather more information from the literature or the materials science community to solidify the relationship.

Once all the known and unexplored relationships are indicated on the map by following the above steps, the first iteration of the map should be complete. If the cartographer is unsatisfied with the size or scope of the materials design space, the cartographer can iterate through the steps detailed above by adding, combining, or dividing blocks as necessary until the desired level of specificity is obtained. Once the map has been detailed, targeted exploration can be used to solidify those unconfirmed relationships as indicated by dashed lines and blocks. Each relationship possess different drivers thus various methods can be used to confirm each linkage. As discussed by McDowell et al.¹², while traditional materials systems information is contained in literature and databases, to qualify presumed linkages of other materials systems may require an integration of methods which may include high-throughput computational or experimental methods¹³, mechanistic models, simulation-based models, data-driven and materials informatics methods¹⁴, and design of experiments tools. To support the efficient verification of linkages, robust and systematic system design methods, such as factorial design and response surface methods¹⁵, can be implemented to leverage the power of the computation and data-driven tools. Using these statistical techniques, the functional relationships between various blocks can be approached sequentially through design of experiment techniques to efficiently explore and verify PS and SP linkages.

Financial considerations, including cost and value are important system features that should not be neglected within the PSPP framework. Although, cost and value may not be a rigorously defined intrinsic property like Young's modulus, yield strength, thermal conductivity, etc., cost and value are nearly always considered during the primary selection and comparison of different materials systems. Ashby suggests that value of materials systems is driven by “market pull” and “scientific push”. As market trends change and scientific advances are made, the perceived value of a materials system will change which dictates the application of the materials system, which is

reflected in the *Performance* column of the map. The value of the system will inherently seek to optimize the cost of materials system, which, within the PSPP framework, are directly impacted by the chosen *Processing* route. Similar to value, cost will bound the scale, scope and complexity of the *Processing* route. To highlight the financial considerations associated with all materials systems, the cost and value are presented as open bounds on the *Processing* and *Performance* columns to indicate their limiting effect on materials systems and materials selection.

Illustrative Example: PSPP Map of an Age-hardened Ni-base Superalloy Fabricated by Additive Manufacturing

Utilizing the aforementioned general guidelines for the PSPP map creation, a map is created for a Ni-base superalloy processed by additive manufacturing (AM) targeting the performance required for hot section components in gas turbine engines. Additively-manufactured metallic components are fabricated through the sequential deposition of metallic alloys to build up to the desired component geometry. For hot section metallic components, particularly Ni-base superalloys, additively-manufactured parts can be constructed from a powder bed fusion AM process where a powdered alloy is fused through controlled melting of the powder by either selective laser melting (SLM) or electron beam melting (EBM). AM is a preferred method for manufacturing high-value components by increasing materials utilization while reducing scrap materials¹⁶, which is critical for the gas turbine components located in the hot section. One of the key issues that arises from AM is the variability in thermal history of additively-manufactured components and its impact on the material properties due to spatial variations in the microstructure.

The PSPP map is an effective tool to aggregate results from AM studies to determine the underlying linkages within the materials system and the structural heredity of this complex manufacturing technique. The PSPP map is a flexible framework that can be adapted to highlight the similarities as well as identify the differences between conventional and AM processing methods. By doing so, the engineer of materials system can better understand the unique structures that are formed in AM and their impact on the performance profile of the additively-manufactured component.

This exercise evaluates Inconel 718 (IN718), a highly weldable, age-hardened Ni-base superalloy¹⁷ that is routinely used in powder bed fusion AM. Unlike most alloys that soften at elevated temperatures, Ni-base superalloys retain and even increase in strength as temperature is increased up to a limit, typically up to about 700°C for IN718 depending on processing and heat treatment¹⁸. Here, the application of IN718 in hot sections of gas turbines is considered for determining the performance profile.

Performance Profile

For this PSPP map, the yield strength, ductility, and viscoplastic (creep) response are properties that define the performance profile targeting components in the hot section of gas turbines. These properties blocks are shown in Figure 4. Yield strength measures the maximum stress that a material can withstand prior to plastic deformation, which is a useful measure of the operating limits for the materials system. Ductility is an indicator of the extent of plastic deformation in the system and the material's ability to strain without fracture. For IN718 ductility can be used as a surrogate fracture resistance. The viscoplastic response of IN718 is primarily associated with creep deformation, which is an important behavior that needs to be minimized for rotating components operating at elevated temperatures.

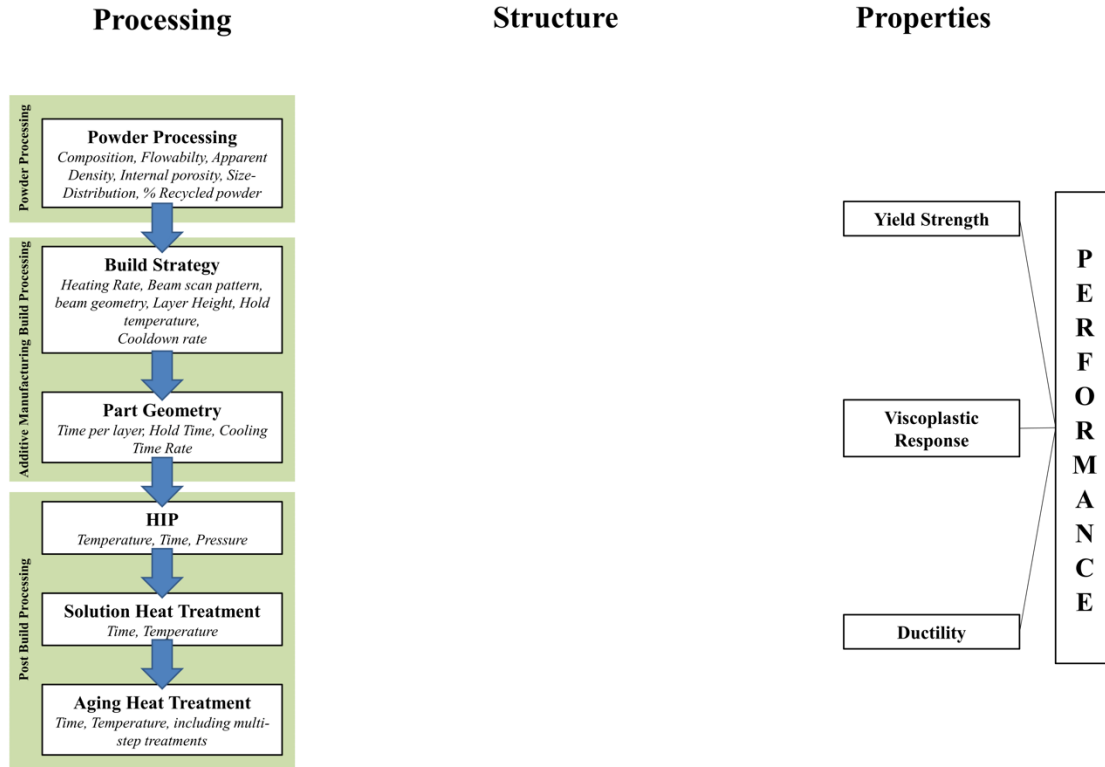


Figure 4: Processing and Properties columns for IN718 fabricated by AM targeting hot-section gas turbine components.

Processing Steps

For additive manufacturing of aged-hardened Ni-base superalloys via powder bed fusion, the processing can be divided into three main stages, as shown in the *Processing* column of Figure 4, with several possible processing parameters for each: (1) the processing of the metal or alloy powder, (2) the additive manufacturing "build" processes of shaping the component, and (3) post-build processes aimed at improving mechanical properties. The variations within the build parameters creates structural variability for each unique AM build. Here, we have focused on a general AM build process that reflects the most recent literature regarding the EBM fabrication of IN718 components.

For powder bed fusion methods, the first step is the processing of the powder, which can be either alloy powder or pure elements. Typically for additively manufactured IN718, alloy powder is used. The specific powder, which acts as feedstock for powder bed fusion AM, is refined to a specific particle size, particle distribution, morphology, and density. The powder process method can create internal porosity or entrapped gases within the powder, both of which can influence the retained porosity in the build. Another factor that influence the quality of the powder process is the percent of recycled powder that was not melted in a prior build step. This recycled powder may have a less spherical and more irregular morphology that can affect its flowability¹⁹.

The next two processing steps relate to the build parameters and influence of the part geometry. Build strategy is an encompassing step that describes the heating and subsequent melting¹⁹ of the

powder by the electron beam to form each solid build layer. For EBM the build strategy process can be divided into two sub-processes: powder coalescence and EBM. Powder coalescence involves the spreading of a powder layer, 50 to 200 μm thick²⁰, and applying a low energy electron beam pass to pre-sinter and adhere the powder into a solid structure²¹. This step ensures that the powder does not ionize and scatter during selective EBM. Powder scattering reduces the depth and consistency of the build layer which in turn reduces the effectiveness of the subsequent EBM process utilizing the high-energy electron beam to fuse together the build layer²¹. Akin to a heat affected zone in welded structures, as the high-energy electron beam passes over the component, the electron beam zone creates local thermal hotspot on the surface that melts the coalesced powder into the desired geometry. Within the fused layer, global thermal gradients naturally form within the build component due to the thermal gradient originating from the local fusion zone. Thermal gradients across the fused layers create long range anisotropy in the grain structure resulting in columnar grains^{22,23} and extensive fine dendrite formation²⁴. Diffusion kinetics, elevated by the build temperature, promote solute segregation within the interdendritic region creating an inhomogeneous distribution of solute atoms within the build. As additively-manufactured builds are tailored to the final component geometry, the component geometry and complexity influence the degree of spatial variation of microstructure and thermal gradients within the component. Invariably, this results in spatially varying microstructures within the component. Hence, the process parameters associated with the part geometry are also critical in controlling the build dependent structures.

The last three processing steps are post-build processes that improve the mechanical properties and reduces the processing artifacts from prior EBM. Hot isostatic pressing (HIP) applies an isostatic pressure at an elevated temperature with the primary purpose to collapse pores that remain after the build process which increasing the component density²⁵. The elevated HIP temperature may induce dynamic recovery and recrystallization of the grain structure through long range diffusion. Following the HIP step, the component is solution heat treated (SHT), which involves heating the alloy to a sufficient high temperature for a sufficient period of time to cause the dissolution of secondary phases that are formed in the preceding processes and then quenching to form a supersaturated solution of solute atoms. Since multiple phases are formed during the solidification process, the SHT may be performed either below or above the solvus temperature of a specific phase of interest resulting in often vastly different microstructures. Solute migration from the interdendritic region allows for the redistribution of solute clusters within the grains and grain boundaries to a more homogenous distribution. Accompanied by controlled quench rates, the disperse solutes are “quenched in” to improve the dispersion and volume fraction of precipitate and dispersoid particles.

The final processing step is the post-build aging heat treatment, which carefully controls the volume fraction, size, and distribution of precipitate phases. In IN718 the aging cycles are designed to promote the growth of γ' and γ'' phases within the grains and carbide and δ phases at the grain boundaries by promoting solute diffusion within the material at elevated temperatures¹⁷. At extended aging times, the aging thermal profiles are controlled to prevent the uncontrolled formation of large δ phases at the grain boundary and topologically closed-packed (TCP) Laves phases within the grain. The aging process can be completed in one step however for complex microstructures, it is common to have multiple steps to control the growth of each type of precipitate as each precipitate phase has different mechanisms and for growth.

Structure

To complete the PSPP map, all of the relevant features of the structure that may influence one or

more of the properties, from nanoscopic to near macroscopic in size, are identified in the *Structure* column, shown in Figure 5. For IN718, Ni is the primary constituent while Cr, Fe, Nb, Mo, Ti, and Al are alloying elements added to strengthen and stabilize the alloy and to provide corrosion resistance. As a precipitation-hardened alloy, IN718 contains alloying elements to promote the formation of precipitate phases, typically systematically controlled by post-build heat treatment. IN718 can contain three different precipitate phases, γ' , γ'' , and δ ²⁶⁻²⁸. The coherent, metastable γ'' phase, $\text{Ni}_3(\text{Nb}, \text{Ti}, \text{Al})$ with an ordered body-centered tetragonal (BCT) DO_{22} structure is the primary strengthening phase in IN718^{17,29}. The γ'' has a disc-shaped morphology lying in a $\{001\}$ plane. The γ' phase is based on $\text{Ni}_3(\text{Al}, \text{Ti})$ with an ordered face-centered cubic (FCC) L1_2 structure. The δ phase is equilibrium, incoherent phase based on Ni_3Nb with an orthorhombic DO_a structure that tends to form at the grain boundaries, providing the beneficial effect of improving the resistance to grain boundary creep fracture while nominally decreasing yield strength³⁰⁻³². The sequence and order of precipitation is shown through a time-temperature transformation plot (TTT), as presented in Figure 5. The γ' and γ'' phases are usually submicron in size. Due to the low strain mismatch between the γ' and γ matrix phase, the γ' precipitates homogeneously throughout the matrix and provides excellent stability against dissolution at high temperatures³³. In contrast to the γ' phase, the γ'' phase forms fine disperse precipitates within the matrix due to a larger strain mismatch³⁴, and therefore requires more energy to form homogeneously and is less stable within the matrix. The equilibrium δ phase is a common intermetallic precipitate phase that is composed of practically the same chemical composition as the γ'' phase, and therefore the metastable γ'' phase is susceptible to transforming to the δ phase during processing or service as the orthorhombic crystal structure of the δ phase is more thermodynamically stable^{31,35}. In addition, since IN718 contain a small amount of C (less than 0.08 wt %), carbides, typically Nb-rich MC type with some M_{23}C_6 form under a similar manner as the δ phase and also typically at the grain boundaries³⁶. These grain boundary carbides decompose under elevated temperatures³³, and exhibit brittle properties. Mo based carbides form at grain boundaries, leading to local solute depletion near the grain boundaries and an immediate precipitate free zone which promotes intergranular failure³⁶. Poor diffusivity of the refractory elements, Nb and Mo, makes it common for them to segregate in the interdendritic regions that promotes the formation of brittle Laves phases particularly in the conventional cast and welded conditions^{33,37}. Solution treatment is key to dissolving the Laves phases as well as the carbides to improve the strengthening from the precipitation of γ' and γ'' phases during the aging treatment. Cr is an additional alloying element added to improve the workability and corrosion resistance of the material²⁸. In IN718, Fe is the balance constituent and provides nominal room temperature strength to IN718. At elevated temperatures, Fe accelerates the aging kinetics in the material by increasing the diffusivity of precipitate elements³⁸. The addition of Fe is carefully controlled as the excess Fe can result in overaging and the formation of unfavourable δ and Laves phases.³⁸

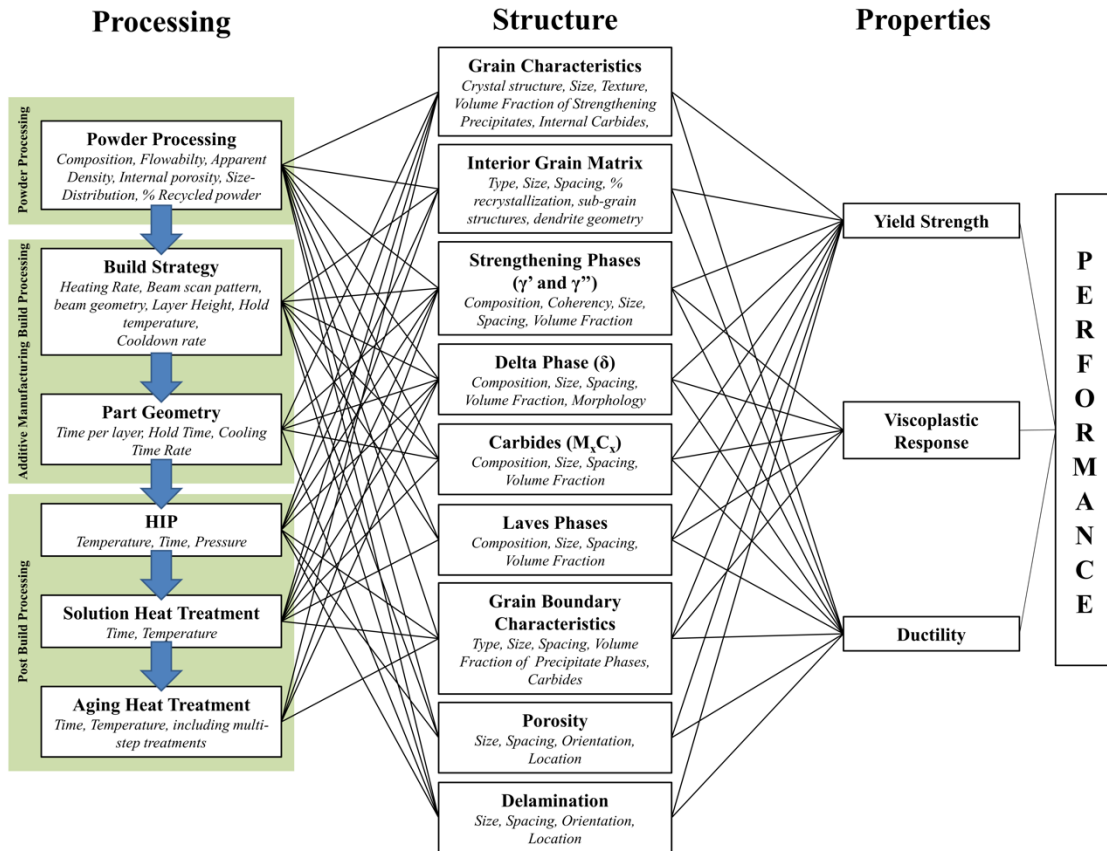


Figure 5: PSPP map for IN718 fabricated by AM targeting hot-section gas turbine components

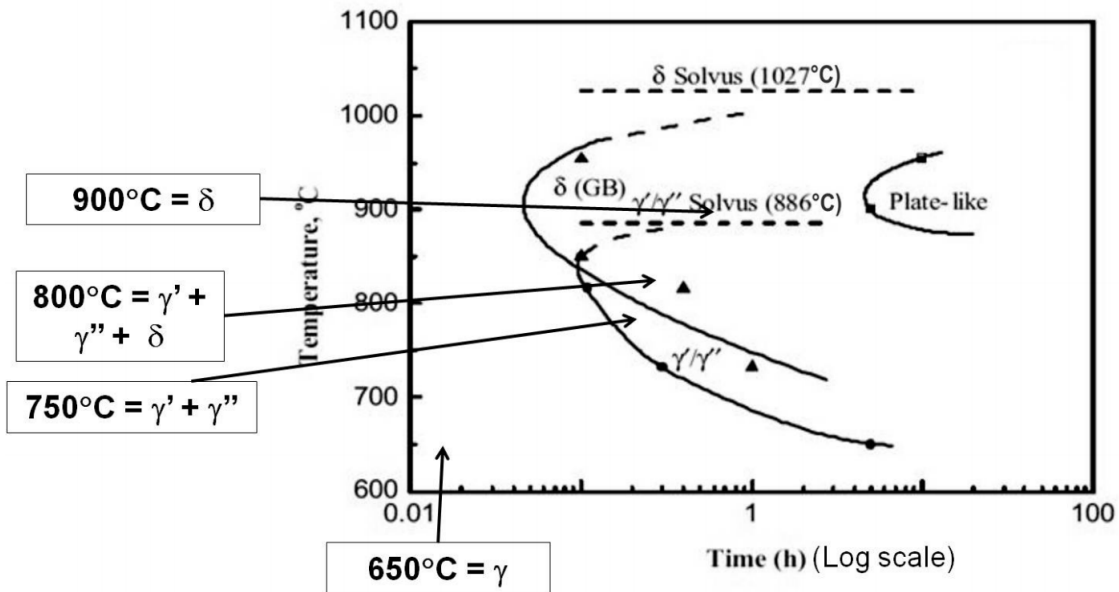


Figure 6: TTT diagram for IN718³⁹

Generally undesirable structures that arise from the powder bed fusion AM processes include porosity and lack-of-fusion delamination. The porosity in additively-manufactured components is either associated with the powder quality, i.e., powders that contain entrapped gases, or shrinkage related to the build strategy²⁴. Delamination is a build-dependent structure that describes the structure of each layer of the build and the interface properties between each build layer. Variations between each “built-up” layer, such as local debonding, incomplete melting, and beam pass configurations create directionally dependent, columnar grain structures²² which impact the interface properties between each build layer and results in anisotropic material properties.

Structure-Properties Linkages – Yield Strength

The primary strengthening mechanism for age-hardened Ni-base superalloys is derived from the γ' and γ'' precipitate phases and to a lesser extent grain boundary strengthening associated crystallographic texture and grain boundary precipitates phases⁴⁰. The γ' phase primarily strengthens through the antiphase domain boundary (APB) energy^{41,42} which prevents dislocation motion in the material through the γ' phase due to the increase in energy required to pass dislocations through the precipitate⁴³. The γ'' phase further strengthen the material through coherency hardening between the matrix and precipitate which prevent dislocation motion due to large lattice mismatch strain between phases⁴⁴. Therefore, the distribution and volume fraction of the γ' and γ'' has a strong influence on the strength⁴⁵. Grain boundary strengthening can also be found in polycrystalline IN718 components which utilizes grain boundaries to impede dislocation motion, thus an inverse relationship exists between grain size and yield strength. As the grains decrease in size, the density of grain boundaries increase which improve the strength of the material⁴⁶. Thus, both the grain structure, crystallographic texture, degree of grain growth, and grain boundary characteristics are important factors that influence the yield strength. An additional strengthening process involves grain boundary precipitates and carbides, including δ phase precipitates and carbides which, at low concentrations, generally improve the creep strength of the material by pinning grain boundaries²¹. At moderate concentrations, the growth of the δ phase is detrimental as the δ phase robs the γ'' phase solute which reduces the extent of precipitation hardening. Although bulk defects are minimized under traditional processing conditions, the powder bed fusion AM process can generate detrimental porosity and lack-of-fusion structures forming planar voids which result in localized weak spots that can severely influence the strength and fracture toughness²³.

Structure-Properties Linkages - Viscoplastic Response

Under elevated temperatures, the structural components that affect the viscoplastic response and associated creep response are primarily the aging precipitates: γ' , γ'' , and δ phases, and the grain characteristics of the additively-manufactured components. The coherent γ' and γ'' precipitation hardening phases are remain stable at elevated temperatures which prevents dislocation shear due to the APB energy actively preventing the movement of dislocations across the crystals at elevated temperatures¹⁷. The γ'' phase further prevents dislocation motion through the limited slip systems in BCT crystal structure of the γ'' phase which prevent dislocations from cutting or cross-slipping through the γ'' phase precipitates. At elevated temperatures, dislocation bowing around the γ'' phase can become a dominant form of dislocation densification which increases dislocation diffusivity and reduces the creep resistance⁴⁷. The presence of the δ phase accelerates the viscoplastic deformation response through the accelerated cannibalization of the γ'' phase, as they share the same precipitation solute atoms required for formation. At elevated temperatures below 700°C²⁸, the δ phase is formed at the expense of the γ'' phase at grain boundaries, reducing

the high temperature strengthening effect of the γ'' phase. At temperatures between 700°C to 880°C, the γ'' phase will coarsen while simultaneously forming δ phase, thus further reducing the creep resistance²⁸.

Structure-Properties Linkages – Ductility

Ductility in IN718 depends on both intragranular and intergranular structures as strain can propagate through the grains or between the grains which impact the resistance to crack nucleation. For IN718, the ductility can be a representative measure of fracture resistance as the mechanistic drivers are similar and increasing ductility often results in increasing fracture resistance. Intragranular precipitation hardening phases, including γ' and γ'' phases limit internal strains by prevent dislocation glide within the grains through APB energy and coherency strains respectively⁴³, thus preventing slip and plastic deformation²⁵ and are often shown to be detrimental to ductility properties. However, for IN718 it has been shown that the type of precipitate can influence the ductility property where the γ'' phase limits ductility, but the γ' phase has more favorable ductility, thus the distribution and type of strengthening precipitates are essential in determining the ductility properties. Similarly, the intergranular properties are important factors in ductility, as the brittle grain boundaries precipitates, decorated with δ phase and carbides, can easily fracture under applied strain⁴⁸ and inhibit crystallographic reorientation required to accommodate the applied strain²⁰. Additionally, additively-manufactured components form anisotropic polycrystalline structures due to thermal gradients from the build process; therefore, the grain orientation and texture will influence the directional ductility due to localized variation in microstructure. Laves phases have also been shown to impact the ductility response as the microvoids formed during formation coupled with weakened solutes are naturally favorable crack nucleation sites⁴⁹. Lack-of-fusion delamination and porosity are particularly significant in the ductility response of additively-manufactured components as they create microvoided locations which coalesce²² and form preferential porosity bands which significantly reduce the ductility response by initiating cracks and fracture within the material which inhibits the fracture resistance response of the material.

Discussion

Engineering materials are complex systems. Invariably students can get lost in the connections and relevance of some of the fundamental science from the reductionist point of view. The PSPP map provides this clarity and framework for a methodical approach to materials education. Creating a PSPP map is an active learning method, engaging students in understanding and defining a materials system. It promotes analysis, synthesis, and evaluation of several topics covered in an introductory course on materials science and engineering. Students are encouraged to identify what they know and more importantly, what they do not know, by creating a map.

PSPP maps provide a standard method to communicate critical information about a materials system from those who develop the system, to those who are interested in modeling it, and beyond. Historically, materials systems have been developed by people with a deep knowledge of the system in question, but computational models have been, and will likely continue to be, developed by systems engineers with a deep knowledge of computational modeling but little knowledge in the mechanisms that drive materials systems. Therefore, it is critical that a standard exists to communicate information about the mechanisms driving the system. The PSPP map provides clarity on what information must be obtained to accurately describe the materials system in its entirety.

To most effectively model the overall Processing-Structure-Properties linkages, multiple models, both data-driven and simulation-based, must be coupled together. If this materials knowledge is captured with reduced-order link functions, it is possible to design alloys using an inductive design exploration method (IDEM)¹², illustrated in Figure 7. This inductive method specifies the desired performance response requirements through a multi-objective function involving a set of properties (here, the "z space") and then working backwards to understand which processing parameters ("x space") will achieve the desired requirements. They are both linked by the structure ("y space"). Additionally, each PSPP linkage can be equated to an existing or non-existing model that reflects the relationship between the individual blocks. As each block is linked to multiple blocks, this indicates that a suite of models, both simulation and empirically based, are required to accurately correlate the property of interest. Recent work has expanded on this method to a computational framework that allows for a larger application space and expedited adoption of the IDEM framework⁵⁰ into pre-existing computational tools. The PSPP mapping is a necessary foundational step in establishing the workflow and functional relationships for IDEM.

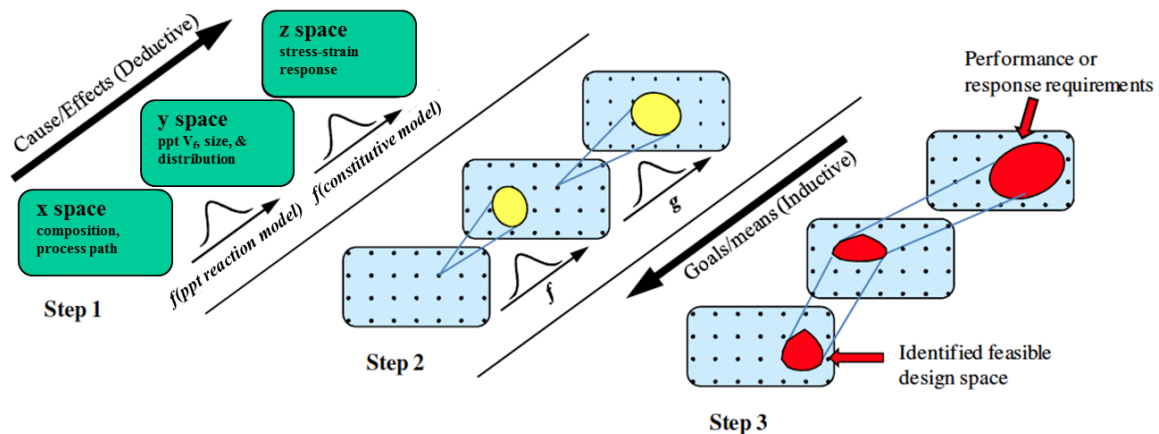


Figure 7: Inductive Design Exploration Method by "McDowell et al"¹².

For novel materials, the PSPP framework allows the cartographer to understand the unique processing steps that modify structures in a new way. As shown in Figure 8 by isolating the structure of interest and mapping the known processes and properties of interest, the student can understand clearly see that the structure in the new material will not have the same origin or resulting effect as the traditional definition of the structure of interest. For the example shown in Figure 8, if the cartographer is interested in the influence of porosity in additively-manufactured IN718 components, the PSPP clearly indicates the processing steps that cause porosity and the subsequent properties that will be affected by the porosity. This map highlights the AM specific processing steps that will influence the extent of porosity and the subset of material properties, which are driven by the desired application and performance needs of the specific materials system, which will be dependent on the structure of interest. This distinction allows the student to understand the unique challenges in the new materials system and allows for the possibility for a new structure definition that best reflects structure of interest. The application of the map is particularly useful in developing the suite of computational, data informatics, and experimental tools to model the linkages in the system, since the map highlights the new linkages that need to be added to pre-existing models to accurately model the structural transformations in the new materials system. Using statistical techniques the functional linkages can be approached systematically through design of experiment techniques to efficiently explore and verify PS and SP linkages.

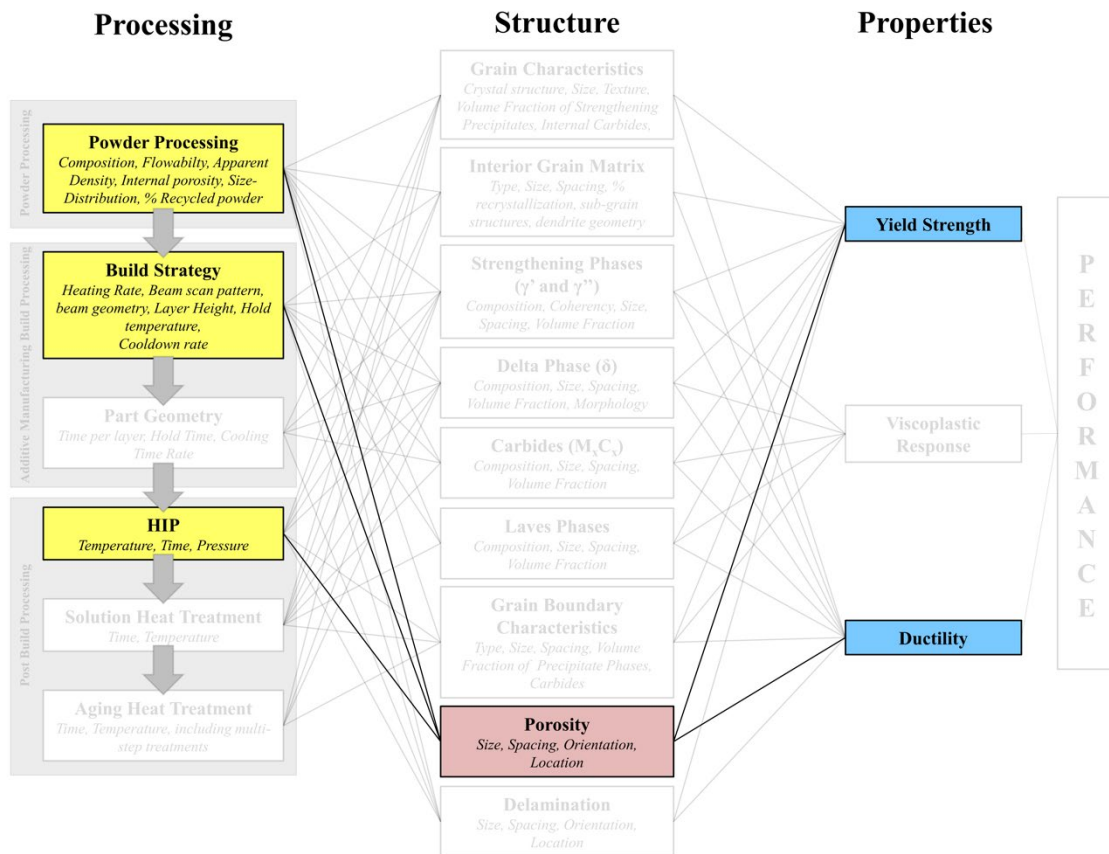


Figure 8: Example of functional linkages that influence porosity for IN718 fabricated by AM

These maps serve as a roadmap for introductory materials science and engineering courses, to

provide the healthy mix of reductionist and systems viewpoints needed to understand and leading to the confidence to design a materials system. Ideally, PSPP maps should be introduced early in the course, and revisited with every new topic introduced to see where it fits on the bigger picture shown by the map. Moreover, students can actively construct a PSPP map for a material to show their current understanding of a materials system and discover what they still do not know about it. The level of detail can vary depending on how the map will be used. For alloy design, rather detailed maps are required to clearly identify gaps in the knowledge of either attributes or linkages. However, for providing students a general system view of the different classes of materials in an introductory course, simpler maps with major processing steps, structural features, and set of important properties while still targeting some application, can be considered.

Summary and Conclusions

PSPP maps provide students a different perspective on materials in that they are in reality complex systems and the design of them requires a systems viewpoint. PSPP maps are a standard tool to effectively communicate materials knowledge critical for advancing materials design. This paper introduces the idea that PSPP maps should be utilized recurrently in materials education.

The development of advanced materials involves a team of researchers and engineers necessitating the establishment of the protocols on the communication of materials knowledge, both to the student and practitioner. This paper details a systematic workflow for constructing PSPP maps and applies the workflow through an example of a precipitation-hardened Ni-base superalloy fabricated by AM for hot-section turbine components. This exercise of creating a PSPP map provides a clear path for conveying to next generation students what is meant by the "materials genome" and how it can be conveyed in PSPP mappings.

It is anticipated that these PSPP maps will inspire our educators to convey knowledge to our young researchers, engineers, and scientists by providing them with more effective ways to convey vast materials knowledge to our next generation. The long-term goal is to have a similar educational impact as Ashby deformation mechanism maps have had on clearly conveying the relationships among temperature, stress, strain rate, and structure on the materials deformation behavior and the impact of Ashby property charts have had in showing trade-offs among properties facilitating materials selection and design. We advocate that these PSPP maps be more widely used in materials education.

Acknowledgements

The authors would like to thank Adrienne Muth for the design of these clear and beautiful graphics, and Dr. David McDowell for useful discussions related to the Materials Genome Initiative, and its goals in bridging modeling and experimentation. This work was funded in part by the Center for Computational Materials Design (CCMD), a joint National Science Foundation (NSF) Industry/University Cooperative Research Center at Pennsylvania State University, University Park, Pennsylvania (IIP-1034965) and Georgia Institute of Technology, Atlanta, Georgia (IIP-1034968).

References

- ¹ Executive Office of the President: National Science and Technology Council, T. Kalil, and C. Wadia, *Materials Genome Initiative for Global Competitiveness* (Washington D.C., 2011).
- ² M.K. Stein, E.A. Silver, and M.S. Smith, *Harvard Educ Rev.* **69**, 32 (1999).
- ³ Workshop on Materials Science and Materials Engineering Education: National Science Foundation, *The Future of Materials Science and Materials Engineering Education* (National Science Foundation, Arlington, VA, 2008).
- ⁴ https://commons.wikimedia.org/wiki/File%3AMaterials_science_tetrahedron%3Bstructure%2C_processing%2C_performance%2C_and_properties.svg archived at <http://perma.cc/M9ND-TAV8>, (n.d.).
- ⁵ G.B. Olson, *Science* **288**, 993 (2000).
- ⁶ G.B. Olson, *Acta Mater.* **61**, 771 (2013).
- ⁷ G.B. Olson and C.J. Kuehmann, *Scripta Mater.* **70**, 25 (2014).
- ⁸ H.J. Frost and M.F. Ashby, *Deformation-Mechanism Maps: The Plasticity and Creep of Metals and Ceramics*, 1st ed. (Pergamon, 1982).
- ⁹ M.F. Ashby, *Materials Selection in Mechanical Design*, 1st ed. (Elsevier, 1992).
- ¹⁰ *CES Edupack 2017* (GRANTA Design Limited, 2017).
- ¹¹ A.N. Goulding, R.W. Neu, and T.H. Sanders, in *ASM International - 23rd IFHTSE* (Savannah, GA, 2016).
- ¹² D.L. McDowell, J. Panchal, H.J. Choi, C. Seepersad, J. Allen, and F. Mistree, *Integrated Design of Multiscale, Multifunctional Materials and Product* (Elsevier, 2010).
- ¹³ R.W. Neu and J. Meredith, *Introduction to High-Throughput Materials Development* (Coursera Inc., Atlanta, GA, 2016).
- ¹⁴ A. Jain, S.P. Ong, G. Hautier, W. Chen, W.D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K.A. Persson, *APL Mater.* **1**, (2013).
- ¹⁵ G.E.P. Box, J.S. Hunter, and W.G. Hunter, *Statistics for Experimenters* (Wiley, 2005).
- ¹⁶ <http://web.ornl.gov/sci/manufacturing/research/additive> archived at <http://perma.cc/2U6J-TSY5>, (n.d.).
- ¹⁷ R. Reed, *The Superalloys Fundamentals and Applications*, 1st ed. (Cambridge University Press, Cambridge, 2006).
- ¹⁸ *MMPDS-12 : Metallic Materials Properties Development and Standardization (MMPDS)* (Federal Aviation Administration, Washington D.C., 2017).
- ¹⁹ P. Nandwana, W. Peter, R. Dehoff, L. Lowe, M. Kirka, F. Medina, and S. Babu, *Metall. Mater. Trans. B.* **47**, 754 (2016).
- ²⁰ A. Spierings, *Additive Manufacturing Mit Metall. Ein Überblick Über Die Forschung* (PRODEX/Swiss Tech Conference, Basel, 2014).
- ²¹ F. Medina, M. Kirka, U. Ackelid, and R. Dehoff, in *Superalloys 2016: Proceedings of the 13th International Symposium of Superalloys* (2016).
- ²² A. Strondl, R. Fischer, G. Frommeyer, and A. Schneider, *Mater. Sci. Eng. A* **480**, 138 (2008).
- ²³ M.M. Kirka, F. Medina, R. Dehoff, and A. Okello, *Mater. Sci. Eng. A* **680**, 338 (2017).
- ²⁴ A. Strondl, M. Palm, J. Gnauk, and G. Frommeyer, *Mater. Sci. Tech. Ser.* **27**, 876 (2011).
- ²⁵ G.A. Rao, M. Kumar, M. Srinivas, and D.S. Sarma, *Mater. Sci. Eng. A* **355**, 114 (2003).
- ²⁶ C.T. Sims, N.S. Stoloff, and W.C. Hagel, *Superalloys II* (Wiley, New York, 1987).
- ²⁷ G.H. Cao, T.Y. Sun, C.H. Wang, X. Li, M. Liu, Z.X. Zhang, P.F. Hu, A.M. Russell, R. Schneider, D. Gerthsen, Z.J. Zhou, C.P. Li, and G.F. Chen, *Mater. Charact.* **136**, 398 (2018).
- ²⁸ G. Fuchs and D. Furrer, in *Handbook of Mechanical Alloy Design*, edited by G. Totten, L. Xie, and K. Funatani (CRC Press, 2003), pp. 585–618.
- ²⁹ M. Sundararaman, P. Mukhopadhyay, and S. Banerjee, *Metall. Trans. A* **23**, 2015 (1992).
- ³⁰ Y. Desvallees, M. Bouzidi, F. Bois, and N. Beau, in *Superalloys 718, 625, 706 and Various*

Derivatives, edited by E. Loria (The Minerals, Metals & Materials Society, Pittsburgh, PA, 1994), pp. 281–291.

³¹ S. Azadian, L.Y. Wei, and R. Warren, *Mater. Charact.* **53**, 7 (2004).

³² X. Xie, J. Dong, G. Wang, W. You, J. Du, C. Zhao, Z. Wang, and T. Carneiro, in *Superalloys 718, 625, 706 and Various Derivatives*, edited by E. Loria (The Minerals, Metals & Materials Society, Pittsburgh, PA, 2005), pp. 287–298.

³³ R. Bowman, *Superalloys: A Primer and History* (2000).

³⁴ F.C. Campbell, *Elements of Metallurgy and Engineering Alloys* (ASM International, 2008).

³⁵ M. Sundararaman, P. Mukhopadhyay, and S. Banerjee, *Metall. Trans. A* **19**, 453 (1988).

³⁶ M. Sundararaman, P. Mukhopadhyay, and S. Banerjee, in *Superalloys 718, 625, 706 and Various Derivatives*, edited by E. Loria (The Minerals, Metals & Materials Society, Pittsburgh, PA, 1997), pp. 367–378.

³⁷ D. Deng, R.L. Peng, H. Brodin, and J. Moverare, *Mater. Sci. Eng. A* **713**, 294 (2017).

³⁸ J.R. Groh and J.F. Radavich, in *Superalloys 718, 625, 706 and Derivatives*, edited by E. Loria (The Minerals, Metals & Materials Society, Pittsburgh, PA, 1991), pp. 351–361.

³⁹ V. Acharya, S. Ramesh, and G.V.S. Murthy, *Characterization of Intermetallic Precipitates in Ni-Base Alloys by Non-Destructive Techniques: Superalloys* (InTech, 2015).

⁴⁰ M.M. Kirka, K.A. Unocic, N. Raghavan, F. Medina, R.R. Dehoff, and S.S. Babu, *JOM* **68**, 1012 (2016).

⁴¹ M.C. Chaturvedi and Y. Han, *Met. Sci.* **17**, 145 (1983).

⁴² M. Donachie and S. Donachie, *Superalloys: A Technical Guide*, 2nd ed. (ASM International, Materials Park, 2002).

⁴³ J.M. Oblak, D.F. Paulonis, and D.S. Duvall, *Metall. Trans.* **5**, 143 (1974).

⁴⁴ E. Akca and A. Gürsel, *PEN* **3**, (2015).

⁴⁵ H. Kitaguchi, *Microstructure-Property Relationship in Advanced Ni-Based Superalloys: Metallurgy-Advances in Materials and Processes* (InTech, 2012).

⁴⁶ G.D. Janaki Ram, A. Venugopal Reddy, K. Prasad Rao, G.M. Reddy, and J.K. Sarin Sundar, *J Mater. Process. Tech.* **167**, 73 (2005).

⁴⁷ B. Pieraggi and J.F. Uginet, in *Superalloys 718, 625, 706 and Various Derivatives*, edited by E. Loria (The Minerals, Metals & Materials Society, Pittsburgh, PA, 1994), pp. 535–544.

⁴⁸ W.J. Mills, in *Superalloy 718 - Metallurgy and Applications*, edited by E. Loria (The Minerals, Metals & Materials Society, Pittsburgh, Pennsylvania, 1989), pp. 517–532.

⁴⁹ W.J. Sames, K.A. Unocic, R.R. Dehoff, T. Lolla, and S.S. Babu, *J. Mater. Res.* **29**, 1920 (2014).

⁵⁰ P.C. Kern, M.W. Priddy, B.D. Ellis, and D.L. McDowell, *Mater. Des.* **134**, 293 (2017).