The Development of a Process-Structure-Properties-Performance (PSPP) Map for Aluminum-Zinc-Magnesium-Copper Alloys Used In Aircraft Applications

A. N. Goulding, R. W. Neu
George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA, 30332
School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA, 30332
T. H. Sanders, Jr.
School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA, 30332

Abstract

In 2011, the White House announced the Materials Genome Initiative, which aims to cut down the cost and time required to discover, develop, and optimize a material and deploy it in a commercial system. One method of achieving this is by integrating experimental test methods, computational tools, and known knowledge databases. While the potential for computational models to speed and assist process-structure-property optimization is not a new concept, one of the key issues in the implementation of models in this space is the lack of a standard method of communication regarding the physical and chemical mechanisms that drive a materials system, and the amount and type of data required to accurately characterize that materials system in its entirety. This work focuses on developing process-structure-property-performance (PSPP) maps as this missing standard communication method. Here we detail the steps that should be taken to generate a map for any system, and then briefly discuss how those steps were applied to high-strength Al-Zn-Mg-Cu alloys. These alloys are highly utilized in aircraft applications and are extremely complicated and commercially viable materials which are repeatedly subject to re-optimization, and are thus a good example of the value of these maps and how they can be used.

Introduction

In 2011, the White House announced the Materials Genome Initiative (MGI), which is based on the idea that advanced materials systems are foundational and transformative technologies. One of the major goals of the MGI is to encourage researchers to integrate experimental test methods, computational tools, and known knowledge databases to find ways to decrease the time and cost the currently goes in to discovering, developing, and optimizing a material system for deployment in a commercial system[1].

One of the potential applications for this kind of integration is in the development and property optimization stage of material development. These stages are often cost and time consuming, largely because of the strong reliance in materials research and development on scientific intuition and trial and error experimentation. Much of the design and testing of new materials systems is currently performed through time-consuming and repetitive experiment and characterization loops. However, once enough experimental work has been done to develop the material system, including understanding the chemical and physical mechanisms that drive the process-structure-property-performance relationships, then computational tools can be used to more quickly and efficiently work towards optimization.

While the potential for computational tools to assist with property optimization is not a new concept, it is surprising that more accurate computational models are not used in many materials systems which could benefit from them. On closer examination, there are still two key issues that are limiting the development and integration of these tools. The first, is that there is currently no standard method to communication critical information about the material system from those who develop the system, to those who are interested in modeling it, and beyond. Oftentimes these materials systems are developed by people with a deep knowledge of the system in question, but the computational models are developed by people with a deep knowledge of computational modeling, and who are usually knew to the material system they are working in. Therefore, it is critical that a standard exists to communication information about the mechanisms driving the system. The second key issue is that there is often a lack of understanding about what information must be obtained to accurately describe the material system in its entirety. Having a standard method of communicating the physical and chemical mechanisms which drive the system could be useful in resolving this issue as well. This work focuses on developing process-structure-property-performance (PSPP) maps as this missing standard communication method. Here we detail the steps that should be taken to generate a map for any system, and then briefly discuss how those steps were applied to high-strength Al-Zn-Mg-Cu alloys. These alloys are typically utilized in aircraft applications and are extremely complicated and commercially viable materials which are repeatedly subject to re-optimization, and are thus a good example of the value of these PSPP maps and how they can be used.

Generating a PSPP Map

Process-Structure-Property-Performance maps as they are described here are meant to be a standard method of communication for the physical and chemical mechanisms that are involved in the system, as well as the data or information required to fully characterize it. Here, we lay out some general guidelines for how to make these maps for any materials system.

When developing a PSPP map for a material, it is important to consider how developed the materials system is. Although the method detailed here is flexible enough to account for both more established systems as well as newer materials that are still in development, the overall process or result may be altered depending on how much is currently known about the mechanisms that drive the system being mapped. Just as the development of a materials system is an inherently iterative process, the mapping of the system will also be iterative, with new maps being developed as new information becomes available. Since these maps are meant to serve as an allegorical tool and help researchers and modelers navigate these often complex and interconnected materials systems, it is unsurprising that they share many of the same characteristics observed in geographical maps. Although the underlying relationships that govern a material system to do not change depending on the application, it is possible that maps with various levels of specificity may exist for different applications or defined materials spaces. Much like geographical maps, PSPP maps are visual standards, but can be customized depending on the features of interest and the level of detail or total size required.

Given the various levels of specificity that are available, an important aspect to consider when building a PSPP map for a material system is the scope, or total size, of the materials design space that is desired. As a general guideline, maps should be large enough to capture all of the features, processing options, or properties of interest, but specific enough to be useful to the application or project they are built for. Ultimately, the scope and level of detail that is captured in the "Structure" column will set the space.

Even though the "Structure" column is pivotal to defining the space included in the map, it is not considered the best place to begin the mapping process. Rather, users who are interested in developing a new map should start with the "Process" and "Properties" columns as a first step. Under the "Properties" column, the user should begin by listing the various properties of interest. If the user has a particular set of "Performance" metrics, sometimes called a "performance profile", these may be useful in determining what properties need to be included in the map. It is recommended that the properties initially be listed and boxed individually as much as possible. After the first iteration of the map has been detailed, properties that share similar driving mechanisms can be grouped for convenience if desired.

Under the "Process" column, it is recommended that the user begin by listing all of the available or currently known processing steps involved in the production of the material defined by the system. Each processing step should be boxed, and within each box the variable parameters involved in that step can be listed and grouped together (e.g. a box containing the "Annealing" step might include variable parameters such as "annealing time" and "annealing temperature"). When the processing route being detailed contains two possible steps that are mutually exclusive, they must either be redefined so that they can be included together in one box, or one must be discarded and the system being mapped will be constrained (e.g. a metal alloy which may be either extruded or hot-rolled can have either a boxed step labeled "Extrusion", a boxed step labeled "Hot-Rolling", or these two processing steps could be simultaneously combined in a more general boxed step labeled "Plastic Deformation"). The "Process" column should generally consist of a set of linear steps that constitute the entire processing route. However, other parameters, such as the parent composition of the material, can also be included. Ultimately, the "Process" column should contain all directly controllable parameters involved in the making of the material being characterized.

Once the "Process" and "Properties" columns have been detailed, the various structural features of the material, which are indirectly controlled through the processing, can be generated. To do this, the user should begin by examining the elements listed in the "Process" column and, using what is already known about the material, generate a list of structural features that are influenced by the different processing parameters. The structural features can be boxed either individually or in relevant groupings depending on the level of detail that is desired. Recall that the scope and detail of the "Structure" column will ultimately define the design space encompassed. Similar to the "Properties" column, if the user is unsure of which structural elements would be well suited to grouping, it is best to leave them boxed individually until the first iteration of the map has been detailed. Afterwards, structural features that are of similar length scales and have similar effects on the processing parameters may be considered for grouping.

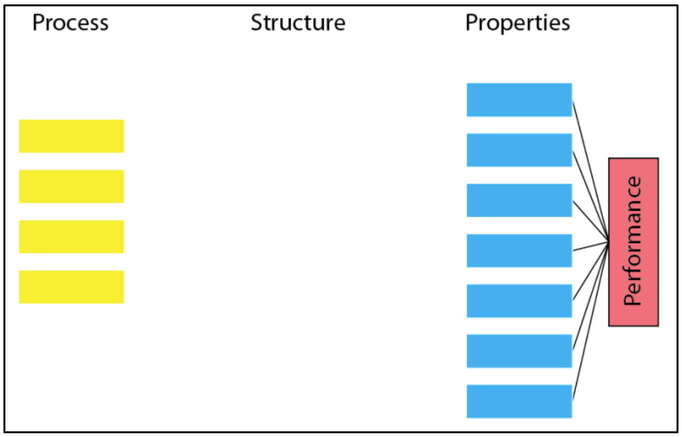

Figure 1: The user should begin the mapping process by generating all the necessary boxes contained in the "Process" and "Properties" columns.

Once the structural elements have been boxed, it is important to map the relationships between the two columns. If a relationship between an element in a processing box and an element in a structural box is known, indicate this relationship by connecting the boxes with a solid line. If a relationship is expected, but not confirmed, use a dashed line. The presence of a dashed line is useful to indicate that a relationship between these boxes is expected, but that further work must be done by the materials science community in order to confirm the presence or absence of this relationship. It is important that the lack of a line connecting two boxes indicates that the two elements in question have been confirmed to *not* share a relationship. Therefore, if the effect of a processing step on the various structure elements is not fully or adequately known, indicate this by dashing the processing box in question. Even if the processing step in question does have some confirmed or expected relationships, this can still be a useful way to indicate to the community that this step may have effects on the structure that are not fully understood. As a point of clarification, while the presence of a solid line should indicate that there is an influence of a processing box on an associated structure box, it is not an indication that the exact relationship is known. Even in situations where the two parameters are known to be, for example, linearly or inversely related, this information should not necessarily be indicated as a part of this map.

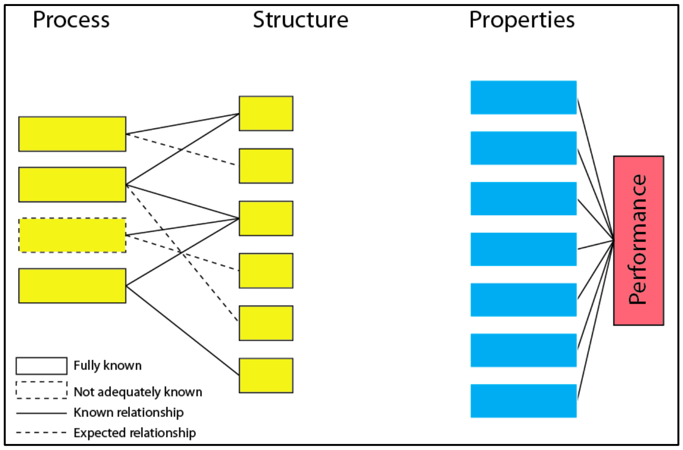

Figure 2: The known and expected relationships between the processing parameters and the structural features should be indicated by a series of solid or dashed lines and boxes.

Once the relationships between the "Process" column and the "Structure" column have been mapped, similar steps can be taken to map the "Structure" column to the "Properties" column. Here, the user should generate a second list of structural features that drive or affect the properties that are listed under the "Properties" column. Once again, if the features that drive a property are unknown or not fully explored, this should be indicated by dashing the box containing that property, as shown in Figure 3.

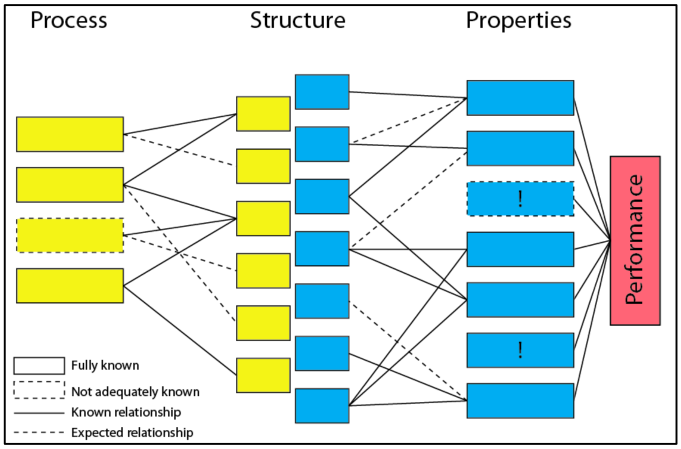

Figure 3: The known or expected relationships between the properties and the structural features that drive them should be indicated with alternatively solid or dashed lines. If the features that drive a property are unknown, this should be indicated with a dashed box around the property in question.

At this point, it is possible that one or more property boxes may be unconnected to the rest of the map because it is unknown what those relationships with the various structural elements may be. However, if a property box is floating and is contained by a solid box, this is an indication that either (1) the user has not included all of the necessary structural elements required to characterize the material, or (2) that the "property" in question is not a true property. For example, yield strength, electrical conductivity, and density are all material properties, which are dictated *only* by the structure of the material. Cost, however, which is driven by many factors not captured in the map, is not a true material property and should not be included in this column.

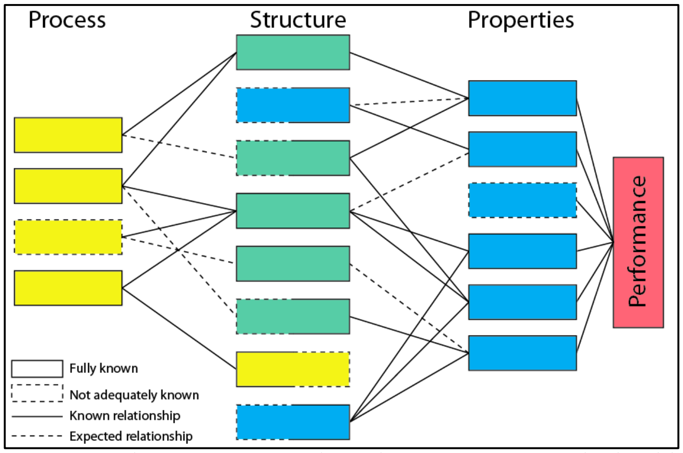

Figure 4: The two structure lists that were generated, should be merged. If the relationship between a structural feature and either the "Process" or "Properties" column is not fully known, this should be indicated by half of a dashed box, as shown here.

Once these two sets of relationships have been mapped, and any misidentified properties have been resolved, the user can proceed with merging the two independently generated "Structure" lists. Here, if a box appears in one list, but not the other, then dash one half of the box to indicate that the relationship between this feature and the opposite column is potentially unknown. It is also possible that, since the structure is indirectly controlled through one or more elements listed under the "Process" column, while one set of processing parameters may have been identified to affect the feature, others are still thought to be missing. Since this indications that more work needs to be done by the community in this area, this would again be indicated by a half dashed box.

For boxes that appeared in only one of the two "Structure" lists, these half-dashed boxes should be solidified *if and only if* it is established that no relationship is missing between the feature in question and the opposite column. If a solidly boxed element in the "Structure" column is not connected to anything in the "Property" column, then it is likely an indication that the structural feature in question, while indirectly controllable by the processing steps, is extraneous to the material system as it has been currently defined. Unless it is likely to be linked to a property of interest at some point in the future, it is suggested that it be removed from the map.

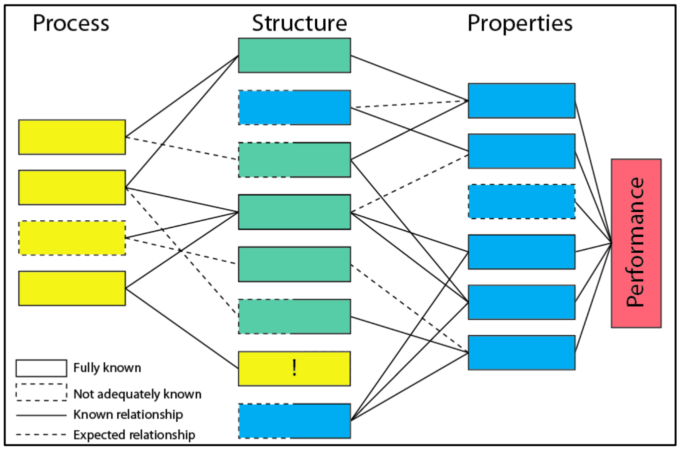

Figure 5: If and only it is established that no relationship is missing between the feature in question and the opposite column, should a half dashed "Structure" box be replaced with a fully solid one.

If a solidly boxed element in the "Structure" column is not linked to the "Process" column then this is an indication that the processing step or steps that control this feature are not included in the existing processing list and it is therefore incomplete. If the processing step that controls the feature in question cannot be added to the map, perhaps because it is not known, then it is still possible to use the map to characterize the material system. But to do so, it will be critical to measure the structural feature in question, since it cannot be indirectly measured by controlling the processing steps that drive it. This information should be communicated on the map by double boxing the structural feature in question.

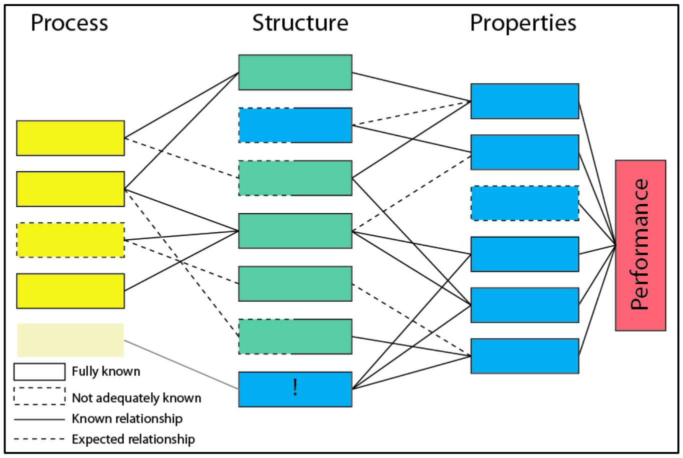

Figure 6: If a solidly boxed structural feature is not connected to an element in the "Process" column, then it is an indication that the directly controllable processing steps listed are incomplete.

Once all of the known and unexplored relationships are indicated on the map by following the above steps, the first iteration of the map should be complete. At this point, if the user is unsatisfied with the size of the materials design space that has been defined, or with the level of detail included in the map, they can iterate through the steps detailed above: adding, combining, or dividing boxes as necessary until the desired level of specificity is obtained. Additionally, once the map has been detailed, targeted exploration can be used to solidify those unconfirmed relationships as indicated by dashed lines and boxes.

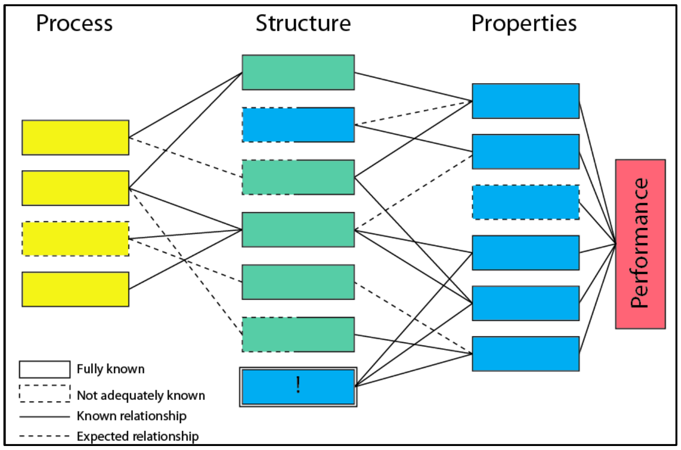

Figure 7: If the directly controllable processing step that drives the 'floating' structural feature in question cannot be included, perhaps because it is unknown, then this information must be included by double boxing the structural feature.

Al-Zn-Mg-Cu System

Now that some general guidelines for how to make these maps for any materials system have been detailed, these steps can be used to create a PSPP map for high-strength Al-Zn-Mg-Cu alloys used in aircraft components. This class of Al-Zn-Mg-Cu alloys, which includes AA7075, AA7050, AA7055, AA7079, AA7449, and many others, has been used in aircraft applications for over 75 years and is well established in the industry. Because these alloys are constantly being developed to provide a wide range of performance profiles for specific applications, they are continually developed. However, the extremely complex relationships that exist between the many processing routes, the complicated microstructural features that extend over multiple length scales, and the variety of properties of interest, make property optimization through computational modeling techniques challenging. In fact, many of these relationships cannot currently be predicted computationally with any real accuracy in this system, even after 75+ years of development[2]. Some initial successes, however, have been made in this space – such as relationships which predict yield strength as a function of a variety of microstructural features[2,3,4,5]. The next step in this materials system is to enable the modeling of multiple elements within this space, possibly through machine learning methods such as artificial neural networks. To do this successfully, a PSPP map for this alloy system must first be developed. Here the authors have used Al-Zn-Mg-Cu alloys as an example to illustrate the steps used to create the map.

Processing Steps and Properties of Interest

One advantage of this material class is that is, to date, quite well developed. As a result, the processing steps and their variable parameters, as well as the effect of changing those parameters on the microstructure are well established. Industrially in these systems, the material is first solidified through direct chill casting methods before being homogenized[6]. While this class of aircraft aluminum alloys is not commonly forged, they are regularly extruded or hot-rolled into stock pieces such as plates, sheets, and bars depending on the application[6]. Since material can only be extruded or hot-rolled, but not both, these steps are contained in one box titled “Plastic Deformation”. After they are formed in to stock pieces, they are typically solution heat treated, quenched, and aged. Occasionally, they can be pre-strained or cold-rolled for stress-relief or to increase the dislocation density prior to aging[7].

Although many properties are typically of interest in this material system, the most commonly optimized and developed properties are the yield and ultimate strength, the work hardenability, the ductility, fracture toughness, and the stress corrosion cracking susceptibility. Other properties such as exfoliation corrosion resistance or density could also be considered, and the performance profile is left general.

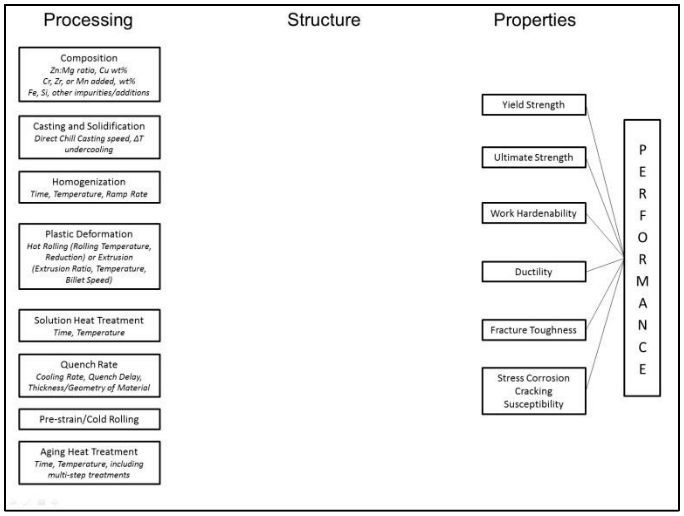

Figure 8: The processing steps involved in making high-strength Al-Zn-Mg-Cu alloys, and some of the most common properties of interest in developing materials for aircraft.

Process-Structure Relationships

Since the material is formed through direct chill (DC) casting, both the casting speed and the degree of undercooling are important and can affect the solidification kinetics[6-8]. Similar to gravity cast systems, semi-continuous casting methods such as DC casting form regions of columnar dendritic growth near the walls of the container, with more equiaxed structures appearing in the middle of the cast. The as-cast material is highly cored with intermetallics in the interdendritic regions[8]. Changing the parameters during this step can affect the solidification kinetics of the casting process, which can lead to changes in the grain size and the size, spacing, and volume fraction of the resulting constituent particles.

Other directly controllable parameters used during this step include additions of Al-Ti-B refiners to change the grain size[6,7,9]. However, care must be taken since small excess amounts of Boron can lead to constituent particles, which have detrimental effects on many properties – including fracture toughness, machinability, and appearance[9]. Cr, Zr, and less often Mn are also added as dispersoid forming elements when the material is formed. The dispersoid particles that are formed using these elements are added to inhibit the recrystallization of the material, but sometimes these additions can form large primary particles during casting instead – leading to more constituent particles throughout the material[6,7,9].

Once the material is cast it is typically homogenized, by heating the material to an elevated temperature for an extended period of time[6,7,10]. The homogenization serves multiple purposes. In addition to redistributing the Zn, Mg, and Cu required to form well dispersed strengthening and grain boundary precipitates, it also serves to redistribute and optimize the precipitation of the Cr- or Zr-containing dispersoid elements which are intended to inhibit recrystallization[6,7,9,10]. The elevated temperature is also used to try and melt as many of the coarse constituent particles as possible. However, care must be taken in setting the homogenization temperature, since many of these constituent particles have relatively low melting temperatures[7,10]. As a result, the time, temperature, and the heating ramp rate, can all affect the dispersion of constituent and dispersoid particles, as well as indirectly affecting the extent of recrystallization through the formation and optimization of the dispersoid particles.

The controllable parameters during the plastic deformation step are obviously different depending on whether the material is hot-rolled or extruded. Regardless, this step is known to have significant effects on the final microstructure, including the texture, the grain characteristics, and the uniformity of the grain characteristics throughout the component[6,7]. Even though this material does not dynamically recrystallize, but rather statically recrystallizes during the solution heat treatment, this step does affect the extent of recrystallization[7,11-13]. As the material experiences deformation, the energy that is added is redistributed inhomogeneously and is often concentrated around coarse constituent particles that remain after homogenization. The more energy that is stored locally in the material, the less thermal energy required during solution heat treatment to begin the recrystallization process. Therefore, the size, spacing, and volume fraction of the constituent particles will also affect the extent of recrystallization, although indirectly, by serving as locations for this added energy to localize. This effect is known as “Particle Stimulated Nucleation” and therefore any processing step that affects the constituent particles, could also have unforeseen consequences on the extent of recrystallization[7].

After the material has been shaped in to a stock piece, it is solution heat treated and then quenched. This step primarily serves to increase the number of vacancies in the system and also increase the amount of primary alloying elements Zn, Mg, and Cu in solution[6,14,15]. Therefore, both of these steps will increase the aging kinetics of the system and have significant impacts on the type, size, spacing, composition, and total volume fraction of precipitates that form both in the interior of the grain and at the grain boundaries. Additionally, since the solution heat treatment is usually conducted at temperatures similar to those used in the homogenization step, it can also melt some of the remaining constituent particles, and as previously discussed the added thermal energy triggers static recrystallization in the material[6,7,14,15].

Prior to aging, the material is occasionally stretched or cold-rolled[7,16]. While further deformation obviously affects the texture of the material, it also can affect the interior of the grain by significantly increasing the dislocation density in these regions. This, in turn, affects the size, spacing, and type of strengthening precipitates that are formed in these regions, since the dislocations serve as heterogeneous nucleation sites[8,16]. During aging, the material can be heated to any one of a range of low to moderately high temperatures for any length of time to encourage the precipitates of strengthening particles in the grain interior and the growth of equilibrium particles at the grain boundary. While aging heat treatments can consist of only one heating step, it is far more common to combine multiple steps together in a single aging process.

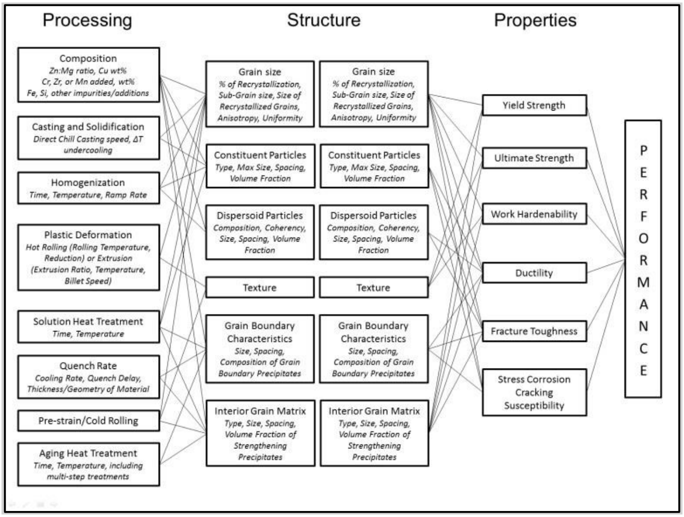

Figure 9: The known or expected relationships between the processing steps and the structural features the influence, as well as the properties and the structural features that drive them are shown here. Since this material system is well developed, no dashed lines or boxes are required.

Structure-Property Relationships

When generating the list of properties that are of interest, we listed each of them individually, as shown in Figure 8. However, sometimes information about the structural features that drive the properties will not be as detailed. For example, in this and many other materials, distinctions between the features that drive the yield strength versus those that drive only the ultimate strength of the material are not always made. And depending on the application and level of detail that is desired in the map, this designation is not always necessary. The main purpose of initially splitting these properties is: (1) to encourage the user to find out if distinctions between the driving mechanisms for each of these properties are known, and (2) to prevent the user from accidentally grouping properties together that are inappropriate. For example, since information about the ductility is also collected as a part of a standard tensile test, users might be tempted to group this property together with the yield strength, the ultimate strength, and the hardening behavior. However, the mechanisms that drive ductility in this system are much more similar to those that drive the fracture toughness. Had the ductility been grouped with the strength and hardening properties, it would have been impossible to distinguish which mechanisms drove which properties. In this material, as in many materials, distinctions between the mechanisms driving the yield strength and the ultimate strength are uncommon. However, as they are very closely related in this material, they are both taken to have the same mechanisms unless shown otherwise.

Although high-strength Al-Zn-Mg-Cu alloys are known for being heat-treatable and precipitation-hardened, there are actually multiple mechanisms responsible for their strength properties[2-6,17]. The most overlooked of these is perhaps the strengthening effect due to the presence of grain boundaries. While the Hall-Petch relationship does hold in these materials for grain sizes at about above approximately 20μm, this effect becomes even more pronounced for smaller grains[17]. Since these materials are often partially recrystallized, the presence of small sub-grain cell structures typically in the range of 2-5μm means that the grain size, the extent of recrystallization, and the sub-grain cell size will all significantly impact the yield and ultimate strength of the alloy[4,5,17-19]. Additionally, the grain size and the shift from large recrystallized grains to unrecrystallized regions of smaller cell structures will also greatly impact the hardening behavior of the material. When dislocations accumulate in fine-grained material, the dislocations are more able to rearrange and annihilate, since they are near grain boundaries. When these dislocations accumulate in larger grains, the distance the dislocation must travel to reach a grain boundary becomes larger than the free slip distance, and so the dislocations become accumulated in the bulk and the material is less able to dynamically recover[17].

In addition to the size and the extent of recrystallization, the texture and the misorientation of the grains and the sub-grain cell structures also affects the yield strength, ultimate strength, and the hardening behavior. As the material is strained, one method of accommodating this excess energy is through the rotation of grains or the polyginzation of the sub-grain cell structures. Therefore, the texture, as expected, will also affect these properties[17,18].

Similar to the effect of grain size, the precipitation-hardening effect is also caused by an increased ability to trap and accumulate dislocations in the material. Here, the formation of coherent solute clusters stabilizes dislocations, since their presence reduces the strain caused by the volume or lattice mismatch that occurs in the matrix. Since small particles are cut by the moving dislocations, their strength contribution is proportional to their average size and volume fraction. When precipitates become large and increasingly incoherent, they become instead physical barriers to dislocation movement, since the only way for a dislocation to circumvent the particles is by bowing into a roughly semi-circular shape between them[6,8]. When this bypassing is done without the aid of cross-slip, it is referred to as Orowan looping, and the strength contribution becomes inversely proportional to the size of the particles[2,6,7,20,21]. It is expected then, that the maximum strengthening effect would be reached when this critical size of the shearing-bypass transition is reached. Indeed the optimization of strengthening precipitate size has been the focus of much of the property optimization work in these material systems to date.

After precipitation hardening has occurred, there are still small amounts of solute that are left in solid solution in the matrix in the interior of the grain boundary. The presence of these solutes contributes to solid solution strengthening. Although this can be a meaningful contribution to the overall strength of the alloy, it is much smaller than some of the others discussed[4]. The amount of strength the remaining solute would be able to impart to the alloy if it was incorporated in to additional precipitates is actually much higher than the contribution from remaining in solid solution. Indeed, new processing methods have recently been developed which increase the total volume fraction of the precipitates in the grain interior, and thereby increase the total strength of the alloy[22].

Fracture toughness is a major design parameter in this class of aluminum alloys, especially as component thicknesses increase. Typically, strength and fracture toughness are considered to be trade-off properties in these materials[6,23]. This view largely stems from the original processing methods that were developed for increasing fracture toughness and aluminum alloys. In these one-step aging treatments, the material has been observed to slowly lose strength as the material is overaged, while the corrosion properties and the fracture toughness are both observed to increase with the increased aging. However, rather than being an inherent trade-off, this change in the properties is driven by a change in the size and spacing of both the strengthening precipitates in the interior of the grain and the equilibrium precipitates at the grain boundary. Here, the slightly elevated temperature these over-aging treatments utilize cause both sets of precipitates to continue to grow. More recently, much work has been done to develop processing methods that allow for the optimization of the size and spacing of these two separate precipitate types – which has in turn led to better strength and fracture toughness or corrosion properties[22-28]. Once again, this demonstrates that it is critically important to understand and be able to distinguish between the structural and physical mechanisms that drive different properties of interest.

Fracture toughness is generally agreed to occur in three distinct phases in these alloys, including (1) void nucleation, (2) void growth, which is also considered to be ductile intergranular fracture since it usually occurs through the growth of voids nucleated near grain boundary regions, and (3) void coalescence, which either occurs by the coalescence of voids and the formation of a void sheet, or through the necking and subsequent failure of the remaining transgranular ligaments[13,14,29]. Because of this transition from intergranular to transgranular fracture at different points of the process, it has been reported that the overall fracture toughness is controlled by this transition. However, a clearer perspective can be gained from considering that an increase in the overall toughness of the material will be gained by prolonging the void growth phase, or through delaying void coalescence[29].

Void nucleation typically occurs through the cracking of coarse constituent particles, which are usually between 1-10μm in size. Since these particles are often quite large and typically appear in clusters, the stress required to break them is quite low, and in many cases they will crack during the multiple thermal and mechanical processing steps required to make the component. Therefore decreasing the size and volume fraction of these constituent particles can significant impact the fracture toughness of the material. However, as the stress increases, voids are also formed at the smaller dispersoid particles, which are typically 0.1-1.0-μm. Thus, it is possible that decreasing the size and increasing the coherency of these particles may also help to increase toughness.

Once nucleated, these voids grow through plastic deformation. As the strain increases, the growth of larger voids can happen concurrently with the nucleation and growth of smaller voids, such as those that form at dispersoids. Although the growth rate of voids that are the same size is independent of void spacing, when small voids are located near larger voids, the growth rate of the smaller voids is significantly accelerated due to strain concentration effects. Decreasing the strain hardening ability can also increase the void growth rate[29]. If the grain interior is very strong compared to the precipitate free zone (PFZ) area near the grain boundary, then void growth is halted, and any additional energy is dispersed in the material through void coalescence along the grain boundaries. This mechanism is responsible for the observed dependence of K_{IC} on the difference in strength between the grain interior and the PFZ. This also explains the severe increase in the amount of intergranular fracture and the overall decrease in the toughness with increasing solute content in Al-Zn-Mg alloys. The increasing solute content increases the strength of the material through the formation of fine particles in the grain interior, thus halting void growth[24]. Therefore the fracture surface goes from being largely transgranular to occurring mainly through intergranular fraction and void coalescence along grain boundaries[24,29,30]. This also helps explain the tradeoff between strength and toughness that is observed with over-aging discussed previously.

Once void growth is halted, the voids will begin to coalesce, and the material will fail. This process can occur either intergranularly through the formation of large void sheets, or transgranularly through the necking and failure of the remaining ligaments. The void distribution, while not observed to affect the growth rate, plays a dominant role in the onset of void coalescence[29]. It has been well observed that the area fraction of grain boundaries plays an important role in determining the overall fracture toughness of an alloy[13,24]. This is due to the acceleration of the void coalescence stage with an increasing areal fraction of the grain boundary, or a decreasing void distribution[24,29]. There is also evidence that supports the theory that the equilibrium particles at the grain boundary facilitate this void coalescence, rather than playing a part in the direct nucleation and growth of voids. Since increasing the size and spacing of the grain boundary particles serves to increase the overall toughness of the material, rather than decrease it. In the over-aged materials discussed earlier, the increase could be accounted for merely by the loss of strength in the grain interior due to the coarsening of strengthening precipitates. But other, more recently developed, processes have shown that this increase is observed even when the interior of the grain is unchanged and the material still possess a high strength [14,23,27,28].

Stress corrosion cracking (SCC) is environmentally assisted fracture, which requires both a corrosive environment and the application of an applied stress to occur. Where typical fracture occurs in three steps consisting of void nucleation, growth, and coalescence, SCC consists of two distinct mechanisms: (1) pitting, which causes a stress concentration and allows for the formation of a crack, and (2) crack growth, which is often measured by the SCC plateau velocity. The stress concentration that must be reached in the initial pitting process before the crack will begin to propagate is given by K_{ISCC}, the threshold stress intensity. Since SCC is effectively accelerated intergranular fracture in the presence of a corrosive environment, it is unsurprising that many of the microstructure parameters that accelerate or affect the fracture toughness and ductility, also affect the SCC resistance[31].

Just as increasing the extent of recrystallization in the material will decrease the overall toughness; increasing amounts of recrystallization will also increase the susceptibility of the material to SCC[13,32]. One mechanism responsible for this is that unrecrystallized sub-grain boundaries, and the dispersoids that are often present at them, are very effective at trapping hydrogen, and therefore their presence can decrease the amount of hydrogen present in the grain boundary regions where SCC is most likely to occur[4,10]. This contributes to an increase in the SCC cracking plateau velocity with an increase in the extent of recrystallization.

Some constituent particles are cathodic with respect to the surrounding the matrix material and can dissolve the material around them through the formation of microgalvanic cells[33]. This decohesion between the particle and the matrix causes pitting, and therefore constituent particles play a role in initiating SCC through the formation of pits that is roughly equivalent to the role they play in void nucleation in the fracture and ductility processes. It was also previously discussed that, although grain boundary particles do not play a role in void nucleation and growth, they are important in the facilitation of void coalescence. Therefore, increasing the size of these particles does not have a detrimental effect on the fracture toughness, and increasing the discrete spacing between them actually has a positive effect. Here, similarly increasing both the size and the spacing of these grain boundary precipitates increases both their ability to effectively trap hydrogen, and increases the amount of time it takes for them to anodically dissolve. [15,22,24,25].

However, changing the chemistry of the microgalvanic cell that is formed between the grain boundary precipitate and the surround PFZ can be more influential on the SCC resistance than changes in size and spacing. It is well known in this material system, that increasing the amount of Cu in the grain boundary precipitates enobles the precipitate, or makes it less electrochemically active[34-36]. Therefore, changing the parent composition of the alloy, or changing the aging process to increase the amount of Cu locally incorporated into grain boundary precipitates will greatly affect the corrosion properties of the material[35,36].

Merge Structure Lists and Adjust for Detail

Once all of the relationships between the three columns have been mapped, the two structures lists have been merged together. Here, the advanced state of this material system is again an advantage, since the two structure columns match and there are no unknown or unexplored relationships that need to be identified. However, this does not mean that the map that has been generated here is static. As discussed in the known structure-property relationships, much work continues to be done to better understand the chemical and physical mechanisms that drive these properties.

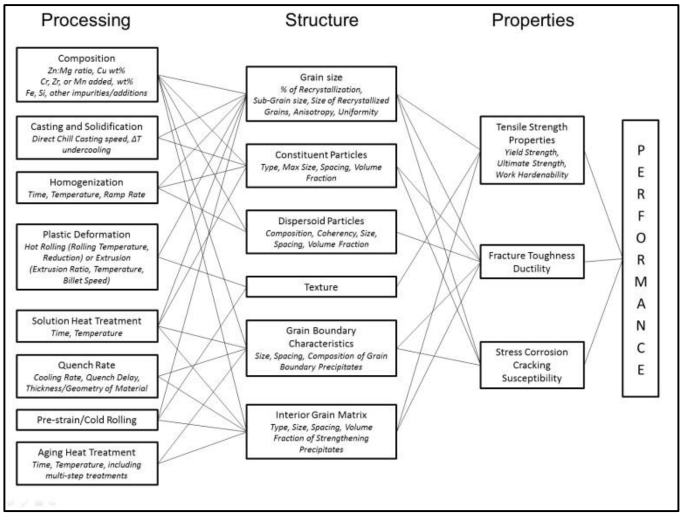

Figure 10: Here, the two structure lists that were generated are merged, and some of the properties have been grouped.

We can also adjust the level of detail by grouping some of the properties we are interested in based on the mechanisms that drive them. Here, we can easily group together yield and ultimate strength, as well as work hardenability. Similarly, we can group fracture toughness and ductility together if desired. Once the PSPP map for a materials system has been developed, it can be used to communicate important information about the physical and chemical mechanisms that drive the system, and about what information must be captured to adequately characterize the material in its entirety.

Discussion

One of the most important things in modeling process-structure-property-performance relationships is making sure that all of the factors that influence the element being predicted are being accounted for. Some of the only successful predictive modeling work in this material system has been in predicting the yield and ultimate strength as a function of various aspects of the microstructure. In each of these cases, this success was due to the ability to individually calculate the different strengthening contributions such as precipitate strengthening, solution strengthening, the strengthening effect due to the presence of grain boundaries, and the strengthening effect due to dislocation-dislocation interactions, and to sum them together using various super-positioning methods.

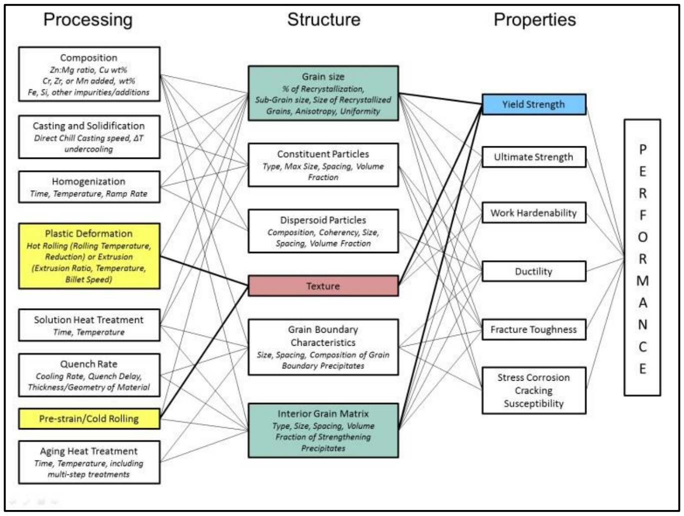

Figure 11: If the yield strength is not modeled directly as a function of the texture of the material, then the model must either account for it indirectly through the processing steps that affect the texture, or the modeling tool will be accurate only for other materials with that texture profile.

The PSPP map, therefore, can be quite useful in making it clear which of these mechanisms needs to be accounted for in such an attempt. But clearly laying out all of the mechanisms that are involved, these individual mechanisms can be more easily decoupled and predicted individually. The map is also useful in understanding which mechanisms may be missing and therefore constraining the usefulness of the model that has been built. This is also true in the case of predicting the yield or ultimate strength as a function of the various mechanisms that were previously mentioned. Using the map, it is easy to see that unless the texture of the material is accounted for, the relationship that was developed may not successfully extend and the predictive model is constrained. In these strengthening equations, the texture is often accounted for with a Taylor factor, which makes rough approximations about the textures that can be accounted for. In this cases understanding that the texture of the material does affect the strength can help users of these predictive modeling tools fully understand any assumptions being made about the material, and adjust their expectations accordingly.

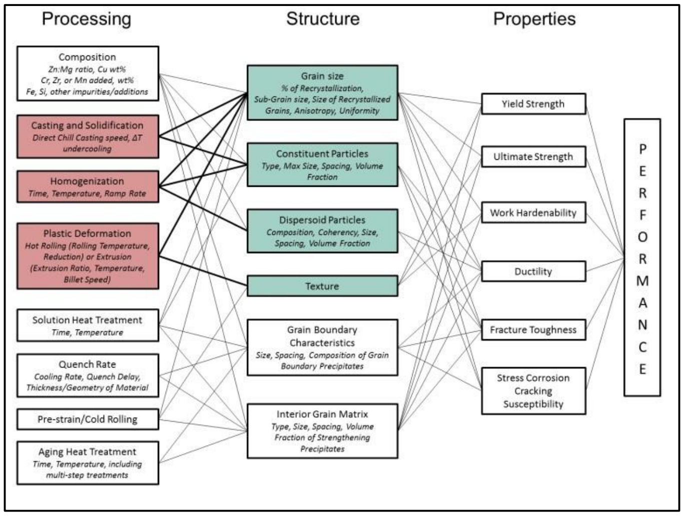

Figure 12: If processing information is unknown, then it is still possible to completely define the material by characterizing the structural features those steps influence.

Another important ability of these PSPP maps is to clearly identify what information must be captured to fully characterize or describe the material. This is especially important in materials systems where some or all of the processing steps are executed by a commercial company. In Al-Zn-Mg-Cu alloys, the casting, homogenization, and formation of a material in to a stock piece is not commonly conducted as a part of academic studies, both in part due to the complexity of these steps as well and the danger than can be involved. Since these materials are made quite commonly industrially, it is far more common to order material that has already been partially or completely processed and simply re-solution heat treat, quench, and age the material for study. Additionally, the casting and homogenization steps in particular are often highly proprietary, and therefore this processing information is rarely if ever reported to the end user. By using the PSPP map for this system, however, it is possible for a user to still fully characterize or describe the material in question, even if these processing details are unknown. Here, we can see that even if the casting, solidification, homogenization, and plastic deformation processes are unreported, the material can still be adequately described by fully characterizing the grain size information, the constituent and dispersoid particle profiles, and the texture. This application of the PSPP map is especially useful when gathering literature databases in a material system, since computational models are only as accurate as the data that is used to develop them. If the data sets that are used to develop and train a computational tool are incomplete, or limited, then the model will be similarly limited at best, or at worst inaccurate.

Acknowledgements

The authors would like to thank Dr. Justin Lamb at Universal Alloys Corporation for his extensive knowledge of casting, solidification, homogenization, and plastic deformation processes as they are currently conducted in commercial aluminum alloy processing today. They would also 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.

References

[1] The National Science and Technology Council, “Materials Genome Initiative for Global Competitiveness”, June 2011.
[2] H. R. Shercliff and M. F. Ashby, "A Process Model for Age Hardening of Aluminum Alloys - I. The Model", *Acta. Metall. Mater.,* Vol. 38, (1990), pp. 1789-1990.
[3] A. Deschamps and Y. Bretchet, "Influence of Predeformation and Ageing of An Al-Zn-Mg Alloy - II. Modeling of Precipitation Kinetics and Yield Strength", *Acta mater.*, Vol. 47, (1999), pp. 293-305.
[4] M. Dixit *et al.*, "Structure-Property Correlations in Al 7050 and Al 7055 high-strength aluminum alloys", *Mat. Sci. and Eng. A*, Vol. 478, (2008), pp.163-172.
[5] M. J. Starink and S. C. Wang, "A model for the yield strength of overaed Al-Zn-Mg-Cu alloys", *Acta mater.*, Vol. 51, (2003), pp. 5131-5150.
[6] J. R. Davis, ed., Aluminum and Aluminum Alloys, (ASM International, 1993).
[7] J. Lamb, “Title of his thesis”, Ph.D. Thesis, Georgia Institute of Technology, December 2015.
[8] D. A. Porter, K. E. Easterling,and M. Y. Sherif, Phase Transformations in Metals and Alloys, (CRC Press, 3rd ed., 2009).
[9] J. B. Hess, “Physical Metallurgy of Recycling Wrought Aluminum Alloys”, *Metall. Trans.*, Vol. 14, (1983), pp.323-327.
[10] J. D. Robson and P. B. Prangnell, "Dispersoid precipitation and process modelling in zirconium containing commercial aluminum alloys",*Acta mater.*, Vol. 49, (2001), pp.599-613.
[11] X. Zhang *et al.*, "Effect of processing parameters on quench sensitivity of an AA7050 sheet", *Mat. Sci. and Eng. A,* Vol. 528, (2011), pp.795-802.
[12] H. Zhang et al., "Hot deformation behavior of Al-Zn-Mg-Cu-Zr aluminum alloys during compression at elevated temperature", *Trans. Nonferrous Met. Soc. China*, Vol. 21, (2011), pp.437-442.
[13] N. U. Deshpande *et al.*, "Relationship between fracture toughness, fracture path, and microstructure of 7050 aluminum alloy: part 1. quantitative characterization", *Metall. Trans. A*, Vol.29, (1998), pp.1191-1201.
[14] N. M. Han *et al.*, "Effect of solution treatment on the strength and fracture toughness of aluminum alloy 7050", *J. Alloys and Com.,* Vol. 509, (2011), pp.4138-4145.
[15] J. Beddoes, “Design of solution heat treatments for aerospace alloys”, *Can. Metall. Quar.*, Vol. 50, (2011), pp.215-221.
[16] N. M. Han *et al.*, “"Effect of solution treatment on the strength and fracture toughness of aluminum alloy 7050", *Mat. Sci. and Eng. A*, Vol. 528, (2011), pp.3714-3721.
[17] R. Mahmudi, “Grain Boundary Strengthening in a Fine Grained Aluminum Alloy”, *Scipta Metall.*, Vol. 31, (1995), pp.781-786.
[18] S. Zhang *et al.*, "Microstructure evolution and deformation behavior of ultrafine-grained Al-Zn-Mg alloys with fine eta' precipitates", *Acta mater.*, Vol. 58, (2010), pp.6695-6705.
[19] S. Chen *et al.*, "Effect of recrystallization and heat treatment on strength and SCC of an Al-Zn-Mg-Cu alloy", *J. Alloys and Com.*, Vol. 581, (2013), pp.705-709.
[20] R. B. Nicholson *et al.*, “The Interaction of Dislocations and Precipitates”, *Acta metal. mater.*, Vol. 8, (1959), pp.172-176.
[21] W. M. Lee and M. A. Zikry, "Modeling the interfacial plastic strain incompatibilities assocaited with dispersed particles in high strength aluminum alloys", *Acta mater.*, Vol. 60, (2012), pp.1669-1679.
[22] J. F. Li *et al.*, "Mechanical properties, corrosion behaviors and microstructures of 7075 aluminum alloy with various aging treatments", *Trans. Nonferrour. Met. Soc. China*, Vol. 18, (2008), pp.755-762.
[23] N. Kamp *et al.*, "Toughness-strength relations in the overaged 7449 Al-based alloy", *Metall. Trans A*, Vol. 33, (2002), pp.1125-1136.
[24] G. M. Ludtka and D. E. Laughlin, "The influence of microstructure and strength on the fracture mode and toughness of 7xxx series aluminum alloys", *Metall. Trans. A*, Vol. 13, (1982), pp.411-425.
[25] J. F. Li *et al.*, "Influence of retrogression temperature and time on the mechanical properties and exfoliation corrosion behavior of aluminum alloy AA7150", *Mat. Char.*, Vol. 60, (2009), pp.1334-1341.
[26] A. Karaaslan *et al.*, "Effect of aging temperature and of retrogression treatment time on the microstructure and mechanical properties of alloy AA7075", *Met. Sci. and Heat Trt.*, Vol. 49, (2007), pp. 443-447.
[27] R N Lumley *et al.*, "Interrupted aging and secondary precipitation in aluminum alloys", *Mat Sci. and Tech.*, Vol. 19, (2003), pp.1483-1490.
[28] R. N. Lumley *et al*., "Development of mechanical properties during secondary aging in aluminum alloys", *Mat. Sci. and Tech.,* Vol. 21, (2005), pp.1025-1032.
[29] T. Pardoen *et al.*, "Multiscale modeling of ductile failure in metallic alloys", *Comptes Rendus Phys.*, Vol. 11, (2010), pp.326-345.
[30] T. H. Sanders Jr. and E. A. Starke, "The relationship of microstructure to monotonic and cyclic straining of two age hardening aluminum alloys", *Met. Trans. A*, Vol. 7A, (1976), pp. 1407-1418.
[31] J. R. Davis, ed., Corrosion of Aluminum and Aluminum Alloys, (ASM International, 1999).
[32] A. S. El-Amoush, "Intergranular corrosion behavior of the 7075-T6 aluminum alloy under different annealing conditions", *Mat. Chem. and Phys.*, Vol. 126, (2011), pp. 607-613.
[33] N. Birbilis *et al.*, "Electrochemical behavior and localized corrosion associated with Al7Cu2Fe particles in aluminum alloy 7075-T651", *Corr. Science*, Vol. 48, (2006), pp. 4202-4215.
[34] N. Birbilis *et al.*, "Electrochemical characteristics of intermetallic phases and in aluminum alloys", *J. Electro. Chem. Soc.*, Vol. 152, (2005), pp.B140-B151.
[35] G. Sha *et al.*, "Segregation of solute elements at grain boundaries in an ultrafine grained Al-Zn-Mg-Cu alloy", *Ultramicroscopy*, Vol.111, (2011), pp.500-505.
[36] R. K. Gupta *et al.*, "Relating the early evolution of microstructure with the electrochemical response and mechanical performance of a Cu-rich and Cu-lean 7xxx aluminum alloy", *J. Electro. Chem. Soc.*, Vol. 159, (2012), pp.492-502.