

Materials Model Development for AA6061 Aluminum

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Abstract

Aluminum alloy 6061 (AA6061) is widely used in industry due to its excellent formability, corrosion resistance, weldability, and strong mechanical properties after heat treatment. AA6061 is hardened through precipitation of alloying elements that act as blockers to dislocation paths in the individual aluminum grains, increasing mechanical performance. During artificial aging, these nano-scale precipitates combine and form the main hardening phase, β'' . The general heat treatment procedure for AA6061 follows a solution treatment, quench, and a direct artificial aging. The focus of this work is to develop the parameters for a materials model for AA6061 which can predict the material response to heat treatment by modeling the kinetics of precipitation formation and coarsening. This work uses data from publications found in the public domain to develop the solution kinetics, artificial aging and coarsening kinetics, and resulting mechanical properties. Another publication was used to validate the developed DANTE model by comparing hardness predictions to hardness obtained in an actual component.

Introduction

Aluminum has a long history in the textile industry in the form of alum, a salt used to aid in dyeing of fabrics. It wasn't until the mid to late 1800s that scientists were able to isolate elemental aluminum. This work continued to grow in the early 1900s to today where over 60 million metric-tons are refined annually. Depending on the alloying elements, wrought aluminum is designated by a series number. 1000 series is very low alloy and is almost pure aluminum. 2000 series is alloyed with copper, 3000 with manganese, 4000 with silicon, 5000 with magnesium, 6000 with magnesium and silicon, 7000 with zinc and 8000 series with other alloying elements such as lithium, iron, and silicon. 1000, 3000, 4000, and 5000 series aluminum alloys can only be hardened through cold working, while 2000, 6000, 7000, and some 8000 series alloys are heat-treatable and can be hardened through precipitation hardening. Casting grade aluminum contains more alloying elements than wrought aluminum, such as silicon to facilitate flow into the cast, and follows a similar numbering sequence as wrought aluminum. 100 series is nearly pure aluminum, 200 series is alloyed with copper, 300 with silicon, magnesium, and copper, 400 with just silicon, 500 with magnesium, 700 with zinc and 800 with tin, copper, and nickel. 100, 400 and 500 series are the only non-heat-treatable casting grades. Precipitation hardening of casting grades tends to be faster than wrought grades due to the higher

amount of alloying elements. Both wrought and casting grade aluminum, which can be heat treated, can be modeled using the DANTE model, with experimental data being fit using methods described in this study.

Solution Treating

Present work in solution treatment of AA6061 was performed by Xu et al. at Hunan University in China. [1] Xu et al. evaluated various solution treatment temperatures and their effect on the time required to achieve maximum hardness at a given aging temperature. The work done by Xu et al. shows that increasing the solution treatment temperature from 490°C to 570°C for one hour has a significant increase in maximum obtainable hardness after artificial aging at 180°C. The maximum hardness increase, per each 20°C temperature division, is significant from 490°C to 550°C. However, between 550°C and 570°C the maximum hardness increase is minimal, showing that the alloying elements are fully saturated when solution treatment is performed at these temperatures. These findings were used to tune the solutionizing model within DANTE, with 1 hour at 570 °C resulting in a fully solutionized condition. DANTE models were then executed using the given heat treatment schedules provided by Xu et al., and solution parameters were compared and tuned to the hardness provided in the publication. The plot in Figure 1 shows the predicted volume fraction of precipitates during solution treatment calculated by the DANTE simulation. Starting with 2.5% of precipitates at the start of the solutionizing process, the treatment at 490°C ends with over 1% undissolved, fully coarsened precipitates, while the 570°C process effectively dissolves all precipitates after the solution treatment. Any fully coarsened precipitates which fail to reenter solution after the solution treatment provide little effect to increase the hardness of the alloy and are considered to be the cause of the hardness drop reported in the publication.

Precipitation Model

The precipitation strengthening of AA6061 starts with a supersaturated solid solution after quenching. If left at room temperature for a long period of time, Mg and Si solutes will begin to precipitate and cluster into vacancies in the aluminum matrix where they combine into Mg and Si co-clusters. For natural aging, this is where the precipitate evolution stops, and the hardness never reaches peak values obtained by artificial aging. If the alloy is heated to artificial aging temperatures shortly after quenching, or after cold storage, the co-clusters continue to form Guinier-Preston zones (GP-Zones), which are more thermodynamically stable and contain more alloy atoms than the co-clusters. These solute-enriched zones are on the scale of 1-5 nm and go on to form the main hardening phase, β'' . β'' precipitates (Mg_5Si_6) are described as needle-like in shape and have an average diameter of a few nanometers and an initial length of about 10 nm. These precipitates act to block dislocation paths, strengthening the material. If the artificial aging temperature is sufficiently high, above 180°C for AA6061, the β'' precipitates will coarsen into rod-shaped β' , β , and, in the presence of copper, Q' precipitates. All non-second order precipitates are indicative of an overaged condition. DANTE's aluminum model allows for up to two (2) separate, distinct precipitates to be modeled and a coarsening model is used to describe the overaged conditions. For this work, focus will be on the main hardening precipitate, β'' . The co-clusters and GP-zones will not be considered in this work. Precipitate A will be analogous to β'' , and the coarsening model will be used to describe the overaged conditions.

Work performed by Pogatscher et al. at the Institute of Nonferrous Metallurgy in Leoben, Austria evaluated a wide range of artificial aging conditions, with the heat-treatment processes well-defined. [2] The work by Pogatscher is extensive and included subjecting some specimens to a natural pre-aging prior to artificial aging. However, the current work will only focus on those specimens in which aging began immediately following the quench. Solution treatment was performed at 570°C for twenty (20) minutes followed by a water quench and subsequent artificial aging in a $Bi_{57}Sn_{43}$ basin at temperatures ranging from 150-250°C, in increments of 10°C. This wide range of temperatures is valuable to heat treatment modeling as it shows the under-aging, peak aging and coarsening behavior of the AA6061 alloy. Each aging condition was simulated using DANTE's Material Simulator (MatSim) and the hardness predictions were compared to the experimental results obtained by Pogatscher et al. The DANTE model parameters were tuned to fit all the data sets reasonably well, with a focus on the typical processing range.

Artificial aging temperatures at 180°C and below are shown in Figure 3. At 150°C, the precipitation is extremely slow compared to the rest of the temperature ranges, which show a much better fit. The precipitation response at 150°C is more typical of a natural aging curve and more data is needed in this temperature range to improve the accuracy of the model. The second precipitate in DANTE, Precipitate B, can be used with this natural aging response if this is an area of concern, but is outside the scope of this work. At 180°C, the first signs of

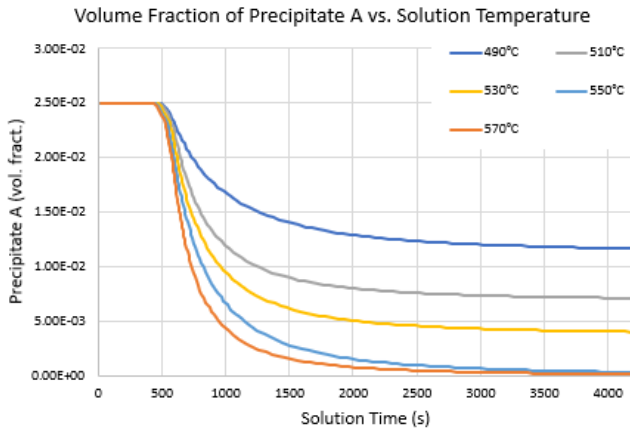


Figure 1: Volume fraction of precipitate A during solution treatment at various temperatures.

Figure 2 compares the measured hardness values for the range of solution treatment temperatures from the Xu et al. publication and the hardness predicted by the DANTE model. The DANTE hardness results are comparable to the publication, and the fit is deemed good. These hardness data are also used to tune and validate the maximum and minimum hardness values of the alloy. The minimum hardness is based on the as-quenched hardness, perfectly devoid of any precipitates. Xu et al. reports these as-quenched values for several specimens and an average was used based on these data, as well as data from the other publications used in this study, to define the base hardness of the AA6061 alloy to be 43 HV. The peak hardness obtained by Xu et al. was 127 HV. This value was compared to the other publications used in this study to tune the maximum hardness granted by a fully-solutionized, peak-aged condition, where all precipitates contribute to the final hardness without coarsening. A value of 3.4 HV/0.1% precipitate was found to give the best fit when all publications from this study were considered. This means for each 0.1% of precipitates which have formed, but not coarsened, the hardness will increase by 3.4 Vickers. With a maximum available precipitate amount of 2.5%, this material can reach a Vickers hardness of $43 + (3.4 * 25) = 128$ HV. The artificial aging temperature prescribed by Xu et al. is 180°C, which causes coarsening of the precipitates during the long aging process and results in a reduction in hardness as shown by the negative slope during aging in Figure 2.

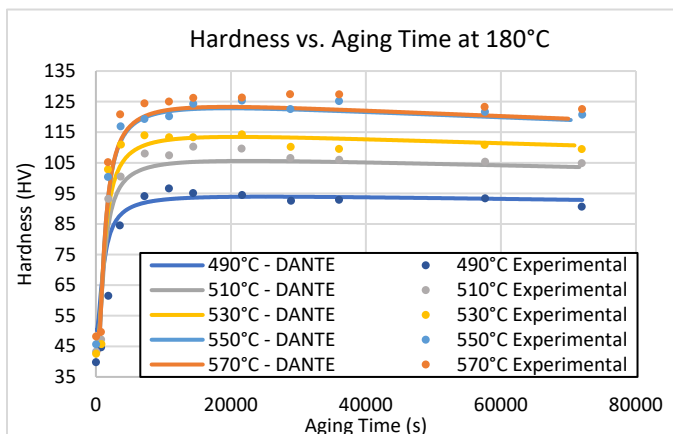


Figure 2: Hardness vs. aging time for various solution treatment temperatures.

coarsening, or overaging, begin to show. The hardness data begins to have a negative slope as the aging time is extended and even drops below the hardness of the lower temperature ranges after seven (7) hours of aging time.

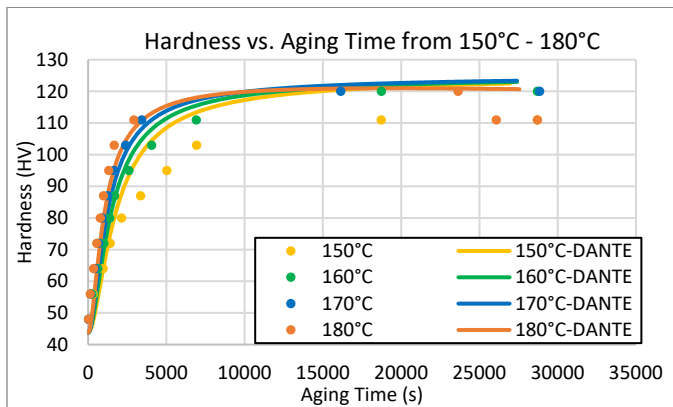


Figure 3: Predicted hardness vs. aging time for temperatures ranging from 150°C-180°C; solutionized at 570°C for 20 minutes.

Between 190°C and 220°C, the coarsening of the precipitates has an increasingly detrimental effect, as shown in Figure 4. As the aging temperature is increased, the time to reach peak hardness becomes shorter. In addition, the magnitude of the peak hardness is severely reduced due to the rapid coarsening of precipitates at these higher aging temperatures. The fitting of the hardness data provided by Pogatscher et al. characterizes the hardness evolution well in both the early precipitate formation and the longer aging behavior.

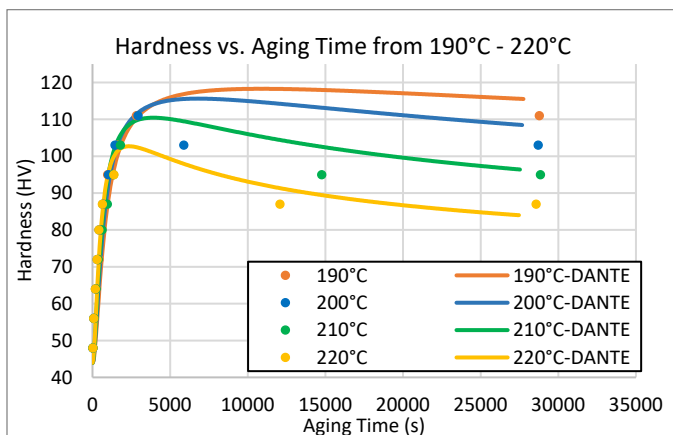


Figure 4: Predicted hardness vs. aging time for temperatures ranging from 190°C-220°C; solutionized at 570°C for 20 minutes.

Artificial aging temperatures at 230°C and above show a severe decrease in peak hardness due to the rapid coarsening of the precipitates, as shown in Figure 5. The samples are shown to reach peak hardness for a given temperature within the first half hour of artificial aging and decrease sharply as aging proceeds. The fitting of this phenomenon is challenging, as the competing forces of formation, coarsening and dissolution all influence the hardness. Despite these difficulties, the fit follows the hardening and softening due to precipitation coarsening well.

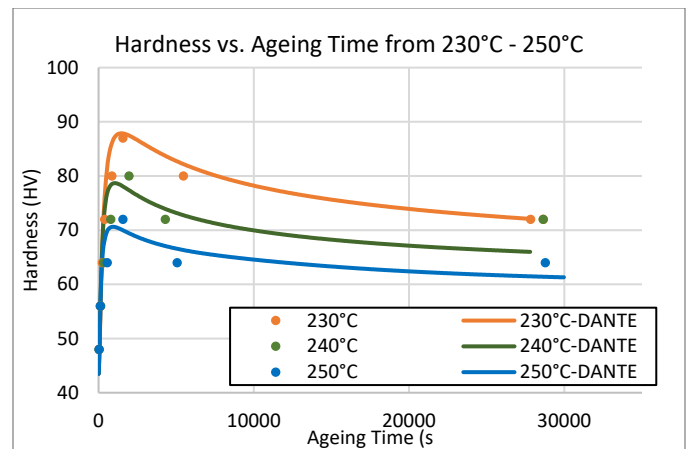


Figure 5: Predicted hardness vs. aging time for temperatures ranging from 230°C-250°C; solutionized at 570°C for 20 minutes.

While these higher temperatures are typically out of the range for heat treatment of AA6061, it is good to fit these data to understand the material response at higher temperatures. For solution treatment, the part must go through these temperature ranges and having a full understanding of the phenomena builds a better model. For instance, higher temperature isothermal holds can better describe the solutionizing rate or shed light on the kinetics of precipitate formation and dissolution at higher temperatures.

For the coarsening model in DANTE, the total volume fraction of precipitate A is broken into eleven (11) different size classes. Size 1 contributes the most to the hardness and size 11 contributes the least. As one size class forms, it can grow to the next size class and so on. The rate of this growth is governed by the temperature and becomes increasingly exponential as the temperature increases. The size class also tracks the average size of the precipitates during the process, which also affects the rate of dissolution during solution treatment as well as any strain produced by the precipitate growth. For the process described by Pogatscher et al., the solution treatment at 570°C is for only twenty (20) minutes. Based on the previous work done with the solutionizing model in DANTE, this short time leaves some size class 11 precipitates undissolved, approximately 0.1%, as shown in Figure 6. This illustrates the importance of having an accurate solutionizing model, as any undissolved precipitates will reduce the peak hardness attainable by artificial aging. The undissolved precipitates also help explain the lower hardness achieved at the 180°C aging performed by Pogatscher et al. (Fig. 3) when compared to Xu et al. (Fig. 2). Furthermore, the fitting of the artificial aging data is based on the hardness evolution during the step, and if pre-existing precipitates are not accounted for the results will be incorrect.

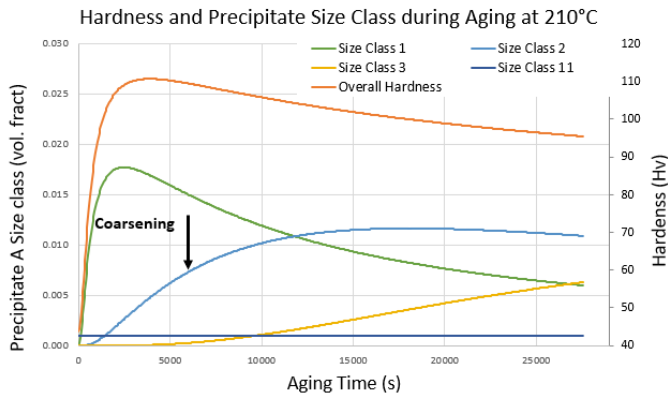


Figure 6: Hardness and precipitate size class evolution vs. aging time at 210°C; solutionized at 570°C for 20 minutes.

Mechanical Properties

Mechanical properties come in two general forms, elastic and plastic. The elastic properties in DANTE, such as Young's Modulus and Poisson's ratio, are simply a function of temperature. Plastic properties are a function of the amount of precipitates in the material, as well as temperature, and consist of twenty-seven (27) parameters that control the yield, hardening and recovery response of the material when strained. A factor is needed to link the precipitation to the plastic mechanical properties. This factor, termed the PPT Factor, is defined in DANTE as: $[(\text{Total hardness}/\text{base hardness}) - 1]$ and is used to gain an understanding of the precipitates' contribution to the overall hardness. After fitting the solution treating and artificial aging parameters, DANTE models were executed using schedules defined in work performed by Ozturk et al. [3] and by Kreyca and Kozeschnik. [4] The resulting schedules produced a range of PPT factors from 0.25% to 1.7%. A PPT factor of 0.25% was used for the No Heat-Treatment (NoHT) condition fitting as some precipitates are expected to exist even after solution treatment and quenching. The PPT factors obtained from the DANTE models for the Ozturk et al. processes for 90-minute and 120-minute aging and the 1-hour aging from Kreyca and Kozeschnik resulted in an average factor of 1.375%. The PPT factor for the 4-hour and 8-hour age from the Kreyca and Kozeschnik publication resulted in an average PPT factor of 1.7%. With PPT factors obtained for each of the heat treatment schedules, mechanical fitting at room temperature of 3 PPT factor conditions; NoHT, 1.375% and 1.7% can be executed using DANTE's mechanical property fitting utility (MecFit). The results of the room-temperature fitting across the range of PPT factors are shown in Figure 7. The 1.375% and 1.7% PPT factor fitting (orange and green, respectively) agrees well with the experimental values reported by Ozturk et al. (90min and 120min) and Kreyca and Kozeschnik (1-hour Age, 4-hour Age and 8-hour Age). The NoHT condition reported by Ozturk et al. fits reasonably well with the 0.25% PPT factor, with the model having a slightly lower yield and slightly more stress at higher strain values.

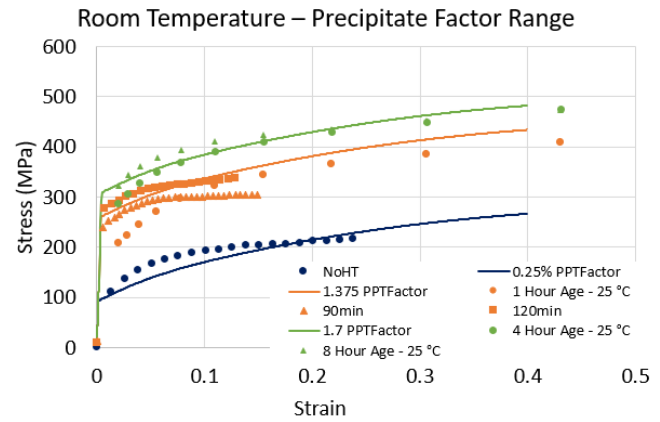


Figure 7: Predicted stress vs. strain curves for room temperature compared to experimental data.

While the work done by Ozturk et al. was great for fitting mechanical properties at room temperature, heat treatment modeling requires mechanical properties over the entire processing temperature range. Using the same method as the room temperature fitting, but with fixed PPT factors of 1.375% and 1.7%, corresponding to the conditions from Kreyca and Kozeschnik, data was fit from room temperature to 500°C. In the work done by Kreyca and Kozeschnik, the samples were artificially aged at 170°C and were then compression tested at elevated temperature on a Gleeble thermal-mechanical simulator. The fitting results are shown in Figure 8. In general, as temperature increases, the yield and compressive stress values decrease. Starting at 200°C, the data shows a notable downward slope as the strain increases. This downward slope increases as the temperature increases and is not captured with the mechanical fitting in MecFit because of the assumed constant PPT factor. The reason for this negative slope is due to the precipitates rapidly coarsening at temperatures above the artificial aging temperature, reducing hardness and mechanical performance while it is being tested in the Gleeble. This is why the DANTE fitting appears to overestimate the stress per strain at the elevated temperatures. A few models were executed where the re-heating in the Gleeble was added to the end of the schedule. The models showed that even in the short testing time of two (2) to five (5) minutes, the PPT factor is reduced significantly at temperatures above 200°C. Due to the previous work with a constant temperature, and a PPT factor range, the DANTE model will capture this change in PPT factor during simulation and adjust the mechanical properties accordingly.

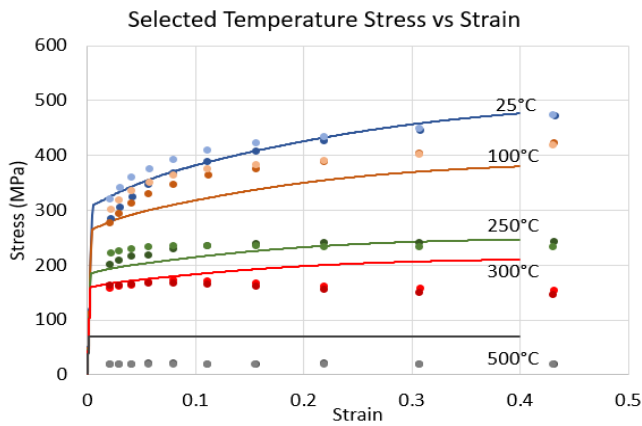


Figure 8: Predicted stress vs. strain curves for selected temperatures compared to experimental data.

Case Study

This case study is a culmination of the previous work; solution treating, precipitation and coarsening kinetics, and mechanical property fitting, and focuses on the hardening of an AA6061 aluminum mirror for telescopes. Newsander et al. performed heat treatment work on large AA6061 mirror blanks like those used in space telescopes. [5] The half-meter diameter test blank was subjected to solution treatment at 530°C for 3 hours followed by a Glycol quench and artificial aging at 180°C for 8-10 hours. An axisymmetric model was built using Abaqus, based on the dimensions given in the publication, and meshed with fine elements near the surface to capture the thermal gradients present in heat treatment processes. The finite-element model consists of 13,766 nodes and 13,496 elements. The heat treatment schedule was executed with six (6) cores and was complete in about ten (10) minutes using an Intel i7 9th generation processor. The hardness contour, shown in Figure 9, reports a surface hardness of 97 HV, with a softer core of 93 HV. The hardness variation from surface to core of the blank is caused by precipitation occurring during the quench when the core of the blank is still hot. These precipitates are considered either fully coarsened or grain boundary precipitates and contribute very little to the overall hardness of the material. The predicted hardness profiles, taken from the two paths shown in Figure 9, were mirrored axially across the centerline of the axisymmetric model, and compared to the hardness data provided by Newsander et al., after converting the published data from Brinell to Vickers hardness. Figure 10 shows the DANTE prediction matches the reported hardness variation of the surface and core well, validating the DANTE model.

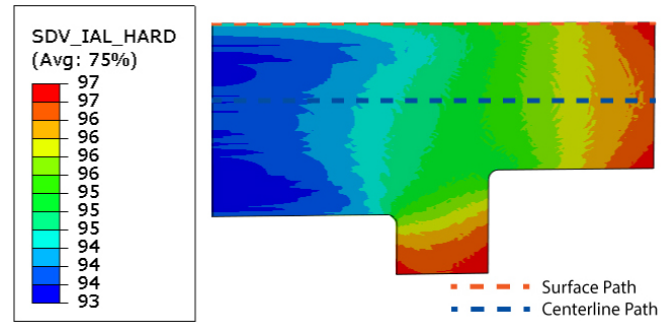


Figure 9: Predicted hardness contour for the axisymmetric model.

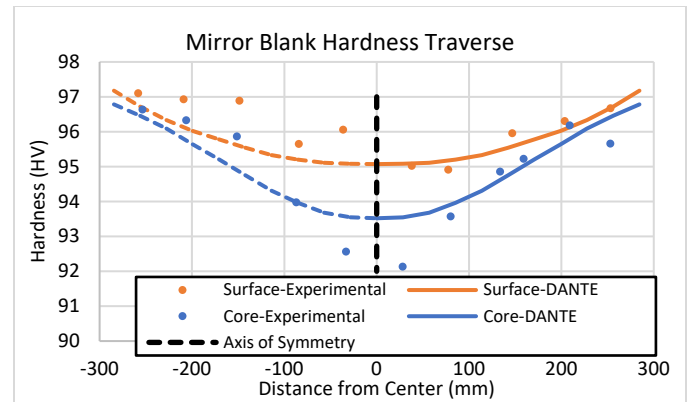


Figure 10: Predicted hardness traverse from the axisymmetric model compared to experimental data.

Further improvements to the results can be realized by modifying the thermal boundary conditions of the simulation. For instance, the data shows a harder surface from left to right in the path plot. This variation is reported to be caused by a non-uniform flow during quenching in the publication by Newsander et al. A nonuniform thermal boundary condition can be applied to the simulation to describe this phenomenon but requires at least half of the mirror blank to be modeled. A second finite element model was constructed in Ansys using the half-mirror geometry. This model consists of 94,192 nodes and 310,182 elements and applies a non-uniform thermal boundary condition by adjusting the heat transfer coefficient during quenching from one side of the blank to the other. The nominal heat transfer coefficient was scaled by a factor of 1.1 times on the right side of the blank, and by 0.9 times on the left side to capture the shift in hardness shown by the measurements, as illustrated in the contour in Figure 11. The DANTE subroutine applies these factors linearly along the diameter of the blank, ensuring a gradual change from one side to the other. Figure 12 shows the predicted hardness traverse from the DANTE simulation compared to the experimental data using the nonuniform thermal boundary conditions and the half model of the mirror blank. The results match the hardness profile within 1 HV.

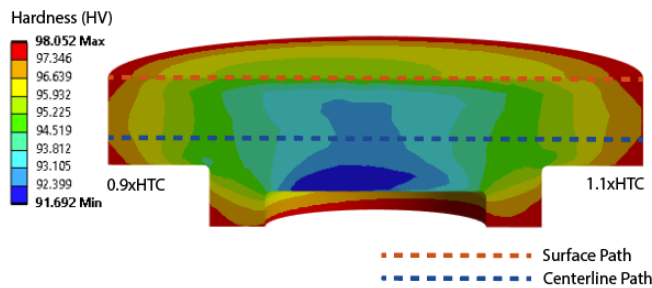


Figure 11: Predicted hardness contour for the half model with nonuniform cooling during quenching.

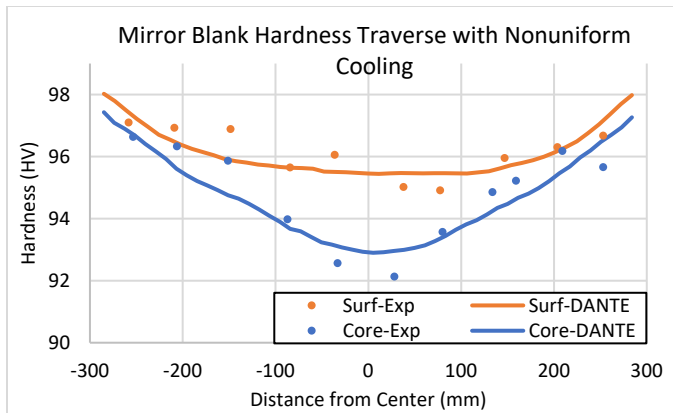


Figure 12: Predicted hardness traverse from the half model with nonuniform cooling compared to experimental data.

Conclusions and Future Work

A DANTE materials model of AA6061 aluminum was successfully developed using data from published papers in the public domain. The model consists of solution treatment parameters fit from work performed by Xu et al. which showed that solution treatment at 550°C to 570°C for one-hour results in a fully-solutionized condition based on hardness, and confirmed by resistivity measurements, after precipitation hardening at 180°C.

For precipitation and coarsening kinetics, data was collected from work done by Pogatscher et al. with aging temperatures ranging from 150°C to 250°C. The bulk of the fitting work focused on these data to accurately characterize the precipitation and coarsening response and is arguably the most important part of the aluminum heat-treatment model. Future work on precipitation can be performed outside the temperature ranges provided by Pogatscher et al. This work's focus was on the main hardening phase, β'' , which uses precipitate A in DANTE to describe the hardening. Isothermal tests using a Gleeble, or similar thermo-mechanical simulator, above 250°C can help to describe the kinetics of precipitation at higher temperatures. These additional tests can be valuable for bulkier, slower to cool, regions of parts. Additionally, precipitate B in DANTE can be used to describe the co-cluster and GP-zone kinetics at temperatures lower than 150°C. This area of study can describe the natural aging process which was outside the scope of this work due to a lack of data. Again, a few isothermal tests can help describe this phenomenon and can be easily added to the DANTE precipitation kinetics.

Mechanical properties were fit from tensile and compression tests performed by Ozturk et al. and Kreyca and Kozeschnik. The fitting requires data from a wide temperature range and with various levels of precipitation, which was described using the PPT factor in DANTE. The room temperature fitting varies the PPT factor to describe increases in yield and tensile strengths from precipitation. The fitting for temperature ranges from room temperature to 500°C, using the fixed PPT factors, showed that yield and compression stresses decrease with temperature.

Lastly, an interesting case study was performed to further validate the DANTE model. The hardness variation across the mirror surface and midline agrees well with data published by Newsander et al. This work illustrates the importance of part geometry and cooling rates when mechanical properties are a concern, paying particular attention to bulkier regions of parts that cool much slower than thinner cross sections.

The material model developed during this work is by no means a complete and refined model. Working from the limited public data provided in publications only serves to develop a base model one can use to ensure they are in the ballpark when it comes to modeling the precipitation hardening of AA6061 aluminum. Each melt of AA6061, and subsequent processing conditions, will vary slightly in its chemical composition and hardening behavior. The material model developed can help save many hours and costs associated with running experiments to develop processes for new components produced from AA6061. DANTE continues to validate and update this material, as well as other steel and aluminum grades, as more data becomes available.

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