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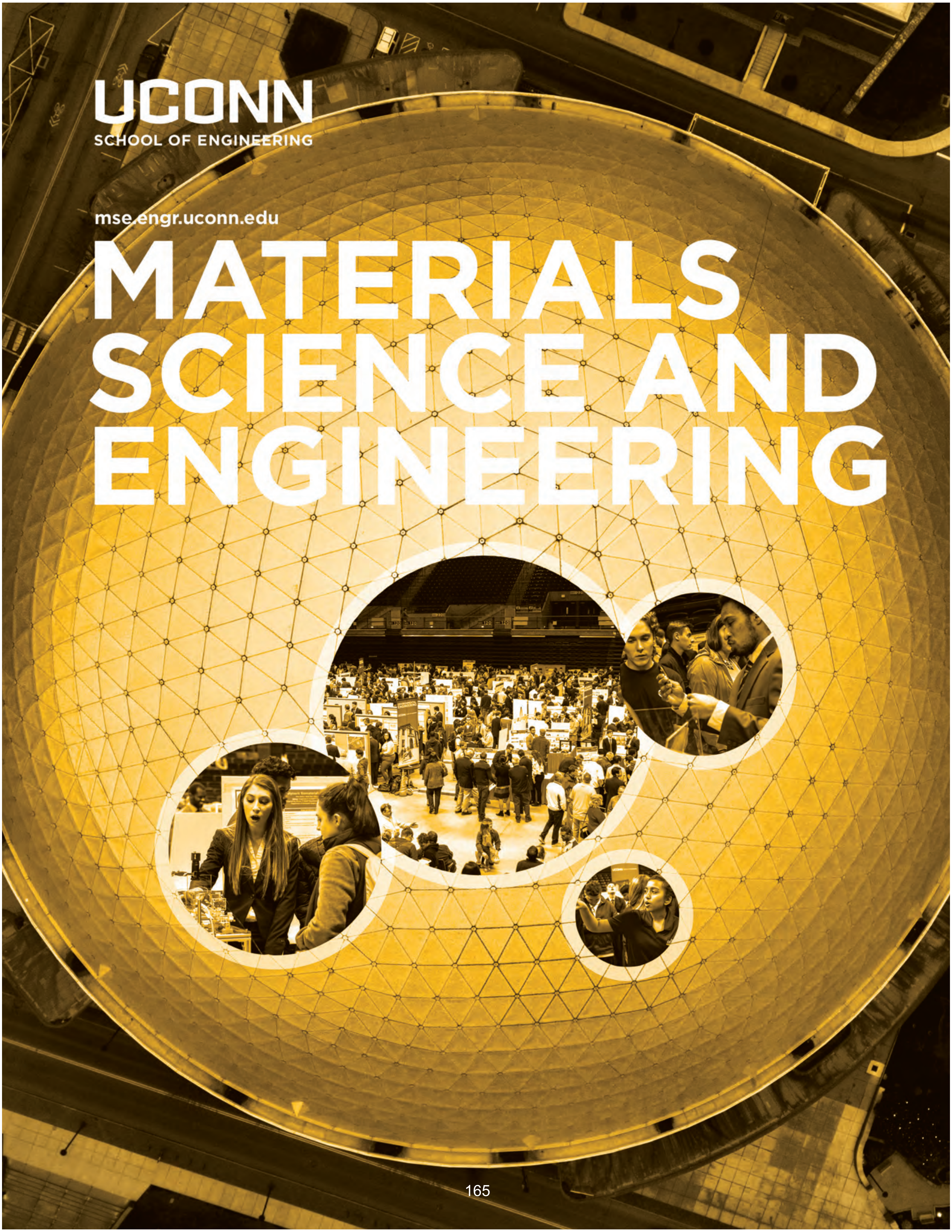
MATERIALS SCIENCE AND ENGINEERING



Mikaela Whittington-Baschoff, Anna McDonald, Baylee Loewen

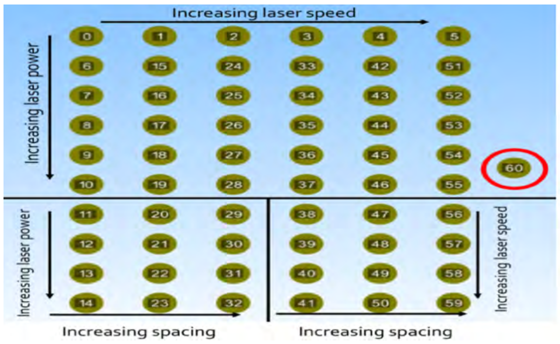
MATERIALS SCIENCE & ENGINEERING

TEAM: 1
SPONSOR: Stanadyne, LLC
ADVISOR: Dr. Rainer Hebert

Additive Manufacturing for Prototype Components

Stanadyne®
Fueling Innovation

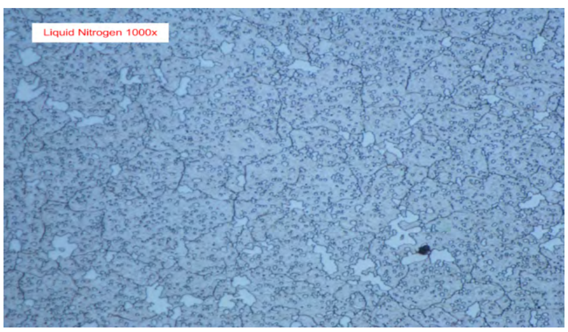
Stanadyne wishes to determine if additive manufacturing (AM) using 440C stainless steel can be used to manufacture prototype components for a gasoline direct injector (GDI). In order to be considered viable, the process must produce components that meet specific tolerances and criteria (porosity, hardness, surface finish). Additionally, AM must have a better lead-time time to generate usable components. The additive manufacturing machine used to produce the components is the Pro300X (located in the Innovation Partnership Building).



This project focuses on three key internal components. In order for the printed components to be deemed successful by Stanadyne, each part must withstand 1000 hours of cyclic stress, the support structures necessary to print the part must be removable/machinable, and the machined surfaces must match the specific tolerance criteria. In addition, the overall printing, and post processing should take no longer than 4 weeks.

The main design aspects of this project include finding the ideal build plate orientation for each component, finding the optimal laser parameters for 440C stainless steel, and successfully processing the printed components to achieve required tolerances and criteria. Essentially, the ideal orientation of the parts is one where the number of required supports needed is minimized, the optimal parameters reduce over porosity, unmelts, and distortions, and successful post processing includes machining and heat treating.

The laser parameters being explored are distance (or spacing), power, and speed. The simultaneous modification of these parameters effects the quality of the printed part. The heat treatment processes being explored are a double temper treatment and a cryogenic treatment. The cryogenic (deep freeze) process involves heating the components to a set temperature, cooling them as quickly as possible without quenching, then submerging them in liquid nitrogen before tempering them once. The two processes produce similar results; however, the deep freeze process is more efficient and can improve the wear resistance more than the double temper process. After treatment, the components are machined to reduce surface roughness and measured for dimensional accuracy.

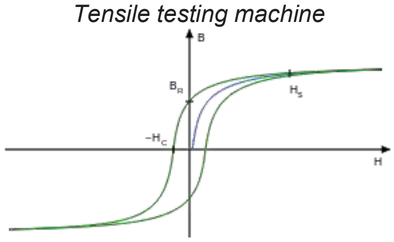


The results are promising. Additive Manufacturing is an extremely efficient process once the proper parameters are determined. The modification of these parameters along with proper processing, produces components with properties and tolerances required by Stanadyne.

Dean Mazzola, Tyler MacLean, Janos Kanyo, Tochukwu Njoku

Stanadyne

Tensile testing machine



B-H curve to display magnetic properties

Magnetic testing devices in Uconn graduate labs

MATERIALS SCIENCE & ENGINEERING

TEAM: 2
SPONSOR: Stanadyne LLC
ADVISOR: Puxian Gao

Hardenable Stainless Steels and Magnetism

Gasoline direct injection (GDI) pumps contain valves that are subject to cyclic loading which necessitates materials that can withstand the high fatigue stresses that occurs. While Stanadyne has industry leading GDI pumps that are made of high-end stainless steels with mechanical properties capable of withstanding this environment, this project is mainly focused on finding less commonly used stainless steels that may be implemented in Stanadyne’s new GDI pumps to increase efficiency and performance. More specifically, there are two different sets of parameters that we are focusing on. The first is finding a stainless steel that displays non-magnetic behavior, similar to that of an austenitic steel, while having sufficient strength and toughness. Along with these non-magnetic properties this steel needs to respond well to heat treatment, meaning maintaining or increasing the physical properties of the steel after being held at elevated temperatures. The second set of parameters outline the goal to find a soft magnetic stainless steel that responds well to heat treatment while maintaining mechanical properties and soft magnetic properties, meaning a strong response to both the introduction and removal of an external magnetic field. The results of these findings will be used simultaneously in the control valve for the new GDI pumps.

The literature review of publicly known and reliable stainless steel data led to the creation of a selection matrix of as many promising stainless steels as could be found. This created a gradient of steels ranging from high mechanical properties and hard magnetic properties to poor mechanical properties and soft magnetic properties. Due to the nature of metal alloying, the most promising steels represent a compromise between the desired soft magnetic and ideal mechanical properties. Properties in the steel were optimized through heat treatments.

Mechanical testing of these stainless steels was completed using a tensile testing machine equipped with two extensometers to collect yield strength, elongation, and young’s modulus. Using data collected during mechanical testing, shear modulus was calculated. Magnetic testing was completed using the magnetic testing device in the graduate labs at UConn. B-H curves were created to show the various points of magnetic data in question. At the end of this testing, we will have a complete selection matrix and suggestion for Stanadyne.

Matthew Prue, Michael Fazzino, and Nicholas Wells Group Photo.

MATERIALS SCIENCE & ENGINEERING

TEAM: 3

SPONSOR: Ulbrich Stainless Steels and Special Metals

ADVISOR: Keith Grayeb, Sean Ketchum

Characterization of Effects of NSCT Scotchbriting Process

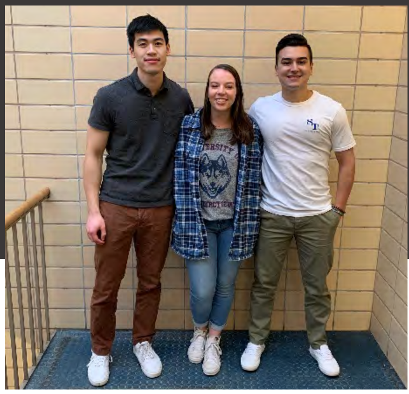
Ulbrich Stainless Steels and Special Metals uses a machine called NSCT Scotchbrite to achieve a product surface finish that is like other industry standard practices such as pickling. The desired surface properties include a high surface cleanliness free of oxides or other contaminants, and a uniform surface roughness. However, a full understanding of the surface properties processed by NSCT Scotchbrite is not available. In order to understand the effect of Scotchbrite on the surface quality of an alloy, the group plans to characterize the effects of Scotchbrite processing (under different process conditions) including oxide presence and depth, and to compare the surface properties achieved by the Scotchbrite with other industry standard methods such as pickling. Based on the correlations established between surface process and surface properties, it is expected that the project will also offer insights on how to improve Scotchbrite processing. Ulbrich Stainless Steels and Special Metals has employed a NSCT Scotchbrite machine for over twenty years for product surface processing. Despite achieving an acceptable surface finish accomplished by empirical experience, a clear understanding of how the Scotchbrite process's effects surface properties is still lacking. Ulbrich has been considering the Scotchbrite processed surface as a special surface finish that is similar to that of pickling, which removes surface oxide.

This assumption has not been validated first hand due to Ulbrich's limited access to advanced surface characterization equipment such as Scanning Electron Microscopy or X-Ray Diffraction. A comprehensive characterization of the surface properties has been challenging with limited equipment available in the facility at Ulbrich. To account for this, this project plans to characterize the similarities and differences between NSCT Scotchbrite and comparable methods in addition to designing a method for Ulbrich to quantify the success of an individual pass on the machine. This project will allow Ulbrich to accurately inform customers as to exactly what the outcome of their processes are to their product.

From Top to Bottom: Ulbrich Stainless Steel and Special Metals Wallingford Facility, Scotchbrite Pad, Ti 35-A Sample

MATERIALS SCIENCE & ENGINEERING

TEAM: 4
SPONSOR: Ulbrich Stainless Steels & Specialty Metals
ADVISOR: Dr. Lesley Frame

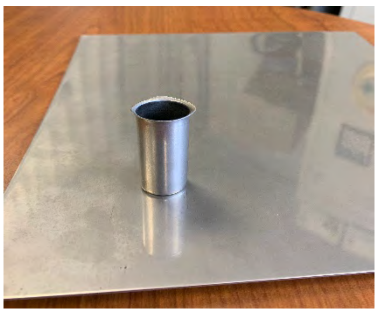


Steven Kha, Grace Quinlan, Joao Carlos Barbosa

Sheet Metal Properties and their Effects on Deep Drawing

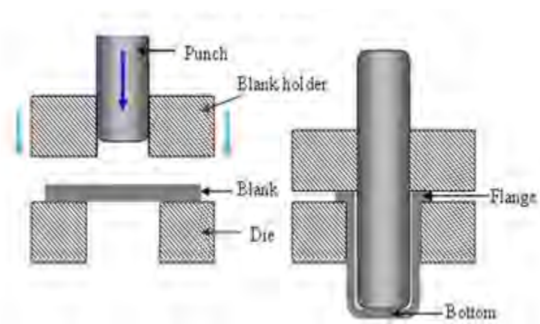
Ulbrich Stainless Steel and Specialty Metals is a company that modifies sheet metals so they can be used for niche applications. Coils of sheet metal are slit to customer specified widths before cold rolling and annealing to achieve desired final properties. Ulbrich's customers produce a wide variety of items including blender blades, nuts, bolts, tubes, cups and pans from the cold rolled sheets.

The main objective of this project is to optimize the processes of cold rolling and annealing for deep drawing of 305 stainless steel as well as determine the limit for deep draw depth after cold rolling. Cold rolling results in the formation of dislocations, which increase the material strength; this process is also called strain hardening. Annealing the material after cold rolling allows for nucleation and grain growth of new grains; thereby increasing the ductility and making deep drawing possible. However, the amount of cold rolling performed prior to annealing can affect deep drawing because a large amount of strain hardening results in a higher tendency for the material to be anisotropic. Anisotropy is undesirable during deep drawing because it causes different grains to have different directional properties. Therefore, it is crucial to optimize the grain structure through defined cold rolling procedures and subsequent heat treatments.



Deep drawing is a process when a metal sheet is radially drawn into a forming die by a punch. Properties that allow for a better deep drawn product include high ductility and high strength. There are many different parameters to take into consideration in order to get a successfully deep drawn part. Parameters of interest include the deep draw ratio, depth of the cavity, punch force and the clamping force. Defects to be avoided during deep drawing include, wrinkling, tearing, galling and earring. Of these four defects, the most common are earring and tearing. Earring is due to the planar anisotropic nature of the sheet which projects unevenness formed along the edge of the flange. Tearing is caused by an increase in tensile stresses which leads to thinning and failure of the metal.

This design project involves cold rolling experiments using different starting thicknesses of 305 stainless steel and different annealing temperatures. After each cold rolling reduction and each anneal, samples are cut and mounted to undergo optical microscopy to track the grain elongation. These samples are compared to already cold rolled and annealed samples provided by Ulbrich in 20-60% reductions. In order to determine the optimal reductions for deep drawing, mechanical testing is done on the samples; specifically tensile testing in 3 different orientations relative to the rolling direction. To test for drawability, a deep draw rig is designed and machined. Abaqus CAE is used to model the deep draw rig and determine ideal parameters for the drawing process. Each reduction is tested on this rig using three different draw ratios. The three draw ratios are further tested by drawing to three different depths to ultimately find the relationship between processing of 305 stainless steel sheet and drawability.

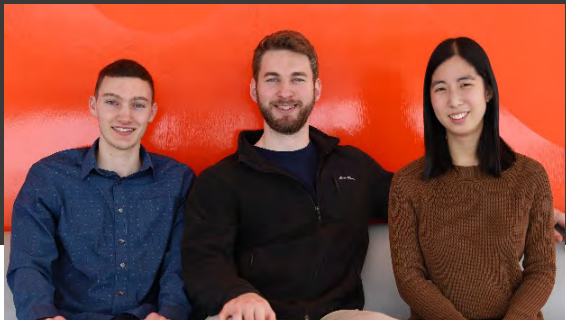


MATERIALS SCIENCE & ENGINEERING

TEAM: 5

SPONSOR: Precision Combustion Inc.

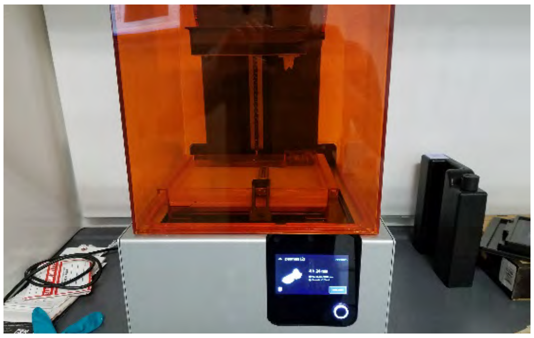
ADVISOR: Dr. Pamir Alpay
Dr. Jeff Weissman (PCI)

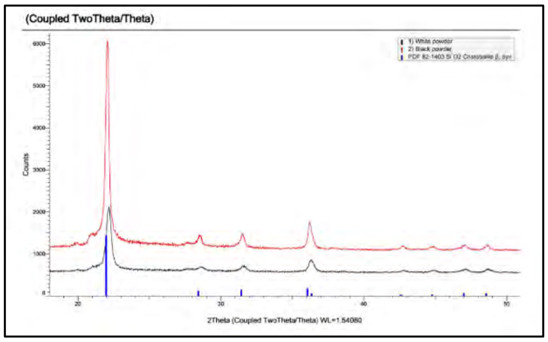


Ryan Corbett, Andrew Spak, Kenna Ritter

Process Design for 3D Printing of Ceramic Components

PCI Precision Combustion, Inc.





Ceramic 3D printing is a new, advanced manufacturing technique. This technique brings the benefits of additive manufacturing such as rapid prototyping, the ability to create complex geometries, and low material waste to ceramic materials. If processed correctly, the printed ceramic components will have all the benefits and potential applications of typical ceramic materials. The process investigated in this project is stereolithography (SLA) printing which is a type of vat photo-polymerization.

Ceramic printing with stereolithography is an additive technology that involves a slurry of ceramic particles in a UV (ultraviolet) curable resin. A UV light will raster across the surface of a pool of the slurry to solidify layers of the resin. The printer builds layer by layer moving the build plate to accommodate new layers of slurry for the UV light to solidify. Once printed, the part is called a “green body”. This green body then has to undergo a complex firing process to finish the product. First, the polymer matrix (the resin) must be burnt out in a process called pyrolysis. After the polymer is gone, the component must then be heated to a sintering temperature. After the ceramic particles are sintered the component can be cooled down.

Precision Combustion Inc. is a clean energy technology company. Their products are used in many fields such as aerospace, gas turbines, fuel cell systems, chemical manufacturing, agriculture, and more. These products fall into four main groups: fuel processors, air cleaners, combustors, and burners/oxidizers. The technologies require materials that can withstand high temperatures and do not react with any of the substances created during these processes.

Precision Combustion Inc. currently uses alumina tubes for their high-temperature reactor that converts gas into fuels. Inside the reactor is a methane-oxygen reaction. The temperatures reach over 800°C, a temperature at which metal tubes would catalyze a combustion reaction necessitating an inert reactor material. The alumina tubes are made of 99.5% alumina with 50% porosity. The goal of this project is to print suitable, fully dense end caps for this tube to contain the reaction. The ceramic particles used in the ceramic-resin slurry are silica, which is compatible with the alumina tube because of their similar thermal conductivities.

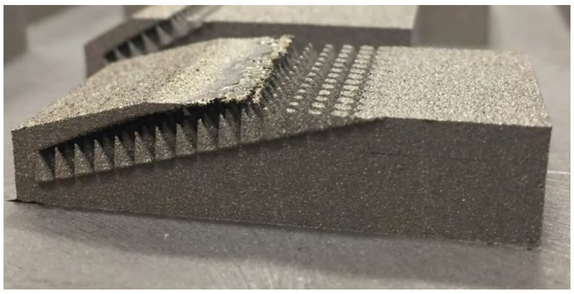
Cayman Cushing (left), William Howard (middle), and Andrew Gagnon (right).

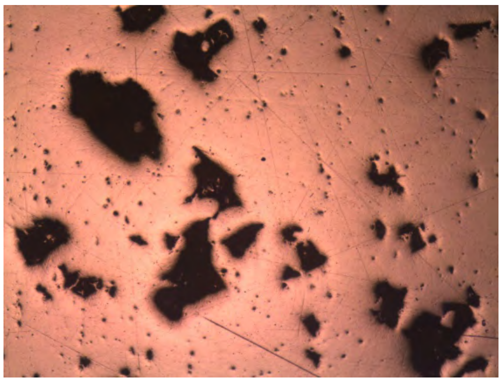
MATERIALS SCIENCE & ENGINEERING

TEAM: 6
SPONSOR: Collins Aerospace
ADVISOR: Colette Fennessy & Loren Brandenburg

Support Structure Design for Powder Bed Additive Manufacturing

Collins Aerospace
A United Technologies Company





During powder bed additive manufacturing, samples have to be built on build plates. The common practice is to use support structures to anchor the parts to the build plate. Special software aid in the design of the support structures and offer numerous design options. Support structures can be solid, lattice grid structures, blades, or cones; many more options exist. Since support structures will need to be removed from the part after the additive manufacturing process, thin walled supports are often desired because they can be removed manually, involving simple hand tools.

The residual stresses that develop during the additive manufacturing process limit the design of thin support structures. Overwhelming residual stresses can cause the support structures to break, causing the samples to warp and the build, eventually, to fail as the machine will stop. The project aims at developing design guidelines for support structures that can be removed manually. Machine parameters, sample geometries, and layout options need to be considered for the specific case of a 3D Systems ProX300 machine.

At the end of the year, the goal of the project is to formulate an additive manufacturing scaffolding guideline for a variety of different geometries. The purpose of the guideline is to have a broad set of rules that should be followed to minimize post-processing time and to ultimately cut down on cost. The scaffold guideline should serve two main functions: bridging the part and holding down the part resisting residual stress-induced deformation. The design should work to find a balance between the two functions. For each of the part geometries, there will be a desired surface finish which correlates to the ease of removal. A balance between surface finish and ease of removal will be factored in the overall guideline.

MATERIALS SCIENCE & ENGINEERING

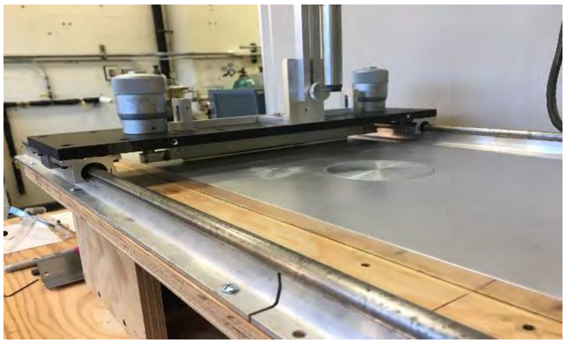
TEAM: 7
SPONSOR: Pratt & Whitney
ADVISOR: Dr. Rainer Hebert

Kierstyn Raines, Tatsuki Katakura, and Meghan Van Wie

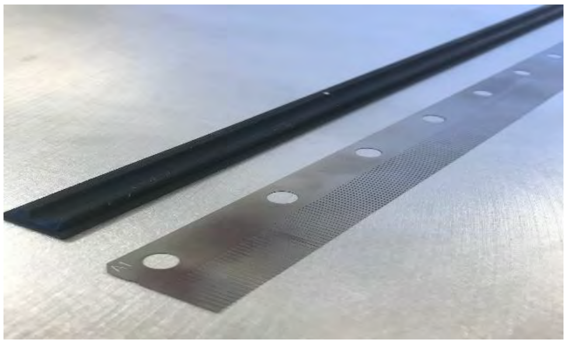
Design and Evaluation of Recoater Systems for Powder Bed Additive Manufacturing

Powder bed additive manufacturing using selective laser melting is a growing field, offering an alternative to the traditional subtractive machining processes. The main benefits include the high flexibility in design and acute understanding of the part production process. Building each part layer-by-layer allows for control over internal properties. This can translate to varying mechanical behaviors and part overall longevity. This method is a generally newer manufacturing technique, thus there is a need for Pratt & Whitney to improve viability of parts and understand possible variations in parameters that contribute towards part quality. Such parameters include recoater blades, powder mesh size, bed density, and layer repeatability.

With a focus on quantifying the variability of powder bed formation, different powders and recoaters can be experimentally tested to evaluate the response. The four types of recoater arm blades are tested in a powder bed simulation apparatus while a camera captures images of powder formation on the build plate. The density and porosity can be determined by this distribution and form the correlation to the overall quality in part printing process. The project explores how to maximize layer repeatability in powder beds. It is known that higher powder bed density minimizes porosity levels which equates to stronger mechanical properties. Additionally, better integrity of printed parts means wider usability of additive manufacturing both in prototyping and product production.



Apparatus of experiments with build plate and metal blade



Recoater blades: rubber and metal comb

MATERIALS SCIENCE & ENGINEERING

TEAM: 8
SPONSOR: Pratt & Whitney
ADVISOR: Dr. Rainer Hebert

Aubrey Tang, Bert Lu, & Steven Gomez

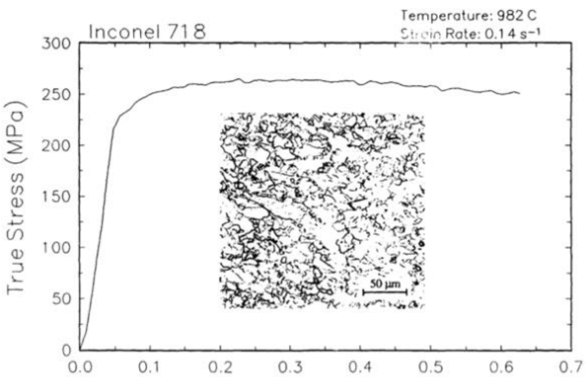
Optimization & Data Analysis of high temperature, high strain rate compression tests with Gleeble Systems

This project has three main objectives. The first main objective is to optimize the interface condition between samples and anvil caps with a systematic study of lubricants in the Gleeble 3500 system. Secondly, this project also aims to achieve uniform temperature distribution within the sample during adiabatic heating. The third objective of this project is to develop an efficient way of achieving the desired strains and strain rates during the compression test.

In order to determine the best lubricants to use in order to optimize the interface condition between the samples and anvil caps, the group chose lubricants that meet the project's requirements. Lubricants selected for this project must be able to withstand high temperatures, as the experiments will be run at above 900℃, and be electrically conductive as the machine passes a current through the sample via direct resistance heating. The group selected to use tantalum foil and graphite foil while also utilizing nickel paste as an adhesive. These lubricants are all able to withstand the temperature the group would like to test, and they are also electrically conductive.

The experimentation involves careful preparation of the sample itself. Thermocouples are used in order to determine the temperature in the specimen and in this experimentation. Two pairs of thermocouples will be used to determine the temperature in the center of the sample and at the edge of the sample as a way to check if there is any uneven heating throughout the specimen.

The critical constraints for this project is time and machine availability. Each test requires 20-30 minutes to complete, which means the total amount of time required for testing is estimated to be 16-25 hours. The Gleeble 3500 is shared among different groups, and the availability of the machine is also limited. In order to successfully complete this project, the group must figure out a method to reduce testing time.



CHAUDHURY, P., & ZHAO, D. (1992). Atlas of formability: INCONEL 718(Final Report, 30 Apr.- 31 Jul. 1992).

Left to right: Beril Tonyali, Avery Gray, Lara Huapaya Rojas

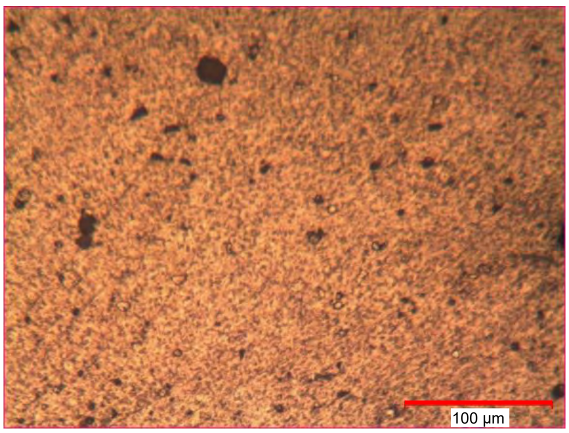
TEAM: 9
SPONSOR: Sikorsky
ADVISOR: Dr. Seok-Woo Lee (Faculty)
Tom Derco, Bill Fallon (Industry)

Post-Processing Heat Treatments of Additively Manufactured Aluminum Alloy, AlSi10Mg

Additive manufacturing (AM) has fostered a lot of interest in the aerospace industry recently because of its printing efficiency, reduced costs, minimal material waste, and higher quality final products. The AM technique known as direct metal laser sintering (DMLS) uses a laser to melt metallic powder particles together. Desired geometries are produced by working in thin layers of powder deposits along the surface, melting them, and building up from the platform in this way until the final product is achieved.

Aluminum alloys are the materials being explored for use in AM technology because it is lightweight, has high strength, and has the ability to be easily alloyed with other elements to enhance or eliminate specific material properties. Wrought 6061 Aluminum is currently the most commonly used alloy in aerospace since it has phenomenal mechanical properties, however its adhesion properties are poor. Although much weaker, AlSi10Mg is one of the first additively available powders to be used as an alternative to wrought Al 6061 because of its excellent bonding capabilities, which is key for AM purposes. Sikorsky is interested in determining what kinds of processing techniques can be used to further improve AlSi10Mg alloys to achieve mechanical properties comparable to those of wrought Al 6061.

The purpose of this project is to understand the structure-properties-processing relationships of heat-treated AlSi10Mg in order to substantially improve the mechanical properties of the alloy. This will eventually lead to a far superior material that can be utilized for additive manufacturing purposes. The approach for this project is to create a design of experiments to test heat treatments varying in time and print orientation. Samples were provided by Sikorsky, where they were printed in XY or ZX orientation. Once received at UConn, samples underwent post-processing heat treatments. Solutionization heat treatments with varying times were the main concern. Heat treated samples were then tested using a tensile tester, and evaluated microstructurally to draw conclusions on structure-properties-processing relationships, and determine optimal post-processing heat treatments.



Images: AM sample obtained from Sikorsky, ready for heat treatment *(top)*. Sample undergoing a tensile test for measurement of mechanical properties *(middle)*. Microstructure of AlSi10Mg that underwent heat treatment at 530°C for 1 hour, 200x magnification. Silicon particles apparent in microstructure *(bottom)*.

Left to right: Jonathan Gager, Spencer Matonis, Zachary Putney, Ryan Wrobel

MATERIALS SCIENCE & ENGINEERING

TEAM: 10

SPONSOR: NASA

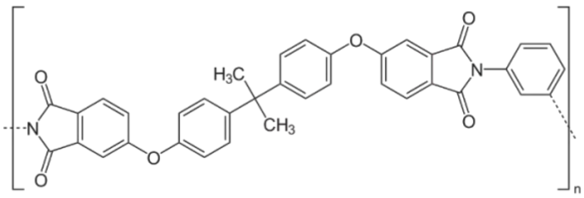
ADVISOR: Dr. Volkan Ortalan (Faculty Advisor)

Tracie Prater, Curtis Hill, Jennifer Edmunson (Industry Advisor)

Development of Novel Feedstocks for In-Space Additive Manufacturing

Currently, there is a sizeable gap between the mechanical properties of plastic versus metal additively manufactured components. The goal of this project is to bridge this gap by doping various thermoplastic materials to enhance the mechanical properties of the composite filament. Along with enhancement of mechanical properties, NASA has shown interest in being able to add functionality to these feedstocks, including a conductive or dielectric filament that could be used in electrical applications.

The primary matrix material being considered is polyetherimide (PEI), commercially known as Ultem. This high-temperature thermoplastic exhibits exceptional mechanical strength, has a high strength-to-weight ratio, and has an exceptional flame, smoke and toxicity (FST) rating. There are two payloads currently on the International Space Station (ISS) that work with Ultem: the Additive Manufacturing Center from Made In Space and the Refabricator from Tethers Unlimited. Potential matrix materials under consideration for electrical applications include polyvinylidene difluoride (PVDF) and high-density polyethylene (HDPE) for their standalone dielectric properties. Commercially well-characterized polymers such as polycarbonate (PC) and acrylonitrile butadiene styrene (ABS) may also be considered and tested.



Dopant materials to improve mechanical strength include short carbon fibers, silicon carbide (SiC) whiskers, graphene, and carbon nanotubes. Dopant particles for electrical applications include graphene and barium titanate ($BaTiO_3$). NASA is also interested in incorporating in-situ resources into the novel feedstocks. Ferromagnetic particles from a lunar simulant could potentially be used in a conductive feedstock, while the non-ferromagnetic particles could be used to improve mechanical properties. Nickel, a common element that is found in Martian regolith, will also be tested for electrical properties.

To achieve adequate particle dispersion through the matrix, a dissolution method is being practiced. This involves dissolving the thermoplastic matrix using a chemical solvent and adding particles to the solution. The solute-solvent ratio is critical to identify an optimum viscosity to suspend particles within the polymer. Once the particles are dispersed through the matrix, the solvent can be boiled off to prevent significant moisture from being in the composite. The composite is then pelletized and fed into the hopper of a Filabot EX2 extruder to create a filament. Data from differential scanning calorimetry and melt flow index testing are used to identify the critical temperature at which each individual composite must be extruded for adequate properties.

The student team (left to right): Piotr Chaber, Brendan Kristie, Chase Sheeley

MATERIALS SCIENCE & ENGINEERING

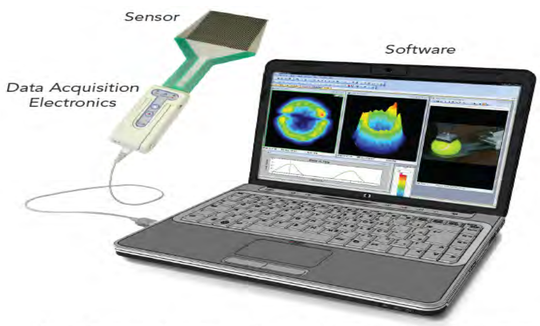
TEAM: 11

SPONSOR: Ensign-Bickford Aerospace & Defense

ADVISOR: Prof. George Rossetti Jr

Design of Improved Methods for Tubing Deformation and Powder Distribution Characterization in Linear Shaped Charges

EBAD Ensign-Bickford Aerospace & Defense RIGHT FOR YOUR MISSION



I-Scan System: Includes software, data acquisition electronics, & sensors (standard Evolution® system shown)

Ensign-Bickford Aerospace & Defense (EBA&D) is a precision explosives manufacturer located in Simsbury, CT. The company is a subsidiary of Ensign-Bickford Industries, Inc. EBA&D has tasked the project team with achieving two major objectives. The first objective is to develop a deformation process for their linear shaped charges (LSC) that allows for manufacturing using copper or a copper-based alloy without introducing defects, such as cracks or thinned walls, during shaping. The second objective is to develop a characterization method for quantifying the packing uniformity of the explosive powder that is contained within the various types of LSCs that the company manufactures.

EBA&D currently manufactures LSCs from aluminum tubing. Transitioning to copper tubing opens new opportunities to expand these products into other markets. LSCs made of lead have shown strong performance, but pose health and environmental risks. Copper is known to perform better than aluminum, but cannot be formed using the current manufacturing process. Adapting the forming process for use with copper or a copper-based alloy would satisfy safety requirements while meeting performance standards for current and future applications. EBA&D also needs a reliable method to quantify the packing of the explosive powder after forming, which greatly affects detonation and the efficiency of the explosive jet, and so is an important quality control metric. An accurate, reproducible and cost-effective method for characterizing powder uniformity does not currently exist within the company.

Major constraints on the solutions to these problems are imposed by the explosive nature of the product. The replacement tube materials must be COTS, fabrication processes must utilize EBA&D's existing manufacturing facilities, and heat treatment is prohibited. Powder characterization methods must be inexpensive and implemented in-house. The adopted approach involves mechanically testing different types of copper in order to gather data showing which is the most ductile and the most susceptible to the cold working done in the current EBA&D shaping process. Greater formability is favorable. Critical parameters in the current process were identified and are analyzed in the project so that adjustments can be made to successfully form LSCs with copper. The powder characterization approach involves scanning by a piezoelectric sensor, which uses software to convert pressure detection into a colored map of density variation.

Adam Li, Jordan Gomes, and Iwona Wrobel.

MATERIALS SCIENCE & ENGINEERING

TEAM: 12
SPONSOR: KX Technologies
ADVISOR: Dr. Stefan Schafföener

Compression Molding of Carbon Block Filters

KX Technologies LLC is a company that specializes in filtration using activated Carbon. Their products are used in multiple common house hold appliances such as refrigerator filters and Brita water purifiers. KX Technologies creates the filters by mixing activated Carbon with a binding agent and then extruding it into a long cylinder. This cylinder is then divided into shorter pieces that form the basis of the filter. The processing technique of extrusion is extremely productive and time efficient, but it also requires a large amount of material to perform. This means that an alternative process must be used if small batches for research needed to be created. As a result, KX Technologies has tasked our group with determining if the compression molding process is suitable for making small batches of their filters.

Compression molding is a processing technique where a mold containing a powder is heated and then pressurized in order to initiate binding and create a singular solid product. For this design project activated Carbon is mixed with a binding agent inside of a cylindrical mold. By applying heat and pressure, the binding agent fuses the powder into a solid cylindrical filter. The disadvantages of compression molding are that it is limited by the size of the mold and that it takes far more time than extrusion. However, compression molding is a good choice for small research samples because it allows for variation without using a large amount of material. The compression molded samples created here at UConn were tested for mechanical properties like porosity, strength, and hardness and then be compared to KX Technologies' extruded samples. If the compression molding technique is deemed viable by KX Technologies they will be able to test new binding agents as well as different compositions for experimental filters.

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MATERIALS SCIENCE & ENGINEERING

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Design of a Machine Learning Algorithm to Design/Discover Layered Materials for Battery Applications

Graphite (layered sheets of carbon atoms) based lithium ion batteries are today's ultimate rechargeable energy storage technology. They have now become the main power supply for laptops, cameras, mobile phones and electric vehicles. However, graphite's low charge capacity will not meet the high demands of the next-generation energy storage capacities. Moreover, the current challenges with the costs and availability of lithium have triggered efforts toward design and discovery of alternative materials to graphene and lithium for battery applications.

Recently, two-dimensional (2D) transition metal dichalcogenides (TMDs) have attracted intensive research activities (Fig. 1). Their excellent electrochemical properties and 2D layered structure like that of graphite show a great promise to be used as a next generation of energy storage material. Characterization of all possible TMDs through experimentation is extremely expensive and time consuming. As a result, present study utilizes powerful computer models and machine learning tools to screen hundreds of TMDs with the goal of computationally guiding experimental work in order to ultimately accelerate the design and discovery process of layered materials for battery applications.

Density functional theory (DFT) is a sophisticated quantum mechanical modelling method that simulate the physics of materials at an atomic level. DFT simulations are used to calculate fundamental properties of over 160 TMD's for its two different phases (Fig. 2) using high performance computational resources at UConn. Results of DFT simulations lead to determination of structural energetics, phase stability, phase transformation, and volumetric expansion of the TMD's upon insertion of lithium, sodium and potassium ions in between the interlayer spacing.

Large datasets built using DFT calculation data were then analyzed using machine learning (Fig. 3) to make correlations between atomic scale descriptors and phase energetics, transformation behavior as well as volumetric expansion due to intercalation. This work set a framework for future DFT and machine learning based discovery/design of layered materials in CMMG in collaboration with EaglePicher LLC.

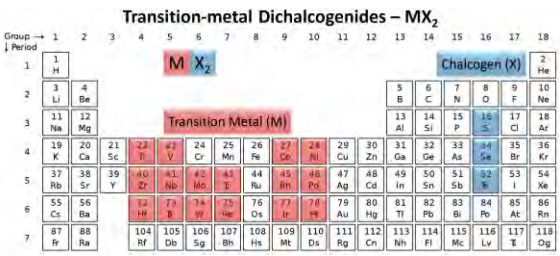

Figure 1. Periodic table highlighting 16 transition metals and 3 chalcogen atoms.

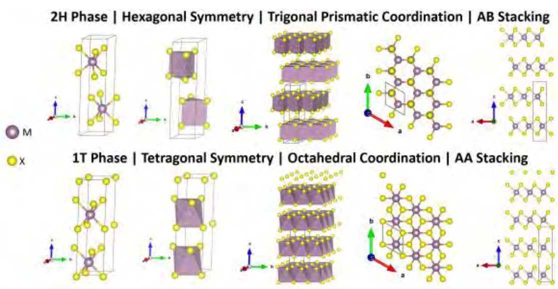

Figure 2. Schematics of 2H and 1T phases of 2D layered TMD materials.

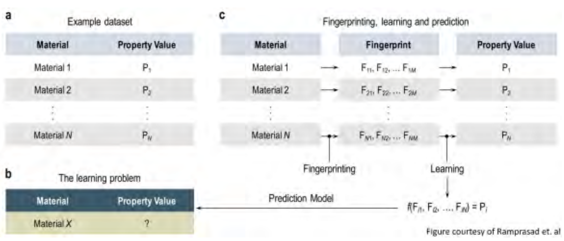

Figure 3. Key elements of machine learning in materials science.

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Optimization of Laser Welding Parameters for Electrical Conductivity

The foremost significant obstacle that stands in the way of conventionalization of electric vehicles is their insufficient range; which could be improved by increasing the energy density of battery cells. Cadenza Innovation, a pioneer in low cost, high energy density, lithium-ion cell technologies, has been implementing their improved 'jellyroll' battery design and novel packaging of "jellyrolls" into a supercell system to address the issue. The company is dedicated to provide the market with safe and reliable lithium-ion cell assemblies.

Cadenza Innovation's supercell assembly.

The main objective of the project is to reduce the joule heating effect in aluminum weld joints of the lithium-ion supercell system. The resistive heating of the welds directly affects the efficiency of the system; which is the most important factor for the emerging electric vehicle technology. Furthermore, Cadenza Innovation requires the formulation and design of a non-destructive testing method to electrically assess the weld joints in their assembly line as the company aims to not only develop the most efficient battery system but also to develop a process that is applicable to mass manufacturing with competitive profitability margins.

Laser weld pattern on Al3003-H14 sample.

Our design team has worked diligently to understand, investigate, and solve the undesired heating effect in the welds of the cell assembly. Through theory and modeling, different combinations of laser welding parameters were arrived at and tested to yield the most favorable microstructure for electrical conductivity. The optimal microstructure for electrical conductivity is found to be when there are large, oriented grains with no intermetallic compounds present at the grain boundaries. However, achieving this is easier said than done when dealing with very fast non-equilibrium heat transport.

Left: NDT Test Rig. Right: Weldment on testing platform.

The secondary goal of this project is to develop a method for non-destructive testing (NDT) of the welds. The physical deliverable for this is in the form of a prototype NDT rig meant to be used in the assembly line for weld verification. The test rig contains an electrical resistivity testing system, specifically designed to ensure that the resistivity of the weld is low enough to carry the high current load without excessive heating.