Investigation of the Use of AFM on the RPI 3D Manufacturing Project

Chris Nkinthorn
MANE 6292: Experimental Mechanics

I. Introduction

THE objective of this research is to model and experimentally verify the physical properties and desired microstructure of 3D manufactured Inconel 718 through the selectively laser melting of deposited metal powder. In particular, the purpose of this paper are fourfold. First, to introduce the process of manufacturing parts through powdered metal deposition and selective laser melting. Secondly, to introduce the overall experimental of the RPI NASA 3D Manufacturing project; its three major subprojects: Testbed, Finite Element, Phase Field; as well the interplay between the three groups. Third, to elaborate on the status research currently being conducted in the finite element subproject. Finally, to investigate the application of Atomic Force Microscopy (AFM) to the mechanics of dendritic growth in the process of solidification of Inconel 718.

II. Experimental Description

In the manufacture of selectively laser melted (SLM) parts, a raw metal substrate is coated with a fine metal powder to be melted using a laser to provide the necessary thermal energy and mirror to direct the laser beam. The powder directly under the beam is fully melted: some material becoming fully liquid and some material leaving as vapor. The laser tracks moves over the powder bead to create a single cross section of of the final metal part. Without the completed layer necessarily being fully cool, another layer of fine metal powder is deposited and the process is repeated until a complete part is manufactured and can be extracted from the powder bed. This process is distinct from the process of selective laser sintering (SLS) which is an other method of additive manufacture.

Sintering is similar as an additive manufacturing process in that a powdered metal is deposited on a substrate and heated using a laser beam. However, this process distinct because it does not fully melt the metal powder. This difference is significant because sintering does not allow for the creation of dendritic crystal structures because the material never fully liquefies. The reason for this is because the solidus temperature is never reached and the processes of liquification and solidification cannot occur. Though this benefits SLS as a less energy expensive process, this also leads to a difference in the possible physical properties of the final part.

A. Methods and Materials

1) Project Organization: The RPI NASA project is divided into three subprojects: testbed, phase field, and finite element. The testbed project is responsible for conducting experimental testing and conducting the experiments at the appropriate process parameters. The phase field subproject is responsible for the measurement of the part's microstructure and physical properties. Finally, the finite element team is responsible for the modeling of the physical properties such as phase, microstructure, porosity, and resulting temperature given process parameters of laser path and power, powder layer thickness, component powder diameter, and component material. The finite element subproject aims to be capable of modeling 3D manufacturing of any part, independent of material. However, the overall project concerns the properties of Inconel 718, specifically and will be used by the testbed subteam for experimental validation. These subprojects interrelated in that information is shared between subteams. The testbed and finite element subprojects share validation of temperatures reached, resulting part porosity, and geometry. The testbed team also shares Gcode which dictates the laser path motion, speed, and output power of the finite element subproject. Gcode is a commonly used in computer aided machining and manufacturing code that has been adapted for use in the SLM project. The finite element subteam then suggests process parameters which would help better model the results presented by the testbed subproject. The finite element subproject also communicates with the phase field subproject in verifying temperature and phase history through defined material points and the corresponding microstructure which result at these locations.

2) Research Status: Currently, the author works under Dr. Antoinette Maniatty in the Finite Element subproject with interests to eventually do work on the phase field subproject studying the parts phase history and resulting microstructure. The following content introduces the process to conduct the author's current work.

B. Data Collection Package

The finite element subproject uses the following process to model the physical properties of material parts created by SLM. This begins by way of creating a solid model part file in SolidWorks, Creo, NX, or another CAD suite. This part file is then converted into a Parasolid file to be opened in Simmodeler. Simmodeler is a program by Simmetrix as part of their Simulation Application Suite and is used by the finite element subteam as a way to create the meshes needed by the Albany code to model SLM. Albany is a implicit, unstructured grid, finite element code created by Sandia National Laboratories, used to model the multiphysics problem presented.The specific Albany problem in this case is Additive Manufacturing Process (AMP). Albany heavily utilizes the Trilinos framework. Trilinos is another project to develop object oriented software for multiphysics problems in science and engineering, focusing on the distribution of its various packages. Albany can also utilize the Rensselaer Polytechnic Institute (RPI) Scientific Computation Research Center's (SCOREC) Parallel Unstructured Mesh Infrastructure (PUMI) software, though this is an optional dependency which is used by the subteam. Albany, Trilinos, and PUMI repositories are all freely available on Github.

Albany is available as a command line tool which can run simulations through a shell interface. The command used is:

```
mpirun -n <number_of_cores> <
    path__to_Albany_Executable>/AlbanyT <
    name_of_input_file>
```

Note that because Albany is is an implicit finite element code, the argument `<number_of_cores>` specifies the number of processor cores to be used to more quickly create the simulation model through parallel computing. Albany requires two files to complete a simulation: an Albany input file, and a material database file, which in this case is `IN718.yaml`.

The argument `<name_of_input_file>` references the main input file. This file serves as a place to reference the other necessary input files such as the material database file, input parameters, output specifications and the solving parameters which are all required by Albany. The final simulation model then has the necessary outputs desired by the subteam: temperature, phase, porosity, and part geometry.

The resulting data is then communicated to the testbed and phase field subprojects as described in the subsection, Project Organization. The resulting simulation outputs should then match the the temperatures, porosity, and geometry of the resulting part measured by the testbed subteam as well as the microstructure predicted by the phase field team. Currently, the finite element subproject does not fully model the process of SLM to the degree desired as some physical processes are neglected in the current code.

C. Modeling Process and Deficiencies

In summary, the subproject models SLM by way a finite element approach to an energy balance of the powder metal liquefying under the thermal energy provided by the laser beam as it travels along a specified path, as dictated by the first law of thermodynamics on some time interval and some bounded domain, using the phase field approach for the interfacial problem presented. The phase field approach is a convenient method for modeling the change between powder solid liquid or vapor as the laser beam heats the powder metal by allowing the interface to become diffuse and a function of state variables. This is used in the weak form of the finite element method to smoothly approximate the Heaviside function at the interface boundary.

In detail, an energy balance on domain Ω for time interval τ can be expressed in terms of the temperature T and state variables $0 \leq \phi_1, \phi_2, \psi_1, \psi_2 \leq 1$ as

$$\frac{d}{dt}e(T, \phi_1, \phi_2, \psi_1, \psi_2) - \text{div}\left[k(T, \phi_1, \psi_1, \psi_2)\text{grad}T\right] - U(\boldsymbol{x}, t, \psi_1, \psi_2) = 0 \quad \text{in } \Omega \times \tau \quad (1)$$

where e is the energy density function; k the thermal conductivity; U the heat flux provided by the laser beam.

This partial differential equation has boundary and initial conditions of temperature which can be described by:

$$T(\boldsymbol{x}, t) = \hat{T}(\boldsymbol{x}, t) \text{ on } \Gamma_1 \times \tau \quad (2)$$

$$-\left[k(T, \phi_1, \psi_1, \psi_2) \text{ grad}T\right] \cdot \boldsymbol{n} = \hat{q}(T) \text{ on } \Gamma_2 \times \tau \quad (3)$$

$$T(\boldsymbol{x}, 0) = T_0(\boldsymbol{x}) \text{ in } \Omega \quad (4)$$

where $\hat{T}$ is a prescribed temperature on part of the boundary Γ_1 in Eq. (2), $\hat{q}$ is a prescribed flux that may be temperature dependent (e.g. Stefan-Boltzmann radiation) on part of the boundary Γ_2 in Eq. (3), $\Gamma_1 \cup \Gamma_2 = \Gamma$, and T_0 is the initial temperature field.

However, the current model is deficient in it does not account for the energy leaving the system by ablation. That enthalpy unaccounted for and needs to be modeled in order to more accurately simulate the results provided by the testbed subproject. Another deficiency is that the temperature history is not maintained between layers of the simulation, which is necessary for determining the phase history of the modeled part. However, the current refactor of the Albany code which began in September 2018, will change the input file arguments and may add in the necessary ability to maintain a temperature history of the simulated part. However, this is not certain as the current refactor is incomplete and may end up being part of another future refactor.

D. Data Analysis

In this section serves the evaluation of the use of atomic force microscopy (AFM) for measurement of the dendritic microstructure of SLM parts is investigated, beginning with an short summary of the process behind dendrite growth. Dendrite growth refers to the creation of microstructure created during the solidification process of materials. This can be seen in the formation of snowflakes through the diffusion of water through air onto the ice crystals. This is because as the liquid freezes, the resulting solid is initially spherical in shape. However, as this spherical solid interface grows, surface instabilities causes the crystal shape to grow faster along energy favorable directions because of the material anisotropy. This leads to a dendrite's distinctive branching shape.

Some work is done using the AFM in investigation of dendritic crystal structure, presently

However, this research using the AFM is limited to poly S lactide on a heated base of 160^o C. This is because a major limitation of studying dendritic growth in IN718, and metals in general, are the very high melting temperatures required, which the AFM cannot support. However, there is a need for the near real time visualization provided by the AFM. Also, because of the material independent phenomena of dendrite growth, this research still serves to study the physical mechanisms in question but would not benefit the author in his particular future research.

If the AFM were to be applied to the 3D Manufacturing project, a small region of laser melted material on powder bed could be used to analyze the local modulii of the resulting part. On successive passes, the local phase may change due to the laser path remelting the already solidified part, which could not be captured by the AFM. This process may still be useful in validating the eventual integration of a temperature history if this comes out of the September refactor, or some future change. This would be done by using the AFM between passes. However, the time elapsed between both layers and measurements would also need to be recorded and simulated by the finite element subteam and related back to the simulated temperature history.

III. Results

Given the degree of precision provided by the AFM, it is expected that the resulting modulii measurements would be very accurate. However, the goal of the subteam the author works on is specifically interested in the modeling of the material whereas validation would be part of the testbed or phase field subteams. In analysis of the results collected from the AFM, which would contain the local modulus as a function of the position, a modulus gradient could be calculated which might show the lower shear stress along the interface of the dendrite crystals. Another possible methodogy would be if the modulus is measured in two orthogonal directions at each location. The basis for this method is that because dendritic growth is a function of the material anisotropy, then the measurement of the local modulii might also be used to back out the material anisotropy.

IV. Conclusion

Though the AFM would provide important, near real time visualization of the processes behind dendritic crystal growth, this instrument would not be useful in the author's future research concerning the modeling of IN718 but would and currently provides useful insight into the governing mechanics behind dendritic solidification.

References

[1] Maniatty, A. M., *Rensselaer Polytechnic Institute*. 3d Manufacturing Model and Analysis. Internal Project Overview, 2018.

[2] Roy, S. and Juha, M. and Shephard, M. S. and Maniatty, A. M..Heat transfer model and finite element formulation for simulation of selective laser melting. *Computatinal Mechanics*, vol. 62.3, pp. 273-284, 2018.

[3] Y. Kikkawa, H. Abe, T. Iwata, Y. Inoue, and Y. Doi. In Situ Observation of Crystal Growth for Poly[(S)-lactide] by Temperature-Controlled Atomic Force Microscopy. *Scientific Reports*, vol. 2.3, pp. 940-945, 2001.

[4] Gibbs, J. W. et. al. The Three-Dimensional Morphology of Growing Dendrites. *Scientific Reports*, vol. 5. art. 11824. 3 July 2015.

[5] Bhadeshia, H.K.D.H. Dendritic Solidification. *University of Cambridge* http://www.phase-trans.msm.cam.ac.uk/dendrites.html