Final Report:

**Supervised linear regression machine learning model to predict the primary dendritic arm spacing**

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# Problem Statement

During the solidification of metallic systems, the microstructure grows in treelike dendritic shape and the morphology of dendrites has a strong effect on the mechanical properties. Spacing between the dendrite arms provides information on segregation patterns and distribution of precipitates between the dendritic arms, which influences the mechanical properties. There are two well-known theoretical models that relate the primary dendritic arm spacing (PDAS) to solidification conditions, namely pulling velocity (V) and temperature gradient (G), and material properties like liquid diffusivity (, the freezing range (, Gibbs‐Thomson coefficient (, and equilibrium partition coefficient (. The two models, named Hunt-Burden (HB) [1] and Kurz-Fisher (KF) [2], are different in the way the material properties are accounted:

HB model   
 . KF model

Despite the previous attempts, there are still important issues to develop a predictive model of PDAS for a wide range of solidification rates. In rapid solidification cases, such as in laser additive manufacturing of materials, the analytical relations and models for PDAS have significant deviations from computational predications and experimental data for the same solidification condition [3]. In this project we want to develop more reliable analytical models for prediction of PDAS in a wide range of solidification rates. For this, a supervised linear regression machine learning model will be used to produce a new relation between PDAS and the solidification rate (pulling velocity and temperature gradient in the model) that works for different material systems.

# Data Wrangling

PDAS data for the PDAS versus solidification rate and for different materials systems is generated for 7 alloy systems, with various solidification velocity range (from 10‐4 m/s to 0.12 m/s), temperature gradient range (from 106 K/m to 107 K/m) of 10 different alloys to generate enough data points for machine learning analysis. Obtaining quantitative prediction of the characteristics of solidification process with phase field simulation approach requires additional knowledge of crystal melt properties, such as anisotropic crystal-melt interfacial free energy and anisotropic kinetic coefficient. A major limiting factor is the scarcity of available experimental data pertaining to crystal-melt interfacial properties. Integrated atomistic and phase-field simulations will be performed in order to investigate the solidification of binary alloys. We will first perform large scale MD simulations utilizing our recently developed second-nearest neighbor modified embedded atom method (2NN-MEAM) interatomic potentials for Al‐Cu, Al‐Ni, Al‐Fe, Al‐Si, Al‐Mg, Ni‐Ti, Ti‐Al, and additional interatomic potentials in literature for Cu‐Ni, Ni‐Fe, and Ni‐Nb to calculate the above-mentioned crystal-melt interfacial properties.

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| --- | --- | --- | --- |
| Alloy | V (m/s) | G (K/m) | Number of data points from PF modeling |
| Ti-3.4 at% Ni | 0.01-0.09 | 107, 8×106, 7×106,6×106, 5×106 | 45 |
| Ti-7.1 at% Ni | 0.01-0.09 | 107, 8×106,7×106,6×106, 5×106 | 42 |
| Ti-10.4 at% Ni | 0.0001-0.02 | 107, 5×106 | 22 |
| Mg-9 at% Al | 0.005-0.12 | 5×106,3×106, 1×106 | 21 |
| Al-6 at% Cu | 0.001-0.06 | 107, 8×106, 7×106, 6×106, 5×106 | 47 |
| Al-8 at% Cu | 0.01-0.08 | 107, 8×106,7×106,6×106, 5×106 | 43 |
| Al-10 at% Cu | 0.008-0.005 | 107, 8×106,7×106,6×106 | 30 |

In a separate study I have performed simulation study to obtain the computational data on PDAS for 7 different alloy systems (250 data points totally), for a wide velocity and temperature gradient range (given in table 1). We have also calculated all the material properties needed for each alloy systems ().

Table 1- Summary of the computational PDAS and the range of velocity (V), temperature gradient (G), and the number of datapoints for each alloy system.

In order to use a regression model, we will take the logarithm from both sides of the PDAS equation for both HB and KF models, while keeping the coefficients on ln(V), ln(G), ln(mat\_HB), and ln(mat\_KF) as unknown in the linear regression models.

Then the data from computational PDAS will input into the linear regression models to obtain A, α, β, and γ.

**References:**

[1] M.H. Burden, J.D. Hunt, Cellular and dendritic growth. II, Journal of Crystal Growth, 22 (1974) 109-116.

[2] W. Kurz, D.J. Fisher, Dendrite growth at the limit of stability: tip radius and spacing, Acta Metallurgica, 29 (1981) 11-20.

[3] W. Xiao, S. Li, C. Wang, Y. Shi, J. Mazumder, H. Xing, L. Song, Multi-scale simulation of dendrite growth for direct energy deposition of nickel-based superalloys, Materials & Design, 164 (2019) 107553.