Quadtree Grids and Dendritic Growth

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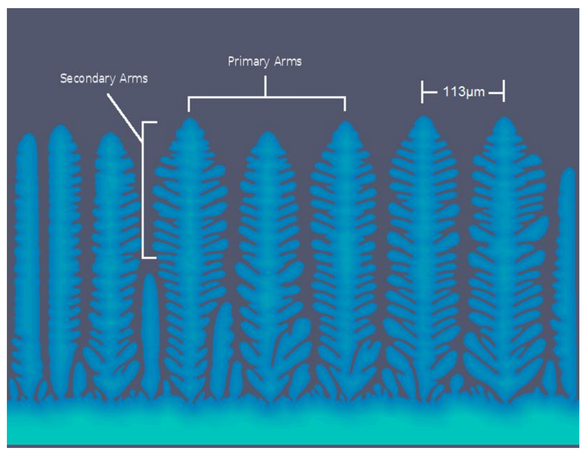
Introduction

Polycrystalline materials such as most metals, are commonly made of dendritic crystals on the micrometer scale. It is of great interest to understand the growth of these crystals, as their characteristics, such as their size and shape, significantly impact the properties of the material. My lab is developing a numerical method and computer simulation that attempts to accurately model the dendritic growth of these crystals during the casting of a metal or alloy. A complete understanding of this process would result in the ability to manipulate these characteristics and ultimately allow for the properties of a metal to be tailored to specific applications. Our simulation aims to provide a fast and free alternative to time consuming and expensive experiments, improving the efficiency of research on this subject.

- Completed simulation:



Applications

The ability to customize the properties of a metal or alloy has a countless number of applications.

- Jet engine turbine blades are exposed to extreme temperatures and forces, and it would be desirable to develop a stronger and more heat resistant alloy.
- The result of turbine blades made of inadequate material:

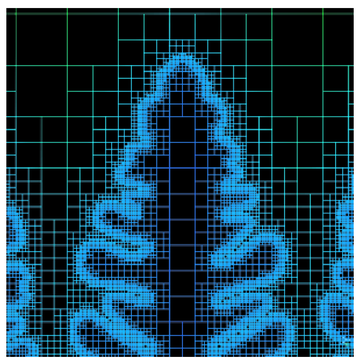
Courtesy of iagblog.blogspot.com

Objectives

- Prove our numerical method.
- Show the simulation is working accurately by matching existing experimental data to data from our simulation.
- Enable extensive research on dendritic crystals.
- Save time and money.

Methods

- Our numerical method solves partial differential equations using a technique called a level set method.
- These calculations are programmed in C++ to create the simulation, and stored using a quadtree grid.
- A quadtree grid uses a variable resolution, which decreases computational time dramatically:



- The simulation outputs files that we view using the visualization software ParaView.
- In ParaView, we make the following measurements:
  - Primary and secondary arm spacing
  - Heat gradient
  - Crystal growth rate
- The following equations were found experimentally to accurately predict the primary and secondary arm spacing in real crystals:

$$PrimarySpacing = k\frac{1}{HeatGradient^{\frac{1}{2}} \times GrowthRate^{\frac{1}{4}}}$$

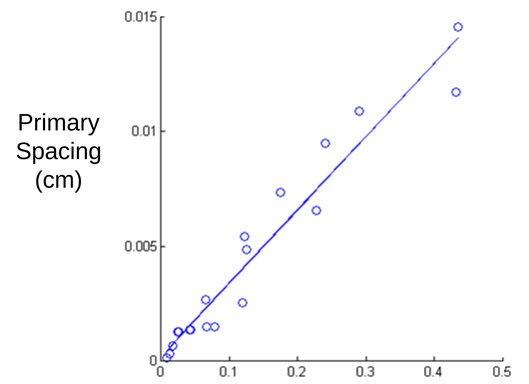
$$SecondarySpacing = k\frac{1}{(HeatGradient \times GrowthRate)^{\frac{1}{3}}}$$

- We enter our measurements into these equations and plot the results using MATLAB.

Results

- From the following equation we expect a linear relationship between the left and right side.
- Each circle on the plot represents a separate simulation.

$$PrimarySpacing = k\frac{1}{HeatGradient^{\frac{1}{2}} \times GrowthRate^{\frac{1}{4}}}$$

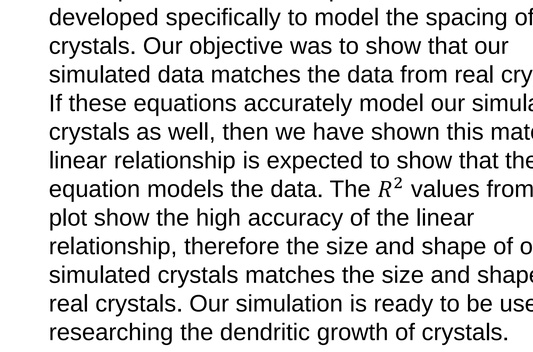


$$Heat\ Gradient^{-1/2} \times\ Growth\ Rate^{-1/4}$$

- The above plot has a coefficient of determination of $R^2 = 0.942$

Results cont.

$$SecondarySpacing = k\frac{1}{(HeatGradient \times GrowthRate)^{\frac{1}{3}}}$$



$$(Heat\ Gradient\ \times Growth\ Rate)^{-1/3}$$

- The above plot has a coefficient of determination of $R^2 = 0.983$

Conclusion

The equations we used to plot our results were developed specifically to model the spacing of real crystals. Our objective was to show that our simulated data matches the data from real crystals. If these equations accurately model our simulated crystals as well, then we have shown this match. A linear relationship is expected to show that the equation models the data. The R^2 values from each plot show the high accuracy of the linear relationship, therefore the size and shape of our simulated crystals matches the size and shape of real crystals. Our simulation is ready to be used for researching the dendritic growth of crystals.

Future Work

- Continue to develop our method
  - Simulations in 3D
  - Convection effect
- Work with Materials Scientists to solve unanswered questions.

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