Automated Hyperspectral Pyrometry of Floating Zone Growths

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Abstract

The floating zone growth technique is a popular bulk crystal growth method for the discovery of new materials and phases. The development of a digital twin for floating zone growths is of interest to accelerate the materials discovery process with this technique. A key component of digital twins is a bidirectional interaction between physical growths and digital models in the form of data-driven model updating. To lay the foundation for data-driven model updating, we develop infrastructure to measure temperature distribution data from the molten zone of Laser Diode Floating Zone (LDFZ) furnace growths. A hyperspectral camera is installed in the furnace chamber and a hyperspectral pyrometry method is developed. For this, we use machine learning to fit hyperspectral data to blackbody radiation spectra and determine temperature. Finally, data streaming is used to automate the data analysis and storage of raw data and analysis results. This allows seamless temperature distribution data collection to provide real-time temperature analysis to experimenters and inform floating zone growth models. Using this infrastructure, we collect our first hyperspectral images and temperature distribution maps from LDFZ growths.

Introduction

The floating zone technique is a popular bulk crystal growth technique for many reasons, including the ability to quickly synthesize small crystal samples and not needing a container in contact with the sample during growth. In this technique, the tips of a crystal rod and a feed rod are heated, and the tips are joined to form a floating molten zone from which a single crystal can be extracted.

A critical parameter in the physics of floating zone growths is the temperature distribution in the molten zone. To advance our understanding of the physics of the molten zone, modelling of floating zone growths simulate the temperature distribution in the molten zone [1]. To inform and validate these models, experimental data for temperature distributions in floating zone growths is needed. In this work, we develop the infrastructure need to collect this data.

Three main steps were completed to develop this infrastructure. A hyperspectral camera was physically placed in the furnace to collect hyperspectral data from growths. A pyrometry method was also developed to determine object temperature from hyperspectral data. Finally, data streaming was used to automate the analysis of hyperspectral images.

Camera Setup

We set up our hyperspectral camera in a Laser Diode Floating Zone furnace (LDFZ). Since the hyperspectral camera captures a line, it needs to move vertically in the furnace to scan over the entire growth. To accomplish this, we attach the camera to a custom mount on a threaded rod. A motor spins the threaded rod, which is fixed in place, causing the camera mount to move vertically.

The motion of this motor is controlled by a Raspberry Pi, which we have programmed to respond to and interact with the camera's control software. The camera is moved up and down repeatedly during image capture.

Hyperspectral Pyrometry

To determine object temperature from hyperspectral data, least squares regression is used to fit spectra to the form of theoretical blackbody radiation spectra, optimizing a temperature parameter in the process. The function form for blackbody radiation from physics theory is given by

$$I(\lambda) = \epsilon \left(\frac{2hc^2}{\lambda^5}\right) \left(e^{\frac{hc}{\lambda k_B T}} - 1\right)^{-1} \equiv \epsilon I_0(\lambda)$$

where h is Planck's constant, c is the speed of light, k_B is the Boltzmann constant, ϵ is the emissivity of the blackbody, T is the temperature of the blackbody, and λ is wavelength.

Given that a wide variety of materials with varying emissivities are used in LDFZ growths, it is a necessary regression parameter alongside temperature. Additionally, emissivity may vary with wavelength, so we use a quadratic approximation [2].

This yields

$$I(\lambda) = \left(a_0 + a_1\lambda + a_2\lambda^2\right) I_0(\lambda)$$

where the coefficients a_0, a_1, a_2 are parameters to be optimized by regression. This emissivity term will also absorb relative scaling of intensities due to the camera's internal correction.

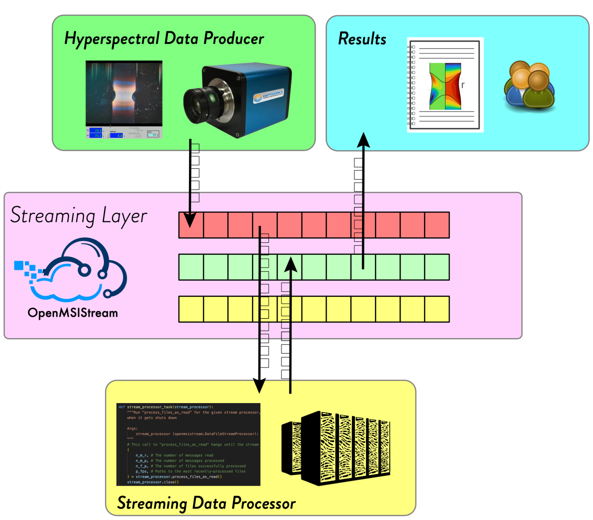
Finally, we add a constant parameter term to account for stray light and relative correction by the camera. The camera may internally make adjustments that shift measured spectra up or down in intensity, so we add a constant offset Ω to account for such shifts in the regression. The final equation for fitting is then

$$I(\lambda) = \left(a_0 + a_1\lambda + a_2\lambda^2\right) I_0(\lambda) + \Omega$$

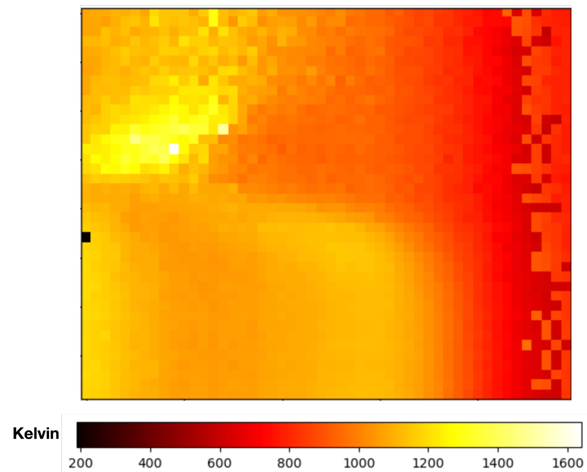
with fitting parameters a_0, a_1, a_2, Ω, T.

Data Streaming

Data streaming is implemented with OpenMSIStream [3]. A producer streams out raw data from the lab, a stream processor performs the pyrometry analysis and streams out the results from PARADIM servers, and a consumer downloads the results in the lab. With this pipeline, the data analysis process is automated, which allows real-time measurement for furnace users and seamless large-scale data collection.



Results and Discussion



Here we have a processed image of a section of the molten zone. We can see the outline of a section of the molten zone as well as a detailed temperature distribution throughout, which is what we desired. There are a few interesting aspects to note and improve on for future work.

Firstly, aligning the camera and focusing in on the molten zone proved to be a non-trivial task, as demonstrated by the absence of the entirety of the molten zone in the shown image. Additionally, more testing and validation of the hyperspectral pyrometry method will be performed. Testing for the method was performed using images not from an active floating zone growth, so adjustments and optimizations may be possible for growths.

We also notice a dark pixel resulting from a failed regression. There are a variety of possible methods that can be explored to reduce the failure rate of regression. The main method used to reduce the failure rate for this image was resolution reduction. By averaging neighboring pixel to slightly blur the image, we are able to remove excess noise that can cause regressions to fail, decreasing the failure rate. We also acknowledge that failures cannot be entirely avoided, and future work will investigate methods to automatically identify and disregard failures when results are used for further analysis.

Finally, we will ultimately use data collected through this infrastructure to inform models and simulations of floating zone growths. Future work will collect and curate a database of temperature distribution images that can be used for this purpose.

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References

[1] Scott S. Dossa and Jeffrey J. Derby. Modeling optical floating zone crystal growth in a high-pressure, single-lamp furnace. *Journal of Crystal Growth*, 591:126723, 2022.

[2] Dong-Xia Qu, Joel Berry, Nicholas P. Calta, Michael F. Crumb, Gabe Guss, and Manyalibo J. Matthews. Temperature measurement of laser-irradiated metals using hyperspectral imaging. *Phys. Rev. Appl.*, 14:014031, Jul 2020.

[3] Margaret Eminizer, Sam Tabrisky, Amir Sharifzadeh, Christopher DiMarco, Jacob M. Diamond, K.t. Ramesh, Todd C. Hufnagel, Tyrel M. McQueen, and David Elbert. Openmsistream: A python package for facilitating integration of streaming data in diverse laboratory environments. *Journal of Open Source Software*, 8(83):4896, 2023.