Systematic Floating Zone Single Crystal Growth for Machine Learning Objectives

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Abstract:

PARADIM is an NSF-sponsored program that provides users access to the platform's world unique equipment in order to expand their research and encourage discovery of new materials at an accelerated rate via materials design. In particular, the development of unique floating zone furnaces has led to a dramatic increase in the discovery of new materials with desirable properties (e.g. magnetic frustration). However, users are often unfamiliar with the equipment, and extensive training is often required for the acquisition of initial results. In order to assist the inexperienced user, machine learning software is being developed by the PARADIM DATA Collective (PDC) for the floating zone furnaces. At present, data were generated from a variety of floating zone growths to develop training sets. By landmarking key points from video footage, a computer can be trained to gauge the success of experiments. Subsequently, a computer can make recommendations to the user for on-the-fly experimental parameter changes should an experiment reach an unhealthy state.

Summary of Research:

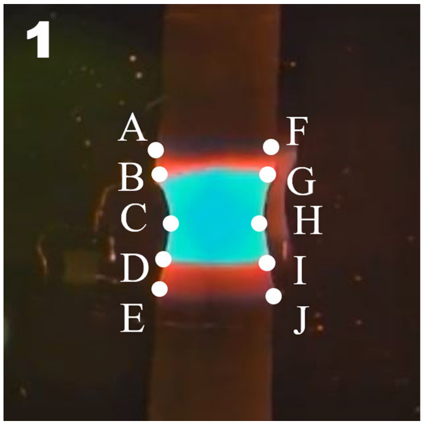
A variety of floating zone growths were completed with parameters systematically manipulated to generate a diverse set of data. Key points of the experiments were selected to be landmarked for the training set. A python script was developed to extract the key parameters, such as laser position and inclination, rotation rate and direction, and feed rate and direction of both rods, and the laser power used, from the video data. Three main types of growth were characterized by the respective widths of the top, neck, and bottom of the molten zone: healthy (Figure 1), thinning (Figure 2), and convex (Figure 3). The potential causes and additional characterization, such as movement of the rods or molten zone, of these three types of molten zones were also determined.

Results and Conclusions:

Analysis of floating zone data led to the determination of three main categories of floating zones: healthy, thinning, and convex. Healthy floating zones, depicted in Figure 1, were characterized by a 11:10:11 ratio of widths of the top: neck: bottom of the molten zone, rods travelling in the same direction, no jerking motion of either rod, and little to no changes in molten zone shape or growth parameters.

In contrast, a thinning molten zone, seen in Figure 2, consists of the width of the bottom solid/liquid interface being much larger than the neck and the top of the molten zone. Thinning molten zones are problematic because they lead to separation of the rods and potentially end the growth. They can be caused by the top feed rate being too slow to keep up with the seed rods travel rate, the power being too low to melt enough of the material, or the rods being too far apart. Thus, a thinning molten zone can be fixed by increasing the top feed rate, decreasing the bottom feed rate, increasing the power, or moving the rods closer together manually.

Conversely, a convex molten zone (Figure 3) has a molten zone neck that is wider than the top and bottom rods, which consequently can cause the molten zone to fall. The top rod moving proportionately too quickly or the power being too high can produce a convex molten zone.



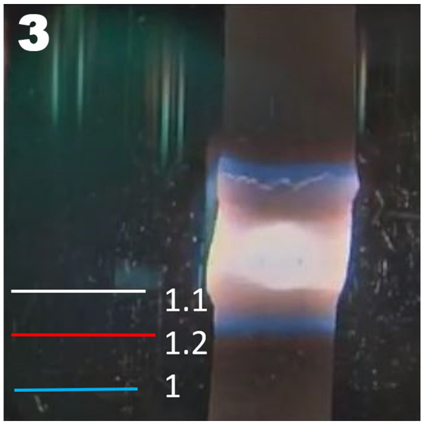
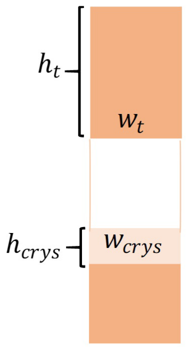


Figure 1, left: Landmarked image of a healthy molten zone marking the edge of the top rod (A,F), top of the molten zone (B,G), "neck" of the molten zone (C,H), bottom of the molten zone (D,I), and edge of the bottom rod (E,J). Figure 2, middle: Thinning molten zone due to user error. Respective widths of various parts of the molten zone characterize it as unhealthy. Figure 3, right: Convex molten zone characterized by the neck of the molten zone being the widest point.

By systematically altering parameters one at a time throughout a variety of experiments, a diverse training set of successful and unsuccessful crystal growths was developed. After inputting this data into a computer program, the computer will recognize not only when a growth is failing, but what parameters must be adjusted. Furthermore, the computer will be able to predict values such as crystal size and density, time left in the growth, and the melting point of the material via simple equations, such as the ones seen in Figure 4.

More complex equations can also be implemented into the program to allow the computer to compute this experimental data automatically. Because the program will have access to thousands of data points, countless calculations will be performed giving the researcher a multitude of data about the material and growth that would have been otherwise lost or time consuming. Such an influx of data will streamline the process of materials research and improve the quality of results.



$$Vol_{crys} = \pi \left(\frac{w_{crys}}{2}\right)^2 h_{crys}$$

$$h_{crys} = \frac{{w_t}^2}{{w_{crys}}^2} * \frac{d_t}{d_{crys}} * h_t$$

$$d_{crys} = \frac{d_t h_t}{h_{crys}} * \frac{{w_t}^2}{{w_{crys}}^2}$$

Figure 4: Sample calculations of crystal height, volume, and density desired from the machine learning program. Note: calculations assume no vaporization.

Future Work:

Further experiments using less traditional floating zone techniques must be conducted so that the data may be added to the training set. In addition to collecting more data, the landmarking program must be selected or developed. Subsequently, the selected training set can be officially landmarked and uploaded to the machine learning program. Once the program has learned sufficiently from the training set, it may be implemented.

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References:

[1] W.A. Phelan, J. Zahn, Z. Kennedy, and T.M. McQueen, "Pushing Boundaries: High Pressure, Supercritical Optical Floating Zone Materials Discovery," Submitted J. Sol. St. Chem. (2018).