Building Open Training Stacks for Image Segmentation of Boron Carbide Experiments

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Abstract:

Recent synthesis of large, single crystals of boron carbide (B4C) in a laser diode floating zone furnace (LDFZ) produced high purity single crystals ideal for characterization and development of advanced protection materials. The LDFZ method is challenging due to the complexity and breadth of tunable parameters. To improve LDFZ operational efficiency and outcome quality, image segmentation is being developed using the Mask R-CNN framework. A new, more precise and broader training set of >900 image has been produced to facilitate retraining the image-segmentation learner and advance application of ML in the LDFZ.

Summary of Research:

The optical floating zone technique is a powerful route to the preparation of single crystals of highpurity materials. Such single crystals are important in the development of new materials for advanced optical and electronic devices. Floating-zone synthesis is challenging, however, due to the complex parameter space (Fig 1). Successful floating-zone work often requires high-level expertise for successful development of new protocols. Recently, image segmentation has proven a promising new route to optimization and acceleration of development of new floating-zone protocols [1]. In this study, we produced an expanded training set to improve and expand application of image segmentation to floating zone synthesis.

Our new training set includes >900 images of each of three classes of molten zones for boron carbide (B4C) synthesis in a tilting laser diode optical floating zone furnace. B4C is an important protection material valued for its lightweight yet extreme hardness and high stiffness. B4C is the third hardest material known, exceeded only by diamond and cubic-boron nitride.



Figure 1. Screenshot of the LDFZ control panel. User has to set and tune all these parameters during typical, multi-hour experiments.

Boron carbide's high strength comes from its icosahedral structure and high-density of covalent bonds. Development and deployment of improved B4C depends on controlled, repeatable synthesis of pure single crystals important to characterizing directional strength and the role of impurities on mechanical behavior. A protocol to synthesize large, single crystals of B4C using PARADIM's laser diode floating zone equipment was developed by Straker, et al. [2], but growing single crystals remains difficult.

Image segmentation can assist monitoring and user control of molten-zone geometry by identifying object classes and locations within an image. The Mask R-CNN segmentation framework of He et al. [3] combines a region-of-interest model with a parallel instance segmentation model providing fast, effective segmentation. Carey et al. [1] created a learner to distinguish three variants of molten-zone geometry. These classes correspond to a stable melt and two unstable melts caused by excessive extraction rate of the growing crystal or excessive feed rate of the pressed powder rod. The trained learner identifies the portion of the image made up of melt and classifies it into one of these three types in under a second and with high confidence [1].

Results and Conclusions:

Images used to create an expanded, higher-precision training set were derived from live video of a furnace growth specifically designed to provide examples of all three classes of interest; good melt, fast bottom and fast top. Video was captured at one frame-persecond and split into individual images. Images were labeled using LabelMe [4], an open source program from MIT and freely available on Github [5], to mark polygonal outlines of the molten zone in each, individual frame. The upper portion of the growing crystal was labelled for a future ML model providing information about the uniformity of growth. Polygon coordinate points and identified classes were encoded in JSON files for the learner framework.

Labeling images focused on the accurate coordinate placement and consistent definitions of polygonal outlines required to produce an accurate ML model. Two polygons per image were labeled (Fig. 3). One labels the molten zone; the second labels newly grown crystal. To accurately define the geometry of the molten zone, polygonal masks were defined by 18 points: four on top and bottom; three on the sides; and one on each corner of the molten zone. To meet the needs of the Mask R-CNN framework, all masks of a given type must be defined identically. Polygons for the new crystal are simpler than the molten zone and able to be defined by eight points: four along the top and four in each corner. The same number of points were used on each image and spaced roughly equidistant. For consistency, images were marked at

235% magnification allowing accurate identification of the molten zone boundary (Fig 4).



Fig 2. Example of labeled LDFZ frame. Magenta polygon marks molten zone; blue marks part of lower crystal.



Fig 3. Detail of contact between molten zone and growing crystal. Lower limit of molten zone is along the bright line highlighted by the bracketing green arrows.

Future Work:

We have labeled ~300 images from each class. These will form the basis to retrain the model of Carey et al. [1] and subsequent evaluation of model accuracy compared to the earlier version. To evaluate accuracy, a training set of an additional 300 labeled images not used to train the model will be used to compare labeled masks and classes to those produced by the trained learner. After evaluation, we'll focus on labeling an additional 900 available images as well as planning a subsequent furnace run to create a training set focused on improving identified gaps in learner recognition.

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