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Image driven machine learning methods for microstructure recognition

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ABSTRACT

Computer vision and machine learning methods were applied to the challenge of automatic microstructure recognition. Here, a case study on dendritic morphologies was performed. Two classification tasks were completed, and involved distinguishing between micrographs that depict dendritic morphologies from those that do not contain this particular microstructural feature (Task 1), and from those micrographs identified as depicting dendrites, different cross-sectional views (longitudinal or transverse) were identified (Task 2). Data sets were comprised of images taken over a range of magnifications, from materials with different compositions and varying orientations of microstructural features. Feature extraction and dimensionality reduction were performed prior to training machine learning algorithms to classify microstructural image data. Visual bag of words, texture and shape statistics, and pre-trained convolutional neural networks (deep learning algorithms) were used for feature extraction. Classification was then performed using support vector machine, voting, nearest neighbors, and random forest models. For each model, classification was completed using full (original size) and reduced feature vectors for each feature extraction method tested. Performance comparisons were done to evaluate all possible combinations of feature extraction, selection, and classifiers for the task of micrograph classification. Results demonstrate that pre-trained neural networks represent microstructure image data well, and when used for feature extraction yield the highest classification accuracies for the majority of classifier and feature selection methods tested. Thus, deep learning algorithms can successfully be applied to micrograph recognition tasks. Maximum classification accuracies of $91.85 \pm 4.25\%$ and $97.37 \pm 3.33\%$ for Tasks 1 and 2 respectively, were achieved. This work is a broad investigation of computer vision and machine learning methods that acts as a step towards applying these established methods to more sophisticated materials recognition or characterization tasks. The approach presented here could offer improvements over established stereological measurements by removing the requirement of expert knowledge (bias) for interpretation of image data prior to characterization.

1. Introduction

Materials characterization is a critical aspect of the material design and discovery process. Recently, there has been much research in the field of materials informatics, a growing research area in which information technology and data science methods are used to interpret and analyze material data in order to accelerate the material discovery, design, and development process [1–5]. Currently, material design relies on chance discoveries and follows a classical synthesis-characterization-theory-computation approach [6]. Further, there is a heavy reliance on individual researcher background and experience which introduces significant bias and potentially error into the process of microstructure recognition, interpretation, and characterization. For example, quantification of microstructures traditionally is done using stereological measurements. Bias is introduced into stereological measurements through the requirement that an expert must first recognize and identify key microstructural features (inclusions, grains, or phases). This bias can be caused by a variety of factors, such as an individual's background, education, and experiences [6].

Although there have been recent advances in the field of quantitative microstructural science, there is still a heavy dependence on expert knowledge to identify what microstructural features are of interest for quantification [7]. Therefore it is desirable to expand upon work previously presented by DeCost and Holm in Ref. [7], and further explore methods of quantitative microstructure representations which do not require *a priori*

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knowledge of microstructural features of interest or significance [6]. This work aims to leverage existing computer vision and machine learning techniques specifically for the challenge of microstructure recognition. While the overlap between computer vision, machine learning, and materials science is currently small [6], this work is a step towards increasing cross-disciplinary studies that challenge the current paradigm for microstructure characterization.

Dendritic morphologies were chosen for this small case-study since dendrites are a well-characterized microstructural feature that exists in a variety of material systems (from single to multi-component). Size, shape, and spacing of dendrites vary depending on solidification behavior and chemistry, thus micrographs of this single feature can vary widely. The sample preparation and imaging methods used also contribute to the variety of micrographs produced from dendritic microstructures. Despite this variability in image data, it is still possible for human experts to look at a micrograph that contains dendrites and identify that it contains this microstructural feature, even though different orientations of dendrites (transverse or longitudinal) look distinctly different.

Computer vision and machine learning methods were applied to the task of identifying a particular microstructural feature of interest (dendrites) from micrographs that do not contain this particular feature (just as a human expert would identify that a micrograph contains dendrites). This recognition task is referred to in this work as Task 1. Task 1 is a high-level microstructure recognition task in the sense that dendrites are a type of microstructural feature that are not specific to a material system. A second classification task (referred to here as Task 2) was also completed, and involved distinguishing between longitudinal and transverse cross-sectional views of dendritic microstructures. This task may be viewed as a logical next step following the identification of dendrites in Task 1. If the micrograph from Task 1 was identified as a dendrite, then a second binary classification task was performed, with the goal of distinguishing between two different cross-sectional views.

The contribution in this work is to investigate multiple computer vision and machine learning methods for microstructure recognition. We hypothesize that the approach and methods presented here can be generalized, and thus applied to a variety of microstructure recognition tasks that act as a necessary first step in characterization of a material system.

2. Alloy fabrication and sample preparation

The alloy fabrication, processing, and metallographic sample preparation procedure followed to obtain images used in this work was based on the process detailed in Refs. [8,9] and is summarized here.

A Materials Research Furnaces (MRF) three probe arc melter was used to fabricate alloys of varying Sn–Ag–Cu compositions. After melting alloys were allowed to solidify and were then prepared for directional solidification (DS). The solidified buttons were placed in a beaker on a hot plate. The button was re-melted while constantly being purged with Ar gas to minimize sample oxidation. The alloy melt was then transferred into a 4 mm inner diameter quartz ampule with a mechanical pump. The rods were allowed to cool, then removed from the ampule, and placed in a larger quartz ampule (5 mm inner diameter) for DS. This ampule was then back-filled with Ar gas, sealed using a hydrogen torch, and inserted into the DS furnace.

DS was performed using a Bridgman-type apparatus in order to refine alloy microstructure. The tube furnace in this apparatus is a Thermolyne Type-21100 fitted with an Omega temperature controller. Following DS, alloys were removed from the quartz ampule, and small sections from the middle third of the rod were mounted in epoxy for metallographic sample preparation. Sections were mounted such that transverse and longitudinal orientations of β-Sn dendrites could be viewed. Samples were ground using silicon carbide (SiC) papers to 600 grit, then polished using 9, 3, and 1 μm diamond slurries. Colloidal silica was used as the final polishing step and as a chemical etchant so that the dendritic microstructure would be readily visible using light optical microscopy.

3. Image data sets

Image data used in this study includes micrographs taken over a span of approximately three years by students in the Lewis Research Group in the Materials Science and Engineering Department at Rensselaer Polytechnic Institute (RPI). All images taken by Lewis Research Group members are of solder alloys with dendritic microstructures. These alloys were manufactured, processed, and imaged at RPI, and a representative process of sample preparation was presented in Section 2. In order to supplement micrographs obtained at RPI, micrographs from the publicly available Dissemination of Information Technology for the Promotion of Materials Science (DoITPoMS) library [10] were used. Example images used in classification are provided in Fig. 1.

Images were grouped into two data sets: Data Set 1 and Data Set 2, corresponding to classification Tasks 1 and 2 respectively. Data Set 1 is comprised of micrographs with and without dendritic morphologies. This data set includes all images with dendrites (longitudinal and transverse cross-sections) from both the Lewis Group and the DoITPoMS micrograph library [10]. All micrographs that do not depict dendritic morphologies were obtained from the DoITPoMS library. Data Set 1 includes 528 images that are each 227 by 227 square pixels. 264 original images were used in making Data Set 1 (132 micrographs containing dendrites and 132 micrographs without dendrites). Each original image is 270 by 500 pixels but includes a scale bar that interferes with feature extraction, therefore each image was cropped to yield two 227 by 227 square pixel images. Thus, 528 images were used for classification.

Data Set 2 is a subset of Data Set 1, and is comprised of micrographs that only contain dendrites, where each micrograph is either a transverse or longitudinal cross-sectional view. Micrographs used in this data set include both images from the Lewis Group and the DoITPoMS micrograph library. Data Set 2 contains a total of 188 images that are each 227 by 227 square pixels. As was done for Data Set 1, original images were cropped to remove the scale bar: 47 micrographs of each longitudinal and transverse sections (total of 94 original images) were cropped to create a 188 images used for classification.

4. Approach

The general approach applied to the task of micrograph classification involved feature extraction and feature selection (dimensionality reduction) to compute feature vectors that were then used for training, validating, and testing various classification models. The same approach was applied to both Data Sets 1 and 2 and is shown schematically in Fig. 2.

Feature extraction is the first step in the process of classifying micrographs. Feature extraction starts with feature detection, where features in an image are local regions of pixels that include an 'interesting' part of a microstructure, such as a corner, edge, or blob-like object. Features detected using computer vision algorithms are not necessarily semantically meaningful, however are pixel patterns that are mathematically repeatable and recognizable, thereby making the region a good feature. Detected features are then described (or represented) in the form of a vector, called