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Exploring the microstructure manifold: Image texture representations applied to ultrahigh carbon steel microstructures



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ABSTRACT

We introduce a microstructure dataset focusing on complex, hierarchical structures found in a single Ultrahigh carbon steel under a range of heat treatments. Applying image representations from contemporary computer vision research to these microstructures, we discuss how both supervised and unsupervised machine learning techniques can be used to yield insight into microstructural trends and their relationship to processing conditions. We evaluate and compare keypoint-based and convolutional neural network representations by classifying microstructures according to their primary micro-constituent, and by classifying a subset of the microstructures according to the annealing conditions that generated them. Using t-SNE, a nonlinear dimensionality reduction and visualization technique, we demonstrate graphical methods of exploring microstructure and processing datasets, and for understanding and interpreting high-dimensional microstructure representations.

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1. Introduction

Comprised of the structures that arise from processing and mediate properties, microstructure is a core focus of the discipline of materials science. Microstructural information is most often conveyed via images obtained through various microscopy techniques (i.e. micrographs), sometimes supplemented by other structural and compositional probes. Traditionally, microstructural images have been evaluated by human experts, both to interpret the micrographs themselves and to connect them to processing conditions and property outcomes. However, recent research in microstructure data science has begun to explore applications of contemporary computer vision to construct microstructure representations suitable for use in machine learning and microstructure analytics tasks [1–4]. For example [3], compare several image texture representations and find that off-the-shelf convolutional neural network (CNN) features can be applied to microstructure analytics tasks (e.g. classification) without fine-tuning any of the CNN parameters. Likewise, Lubbers et al. [4] apply bilinear CNN representations [5–7] to synthetic lamellar structures, and relate this representation to the generative microstructure model

parameters (i.e. lamellar spacing and orientation and noise). While promising proofs of principle, these studies used comparatively simple and well-parameterized microstructures. To move towards quantitative application of generic computer vision techniques, we require real-world, technologically-relevant microstructure systems exhibiting the complex, hierarchical structures that challenge conventional microstructure segmentation and quantification.

To this end, we introduce the CMU-UHCS (Carnegie Mellon University Ultrahigh Carbon Steel) dataset [8,9], based on the work of Hecht et al. [10,11]. This dataset consists of 961 scanning electron microscopy (SEM) micrographs of Ultrahigh Carbon Steel (UHCS) subjected to a variety of heat treatments and taken at several different magnifications. The dataset spans several complex and hierarchical microconstituents typically found in UHCS and other technologically relevant alloy systems, offering a compelling real-world microstructure data science challenge.

UHCS (steels with 1–2.1 wt% carbon) are intermediate in content to high carbon steel (0.6–1 wt% C) and cast iron (2.1–4.3 wt% C). Due to their high carbon content relative to conventional steels, a characteristic microstructure feature of these alloys is proeutectoid cementite (Fe_3C), typically forming a network associated with the grain boundaries of the high-temperature austenite phase. The hard, brittle carbides help lend UHCS its well-known high strength and wear resistance, but highly-connected intergranular proeutectoid cementite networks can be detrimental to toughness and ductility by providing extended pathways for crack

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propagation [12,13]. Recent UHCS research has focused on mitigating this weakness by optimizing the network microstructure through various heat treatments [14] and addition of minor alloying elements [15,16]. Hecht et al. recently developed a quantitative measure of the proeutectoid cementite network connectivity, relating this to annealing schedules and toughness measurements [10]. In a similar study, Hecht et al. explored the effect of annealing conditions on spheroidite morphology [11]. The present UHCS microstructure dataset is built on the characterization efforts for these two UHCS studies.

In this study, we use the UHCS dataset to compare state-of-the-art CNN-based image texture representations with the classic bag of visual words (BoW) representation [17,18]. As microstructure representations, the BoW has the theoretical advantage of strong explicit scale and rotation invariance, while CNNs notoriously outperform BoW on typical natural image recognition tasks (e.g. facial recognition, object detection and identification, scene classification). We evaluate each image representation using both supervised and unsupervised learning methods, and demonstrate how these techniques can be used together for exploratory microstructure analysis. Specifically, we used a Support Vector Machine (SVM) [19] approach to classify microstructures both by primary microconstituent and annealing condition. We complement this understanding by applying the unsupervised dimensionality-reduction technique t-SNE (t-distributed Stochastic Neighbor Embedding) [20] to visualize the high-dimensional distributions of each microstructure representation, relating this structure to available annealing schedule and imaging metadata.

Our primary contributions in this report are:

- A real-world dataset of complex, hierarchical microstructures annotated with microstructure constituent metadata, as well as partial imaging and processing metadata, such as heat treatment, cooling procedure, and magnification [8,9].
- Evaluation of several competitive computer vision techniques, with discussion of their relative strengths and weaknesses for a range of real-world microstructure analytics tasks.
- Exploration of microstructure data visualization techniques for inferring processing – microstructure – properties relationships for realistic complex, hierarchical microstructure systems.
- Considerations of microstructure data bias and quality that will be essential to developing reliable data-driven microstructure models and standards.

2. Methods

2.1. UHCS dataset

The UHCS dataset [8,9] consists of 961 SEM micrographs of commercial UHCS subjected to a range of heat treatments by Hecht et al. [10,11]. These micrographs span a wide range of magnifications, and include both secondary electron (SE) and back-scattered electron (BSE) images. 598 micrographs also have annealing schedule metadata: annealing time, temperature, and cooling method, as described in more detail in Ref. [8]. All 961 images are labeled with their primary microstructure constituents as illustrated in Fig. 1. Most of the micrographs focus on the spheroidite morphology (Fig. 1(a)), the proeutectoid cementite network (Fig. 1(b)), and pearlite (Fig. 1(c)). A smaller number of micrographs contain two primary microconstituents, such as pearlite containing spheroidite (Fig. 1(d)), Widmanstätten cementite (Fig. 1(e)), and martensite (Fig. 1(f)). Table 1 shows the distribution of each of these primary microconstituent labels. We used the full set of 961 labeled 645×484 pixel micrographs to generate the data visualizations in

Section 3.2.

For the primary microconstituent classification experiments, we considered only a subset of these labeled micrographs: 200 randomly selected micrographs each from the spheroidized cementite, proeutectoid cementite network, and pearlite/pearlite + spheroidite classes, for a total of 600 images. We also consider an expanded dataset constructed by cropping four 224×224 sub-images from the center of each micrograph in the original dataset, so that the expanded dataset consists of 2400 images. The single red and four yellow frames in Fig. 1(a) indicate the image regions used for microstructure feature extraction in the full-sized and cropped image sets, respectively.

The annealing schedule classification task was limited to the micrographs collected to study the spheroidite morphology. The dataset contains spheroidite micrographs resulting from 23 distinct annealing schedules. Within this subset of micrographs, we limit the classification dataset to the 13 annealing conditions with at least 15 micrographs. Where more than 15 micrographs with a given annealing condition are available, we randomly select 15 micrographs to obtain a balanced classification dataset. The resulting annealing condition classification datasets consist of 195 full-sized micrographs and 780 cropped micrographs.

2.2. Image representations

In this microstructure representation study, we explore and compare two computer vision approaches for computing generic image representations: Mid-level image patch descriptors [18,21] and convolutional neural network (CNN) representations [22–24].¹ The mid-level features approach is attractive due to its relatively strong invariance to image scale and orientation; its focus on identifying and characterizing individual features is also intuitive to the materials scientist. However, CNN representations are generally regarded as richer, more hierarchical, and more effective than mid-level image features, even when transferring CNN parameterizations from one task to another (in this case completely unrelated) task [26,27]. These advantages stem from the structure of modern CNNs as used in computer vision: deep CNNs are constructed as a hierarchical series of convolution filterbanks that extract image features, interspersed with local aggregation (pooling) functions that derive high-level image features by composing lower-level features [22].

2.2.1. Mid-level image features

The baseline feature extraction method in this study is the bag of visual words (BoW) method, which represents an image as a distribution of local image descriptors (i.e. visual features). As previously reported in detail [1,2], we applied both the Difference of Gaussians [28] and the Harris-LaPlace [29] interest point detectors to select distinctive image regions with characteristic scales and orientations. We then used oriented SIFT descriptors [28] to characterize the visual appearance of each interest point, and k-means clustering [30] to quantize the SIFT descriptors into a visual dictionary with 100 (BoW₁₀₀) visual words (i.e. SIFT cluster centers). Each image is then represented by its microstructural fingerprint: A normalized histogram measuring the occurrence frequency of each visual word within the image. BoW representations can be compared with various similarity metrics for discrete probability distributions, such as the Hellinger and χ^2 kernels [18]. Presently, we use the χ^2 kernel, which for two normalized m -dimensional

¹ In addition to these topical review papers, Szeliski's *Computer Vision* [25] is an excellent introductory text covering a broad selection of foundational topics and concepts in computer vision.

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