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Sparse modeling of space- and time-varying diffraction response of a progressively loaded aluminum alloy

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ABSTRACT

High energy X-ray diffraction data collected *in situ* during loading experiments permits probing of the crystal structure of a plastically deforming material sample. An elastoplastic deformation is associated with heterogeneity in both crystal orientation and lattice spacing—each manifesting as azimuthal broadening and radial broadening of diffraction peaks respectively. Quantifying the spreading effect is challenging, especially in cases where the sample has a granularity between that of a single crystal and fine grain or powder material. The approach developed in this paper begins by modeling the intensity signal in the vicinity of a Debye-Scherrer ring as a sparse, nonnegative superposition of Gaussian basis functions drawn from an over-complete dictionary. Processing automatically selects from the dictionary basis functions whose widths and amplitudes are representative of the data. The chosen basis functions are used to compute scalar measures of radial and azimuthal broadening for the set of diffraction peaks composing a Debye-Scherrer ring. To demonstrate the utility of the approach, we show that analysis of diffraction peak shape information from an aluminum alloy 7075 T651 (AA7075 T651) sample provides insight into the origin of material state that would have otherwise have been difficult if not impossible to extract using conventional methods. Furthermore, the extracted information revealed a deformation response linked to the processing history of the sample.

1. Introduction

1.1. High Energy X-ray Diffraction and Structural Materials

The development of advanced sensing and associated data processing methods along with plasticity models promises the ability to introduce improved or specialized structural materials across a range of applications [1]. Much research in this context has leveraged computational tools and nondestructive sensing to study crystal-scale interactions at play during plastic deformation. Electron back-scatter diffraction, neutron diffraction, and x-ray diffraction are modalities which capture the state of a poly-crystalline material. Electron backscatter diffraction produces high resolution imagery of crystals, but only targets the surface [2]. Neutron diffraction offers subsurface capability compatible with *in situ* experimentation [3]. In contrast to neutron diffraction, high energy x-ray diffraction (HEXD) from a synchrotron source operates well on smaller diffraction volumes, extracting more detailed information from the constituent grains during *in situ* loading [3].

The mechanical state of crystals can be described in terms of changes in the HEXD signature of a crystal [4]. Crystals satisfying the Bragg condition diffract signal into spots along rings on a two-dimensional detector as in Fig. 1. These diffraction rings are known as Debye-Scherrer rings. The diffraction angle, 2θ (or radius of the ring r),[1] is inversely proportional to the lattice spacing of a crystal, d_{hkl}, by Bragg's law [5],

$$n\lambda = 2d_{hkl}\sin\ \theta_{hkl} \tag{1}$$

where λ is the wavelength of the x-ray beam, $\{hkl\}$ are Miller indices specifying the crystal's family of lattice planes, and n is a positive integer. The azimuthal angle, η, of the diffracted beam is determined by the orientation of the diffracting crystal.

Of particular interest are the translation and broadening of diffraction spots both radially and azimuthally. An external force that uniformly strains crystals causes the spacing of lattice planes to decrease or increase, resulting in a radial translation of the diffraction

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[1] Diffraction angle referred to as 2θ and r interchangeably throughout this paper

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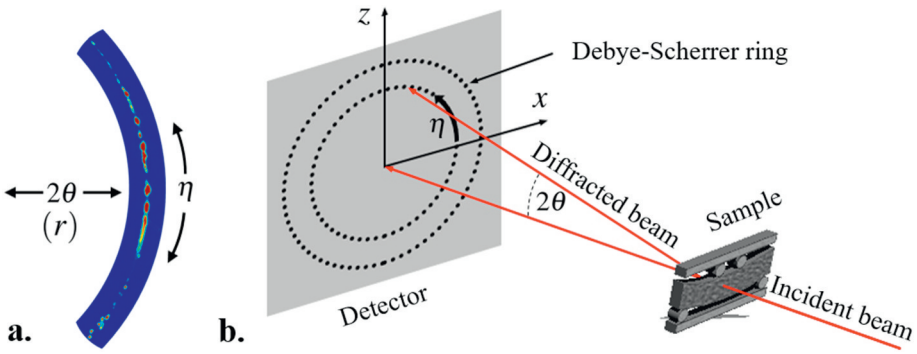

Fig. 1. (**a**) Segment of x-ray diffraction ring with coordinates labeled (**b**) Diagram shows HEXD experimental setup involving a two-dimensional detector, x-ray beam, and rectangular sample in a four point bend load frame. The sample is free to move in the *x* and *z* directions to adjust the point of incidence of the beam on the sample.

signal. The bulk azimuthal rotation of a crystal causes its diffraction signal to translate azimuthally by the same angle. Rotations of crystals along other coordinates may entirely change the set of lattice planes satisfying the Bragg condition.

Broadening of diffraction spots begins to occur as these deformations become heterogenous at the onset of plasticity. It is possible for diffraction spots to broaden, expand or remain stationary as crystals' states evolve. Crystal lattice spacing heterogeneity will result in a radially broader diffraction signature; crystal orientation heterogeneity, in an azimuthally broader diffraction signature. Measurement of these spot broadening effects allows us to study the evolution of the deformed state of a material [6,7].

1.2. Effect of Material Granularity on Interpretability

The interpretability of diffraction rings varies with the size of the diffraction volume relative to the crystal size. In powder diffraction of a sample of fine-grain crystals with uniformly distributed crystallographic orientation, large diffraction volumes give rise to homogeneous diffraction rings depicted in Fig. 2b. Here, broadening analysis is limited to changes only in the 2θ coordinate [8]. Alternatively, when only a few crystals populate the diffraction volume, the diffracted signals associated with individual crystals form discernible spots along the ring as in Fig. 2a. These spots can be localized and fit to a peak function parametrically to evaluate lattice spacing and misorientation heterogeneity [9].

Engineering materials often lie at an intermediate scale as in Fig. 2c; the diffraction data of such samples contain a complex mix of localized, spot-like structure superimposed on diffuse rings. Azimuthal averaging though certainly possible, discards significant information embedded in the heterogeneous intensity structure seen in these rings [9]. Adapting the methods of [6,7] designed for the coarse-grain data requires that individual spots be identifiable in the data as in Fig. 2a. Not only is this labor intensive for highly populated Debye-Scherrer rings, but can also require subjective choices in treating structures that are physically close or overlapping on the detectors such as those in Fig. 2c. The possibility of encountering such data complicates the task of spot broadening quantification.

1.3. Contribution

In this paper, we propose an approach that complements existing work by focusing on these real-world materials with a mixture of coarse and fine grain material characteristics. As noted above, because of the highly heterogeneous nature of the data, fitting individual peak-type functions to single spots is not particularly meaningful or even possible. Rather we take a fundamentally different approach and seek a representation of the data around each ring as a linear superposition of peak functions of various widths centered on a grid of points in radius and azimuth. The set of such functions available for fitting is called a *dictionary*. As illustrated in Fig. 3, distinct spot-like structures in the data, are automatically captured using a small number of these basis functions dominated by one or two which capture the basic spread of a spot in both radius and azimuth. Alternatively, regions of a ring displaying more homogeneous powder-type characteristics are represented using a few basic functions that are less azimuthally localized. The approach collectively fits the entire diffraction ring by a combination of peak functions to overcome the heterogeneous nature of the data and capture the deformation-induced azimuthal evolution.

As we explain in greater depth in Section 2.1, the number of functions comprising our dictionary is exceptionally large, on the order of 10^{12}. Compressive sensing (CS) methods provide an algorithmic framework for automatically determining a small collection of, in a sense that can be made precise, the “most informative” elements of this dictionary. That is, CS techniques produce a representation of the diffraction data comprised of a sparse superpostion of elements in our dictionary. Having arrived at a set of corresponding basis functions, we can statistically analyze their widths to quantify spot broadening. We quantify the degree of azimuthal and radial broadening developed in a ring by measuring the fraction of signal contributed by the broadest basis functions. The resulting process can be thought of as an automated extension of the method used in [6,7] to quantify spot broadening for large grain data.

While drawing influence from machine learning, the approach developed here differs from purely data-driven methods that rely entirely on data to “train” the model. Such techniques may be appropriate for problems where the physics are unknown or too complex to be modeled, but for problems such as the ones of interest here, one knows a

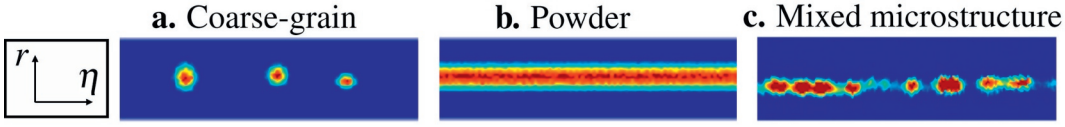

Figure 2: Examples of HEXD data. (a) Coarse-grain samples containing

Fig. 2. Examples of HEXD data. (**a**) Coarse-grain samples containing few, uniformly oriented crystals in diffraction volume result in distinct spots. (**b**) Powder samples contain many crystals in diffraction volume resulting in Debye-Scherrer rings; (**c**) Mixed microstructure is more typical in engineering alloys— they have some intermediate number of heterogeneously structured crystals.