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A framework for generating synthetic diffraction images from deforming polycrystals using crystal-based finite element formulations

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ABSTRACT

A framework for generating synthetic diffraction images on X-ray detectors from individual grains within polycrystals under *in situ* loading is described. Crystal plasticity-based finite element simulations of three-dimensional (3D) polycrystalline aggregates undergoing deformation were utilized to mimic a far-field High Energy Diffraction Microscopy (HEDM) experiment. The smearing of the diffraction spots on a two-dimensional (2D) area detector was consistent between the experiment and simulation for a target grain within a polycrystalline sample of a Cu–Cr–Zr alloy. The influence of crystallographic neighborhood and grain shape on the diffracted intensity distributions of the diffraction spots, the stress distribution and the misorientation distribution within a grain is also investigated. Key features of the diffraction spots are examined, differentiating between changes with applied stress and changes due to lattice misorientation associated with plastic straining.

1. Introduction

High-energy, three-dimensional, X-ray diffraction techniques are a new generation of experiments which enable non-destructive characterization of the microstructural and micromechanical response of individual grains within the bulk of a deforming polycrystal [1,2]. These data are collected by area detectors in the form of diffraction images, which are measured intensity distributions of the diffracted beams. In contrast to being a distinct, sharp point in intensity expected from a perfect crystal, an intensity distribution is a more diffuse pattern that arises from crystallographic imperfections such as dislocations, lattice misorientations, and variations in spacing of atomic planes. Because there are a multitude of reasons for an intensity distribution to broaden, the prospects of deconvolution of a measured intensity distribution to quantify the influence of any single source of broadening are quite low.

An alternative strategy for interpreting intensity distributions provided by diffraction images is to simulate the passage of a beam through a virtual sample and compute the diffraction based on the microstructure within the sample volume. Contributions to the diffracted intensity distributions from many potential sources are superimposed to generate a synthetic diffraction image which can be compared and contrasted to the measured image to understand the significance of the contributions from these sources. This alternative falls within a class of methods referred to as forward modeling. In diffraction, forward modeling consists of projecting a simulated diffracted beam onto a surface that coincides with the detector in an actual experiment. Suter et al. [3] have developed a forward modeling Monte Carlo scheme for quantitative reconstruction of grain and orientation maps from high-energy X-ray diffraction microscopy data. Forward modeling of Laue diffraction patterns from pure Ni foil samples have also been conducted using a discrete dislocation dynamics model and a strain gradient crystal plasticity finite element model [4,5].

Crystal-based finite element simulations in conjunction with forward modeling offer much promise. Virtual samples used in finite element simulations can be instantiated with spatial distributions of important microstructural features that evolve with deformation according to accepted or proposed theories. The heterogeneity of the microstructure and strain within the virtual sample can be captured in the intensity distribution of a virtual detector image via forward modeling.

When effectively coordinated, the integration of experiments and simulations offers the ability to build a more complete picture of the micromechanical evolution of individual grains within an aggregate than would have otherwise been possible with either capability alone. Comparisons between experiments and simulations have typically been conducted by comparing stresses or strains at the crystal level. Polycrystal diffraction methods using X-rays and neutrons have been extensively used to determine residual strains in the unloaded state following plastic deformation (*ex situ*) as well as the evolution lattice strains during loading (*in situ*). A shift in a diffraction peak is associated with a change in the average lattice spacing among crystals with a common

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lattice plane normal aligned with a particular sample direction. Data from neutron diffraction experiments have been used in the validation and calibration of various polycrystal deformation models such as the Taylor [6], self-consistent [7–11], and finite element models [12–15]. While lattice strains for only a limited number of reflections can be measured using neutron diffraction, X-ray powder diffraction techniques have the ability to measure lattice strains in many different directions simultaneously [16,17]. Although lattice strains in individual grains cannot be spatially resolved using powder diffraction techniques, stress or strain distributions as a function of lattice orientation can be constructed [18–20]. While lattice strains for individual grains within the bulk of a sample have been measured using high-energy synchrotron X-ray diffraction and compared to lattice strains computed using crystal-based finite element simulations [21,22], the goal of the current work is to move the comparison between the experiments and simulations downstream to the detector by generating virtual diffraction images.

The methodology presented here builds on previous efforts to model diffraction experiments with *in situ* mechanical loading using finite element simulations of virtual polycrystals. In this paper, we lay out a forward modeling framework for use with finite element simulations of elastoplastic, large strain deformations of virtual polycrystals to facilitate comparison of diffraction intensity distributions between experiments and simulations for individual grains within fully three-dimensional aggregates. This framework, which is referred to as a virtual diffractometer, explicitly deals with the spatial position of the grain, its shape, and various aspects of its mechanical state in constructing a diffraction spot. This approach avoids the ambiguities that can arise in trying to invert image data to obtain, for example, lattice strains associated with a particular grain in a polycrystalline aggregate. Instead, the modeling burden is placed on the mechanical model for deformation (the finite element formulation) and the virtual diffractometer.

This article is organized as follows. Section 2 presents a description of how diffracted intensities from crystals are produced and an overview of the type of diffraction experiment that was simulated using the current modeling framework. Section 3 describes the framework of a virtual diffractometer for generating synthetic diffraction images from finite element-based representations of virtual samples or virtual polycrystals. A demonstration of the current framework is presented in Section 4 by simulating a far-field High Energy Diffraction Microscopy (HEDM) experiment conducted on a Cu–Cr–Zr alloy under *in situ* tensile loading. Comparisons are made between the simulated and measured diffracted intensity patterns (spots) for an interior grain in the sample at various stages of macroscopic loading. The use of the virtual diffractometer as an investigative tool is also demonstrated by examining the stress distribution and the lattice misorientation distribution within the grain.

2. Diffracted intensity distributions from polycrystals

A perfect crystal is composed of regularly spaced atoms which act as scattering sites for X-rays. When an incident X-ray beam strikes a crystal, scattering of the X-rays by the atoms occurs. Due to the periodic arrangement of these atoms, X-rays scattered in certain directions will be in-phase and constructive interference of the X-rays will occur in these directions. A diffracted beam is composed of a large number of scattered X-rays undergoing constructive interference in a particular direction. The directions of these diffracted beams are governed by Bragg's law:

$$\lambda = 2d \sin\theta \tag{1}$$

where λ is the wavelength of the incident X-ray beam, d is the lattice plane spacing for a particular diffracting plane of atoms, and θ is the angle between the incident beam and the diffracting plane.

In a diffraction experiment using a monochromatic X-ray beam, when diffracted beams strike a detector, diffraction spots are observed. Each diffraction spot observed on the detector has a corresponding position, intensity distribution and shape. For grains with sufficiently perfect lattice arrangement, the diffraction spots appear as sharp peaks with a narrow spread in intensity on the detector. However, when a grain undergoes deformation, changes can occur in its lattice arrangement, which manifest as changes to the position and intensity distribution of the diffraction spots.

The radial position of a diffraction spot on the detector, 2θ, is directly related to the lattice spacing of the diffracting plane. A shift in 2θ of a diffraction spot corresponds to a change in lattice spacing, which is interpreted as a normal component of the elastic strain (lattice strain). Dislocations, lattice misorientations, and stress distributions can also cause spatial variations of the crystal lattice. There can also be gradients of stress across a crystal due to heterogeneous deformation. These changes manifest in the diffraction spots through changes in the intensity distribution and shape. A sharp diffraction spot from an undeformed crystal undergoes smearing and the intensity distribution becomes more diffuse.

Synchrotron light sources produce high energy and high flux X-rays with sufficient penetration power for non-destructive grain scale characterizations of polycrystalline bulk materials during *in situ* loading. Various diffraction techniques have been developed to determine the spatial position, morphology, lattice orientation and lattice strains for individual grains [2,23,24]. By reorienting the sample, lattice strains can be measured in many different directions, enabling the full elastic strain tensor to be determined for each grain.

When measuring diffraction spots from individual grains, three types of detector configurations can be utilized [25]. These are classified into the near-field, far-field and very far-field diffraction geometries. In the near-field diffraction geometry, the detector is placed close to the sample such that spatial and orientation resolution are increased at the expense of 2θ resolution [3,26]. Spatial orientation maps of grains are generated using the near-field geometry. For the far-field geometry, the detector is placed at an intermediate distance from the sample, such that the diffraction spots appear on complete Debye–Scherrer rings on the detector. Volumetric averages of orientation and elastic strain tensors for individual grains are measured in the far-field geometry [24]. In the very far-field geometry, the detector is moved even farther away from the sample and a single diffraction spot is observed on the detector at very high angular resolution [2,27,28], enabling strain maps within the grain to be constructed in reciprocal space.

2.1. HEDM experiments

In the current work, the focus is on a framework to simulate a far-field HEDM experiment and generate synthetic diffraction spots from a target grain within the interior of a virtual polycrystalline sample. The HEDM diffraction technique is essentially a rotating crystal method conducted in transmission, employing high energy synchrotron X-rays ($E \geqslant 50$ keV) and high speed 2D area detectors to measure diffracted intensities from individual grains within polycrystalline bulk materials [2,24].

The HEDM experimental technique is currently implemented at beamline 1-ID-C at the Advanced Photon Source (APS). The experimental geometry of a far-field HEDM experiment is depicted in Fig. 1a. A sample is mounted on an ω-rotation stage, where ω is a rotation about the sample loading axis, Y_s. The sample is loaded *in situ* and diffraction measurements are conducted during pauses in loading. Grains within the illuminated volume of the sample which satisfy the diffraction condition generate diffracted beams.