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Automated Data Acquisition and Indexing of Electron Channeling Patterns using the Dictionary Approach

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Defect analysis using a Scanning Electron Microscope (SEM), commonly known as Electron Channeling Contrast Imaging (ECCI), has received much attention in the recent past. Traditional defect analysis has for decades relied on Transmission Electron Microscopy (TEM) modalities, such as the bright field-dark field and weak beam imaging, and Scanning Transmission Electron Microcopy (STEM) diffraction contrast imaging methods. While the spatial resolution of ECCI is somewhat lower than that of the TEM based methods, ECCI provides more flexibility in sample preparation and data acquisition from bulk samples. The method relies on the variation of backscatter yield near lattice defects. However, to achieve quantitative defect analysis, the exact diffraction conditions need to be known, which, in turn, requires accurate determination of the crystal orientation. Electron Channeling Patterns (ECP), the diffraction modality associated with ECCI, are somewhat challenging to index. The method of the Hough transform, used for indexing EBSD patterns, does not always work with ECPs due to the limited angular range of the channeling pattern. In the absence of a general method to index ECPs, there is a lack of commercial and open source software packages to automate this process. While there have been efforts to integrate ECCI with the Electron Backscatter Diffraction (EBSD) method [1] for orientation mapping, it would be convenient if the orientation determination could be performed without the use of extra hardware and in an automated fashion. Furthermore, with the advent of fully scriptable microscopes for stage control and data acquisition, it has become possible to automate the data collection process for rapid ECCI-based defect characterization and analysis.

In this contribution, we present a general method to accurately index ECPs. Our approach belongs to the broader class of dictionary-based methods, which operates in a “plug and play” fashion and serves as a unified approach to indexing all diffraction modalities. This approach is represented in Fig. 1. The first step is to generate a Generalized Forward Projector (GFP) or simply a forward model of the experiment. This step captures the relevant physics of the physical process and can replicate the experiment given the right set of parameters. For the specific case of ECPs, we use both the theory for stochastic and dynamical scattering of electrons, in conjunction with the appropriate detector and noise model with lens aberrations to get the correct forward model. The next step is to uniformly sample the fundamental zone of orientation space, $SO(3)$, and apply the forward model, with the correct set of detector, noise and aberration parameters, to all sampled points to generate a “pattern dictionary”. The uniform sampling of orientation space is achieved using a novel cubochoric parametrization, which is hierarchical and highly convenient [2]. This method maps a set of uniformly spaced points in a cube to the northern hemisphere of the unit quaternion hyper-sphere. The resulting pattern dictionary serves as a look up table in the next step, which involves matching the experimental patterns against the dictionary, using either a simple dot product or mutual information. Adaptive Histogram Equalization (AHE) is performed on both the experimental and simulated patterns as a pre-processing step before pattern matching. The final step is refining the match by either a sub-sampling of the orientation space around the matched point, or using a Derivative Free Optimization (DFO) algorithm to best fit the pattern. A similar algorithm has been shown to successfully index EBSD patterns [3]. Furthermore, the robustness of this approach against noise is about an order of magnitude higher than that of the regular Hough transform-based algorithms used for EBSD indexing [4]. The result of using the dictionary approach on a single ECP of austenitic stainless steel is shown in Fig. 2(a) and (b). The agreement between the two patterns is quite good which allows for the determination of the orientation (Euler angles) with high accuracy. We will describe our efforts to Python-script a TESCAN-MIRA3 SEM with beam rocking apparatus for automated data acquisition by controlling both the stage and the detector (secondary and backscatter). The ultimate aim of this exercise is to automate data collection in the ECCI modality by indexing the ECP and achieving multiple two beam orientations by autonomous navigation in orientation space using sample tilt and rotation. This will enable high-throughput collection of large numbers of defect images from different regions in the sample.

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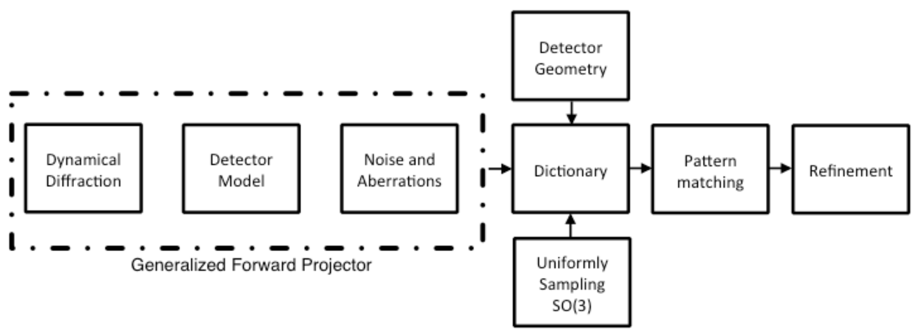
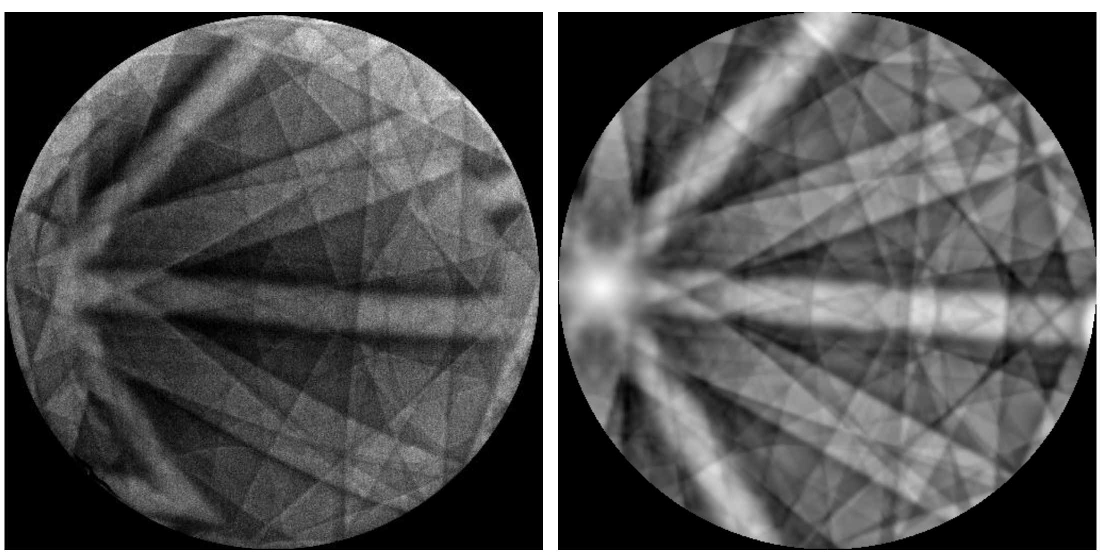


Figure 1: Plug and play model for the dictionary approach to indexing diffraction patterns.



(a) (b)

Figure 2: (a) Experimental ECP for stainless steel. (b) computed channeling pattern after using the dictionary approach.

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