Forward Models for 3D Materials Characterization by SEM and TEM Modalities

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In 3D materials characterization, one generally aims to reconstruct a quantity as a function of position; this quantity can be a scalar (density), vector (magnetization), or tensor (strain) field, and both destructive (serial sectioning) and non-destructive (tomography) techniques are used for data acquisition. Extraction of such field data from 3D measurements belongs to the broad category of "inverse problems" and is not guaranteed to be a stable process nor to result in a unique solution. From a reconstruction point of view, convergence and uniqueness are generally improved by imposing a regularization algorithm. This can be a simple nearest neighbor smoothness constraint or a complex physics-based prior model. In addition, the reconstruction can be stabilized significantly if a reliable and accurate forward model is available for the formation of the signal, given the sample; in other words, if one can predict what the data ought to look like for a given sample, then it becomes much more likely that the experimental data can be interpreted correctly.

In this contribution we review several forward models for important characterization modalities, including electron back-scatter diffraction (EBSD) and vector field electron tomography (VFET). The general concept of a forward model is illustrated schematically in Fig. 1: one or more instruments (blue) generate particle beams that interact with the sample (center). The beams are modified by the sample and its internal fields, and signals emanate from the sample; these are then intercepted by detectors (red) which impart their own fingerprint (e.g., in the form of a point spread function) and produce the measurements. The general task of materials characterization is then to invert this process, and to extract the sample fields from the measurements. In the case of EBSD measurements, in particular in the context of 3D serial sectioning, time is of the essence, and fast pattern acquisition is necessary, often leading to patterns with low signal-to-noise ratio which can not be easily indexed by commercial packages that rely on feature-extraction. Instead, direct forward modeling of the patterns allows for a robust indexing approach, as illustrated in the [001] inverse pole figures of Fig. 2; the sample is polycrystalline Nickel and the data on the top row was acquired using optimum detector settings whereas the bottom row shows the indexing results for a low signal-to-noise ratio.

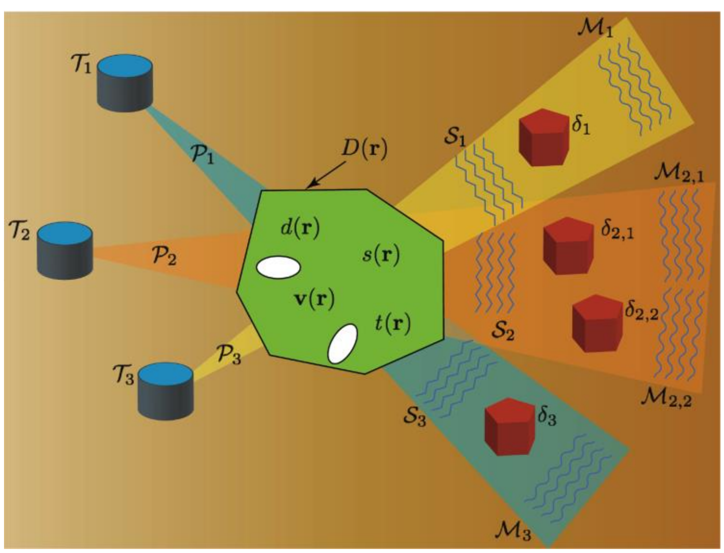
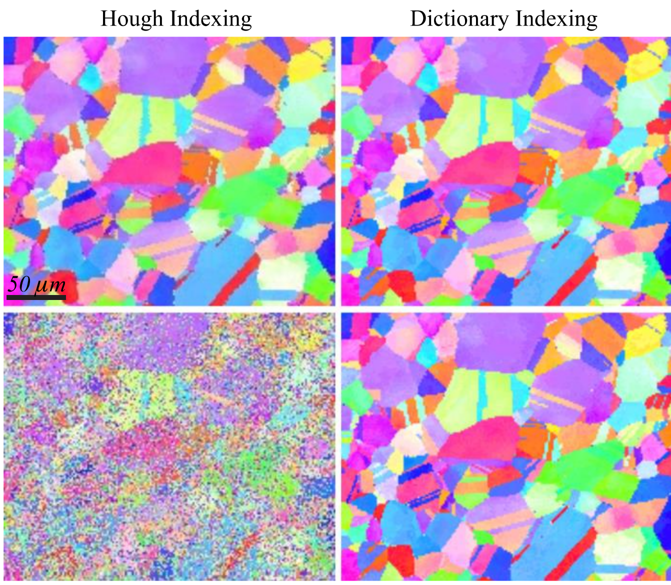


Fig. 1. Schematic illustration of the signal formation process in materials characterization modalities.

In Lorentz TEM, the phase of the electron wave is modified by the presence of a magnetic vector potential **A** in the beam path; this integral can be regarded formally as the "vectorial X-ray transform" of **A**, which suggests that it should be possible to reconstruct **A** in 3D, starting from tomographic LTEM data. We will show that an accurate forward model of the image formation process enables 3D reconstructions in a Bayesian model-based iterative reconstruction (MBIR) algorithm. Fig. 3 shows a 3D view of the magnetic vector potential around a planar array of Permalloy islands; the voxel size is of the order of 6 nm. We will conclude this contribution with a brief review of other forward modeling efforts.



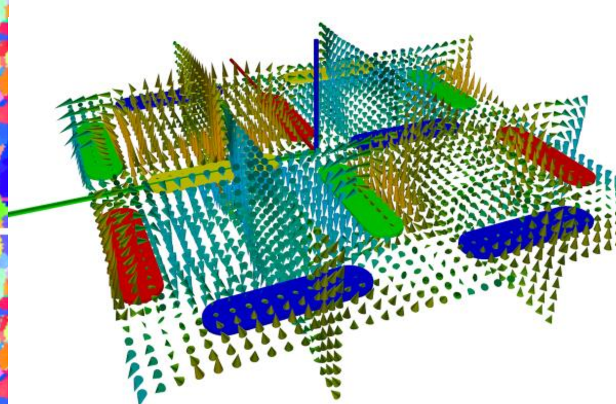


Fig. 2. Hough-based indexing (left) vs. dictionary indexing (right) for a polycrystalline Ni sample; the [001] inverse pole figures on the top were obtained from 186x151 patterns with a high signal-to-noise ratio; the bottom shows how the Hough-based indexing fails for low signal-to-noise ratio patterns whereas the forward model based indexing approach is robust against noise.

Fig. 3. (Right) Reconstructed magnetic vector potential for a 2D array of Permalloy islands; the color indicates the magnetization direction of each island. Note the circulation of the vector potential around the islands.

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