

## Evaluating spherical models of EBSD patterns for forward modelling indexing

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The application of full pattern matching-based forward modelling indexing techniques of EBSD and transmission EBSD patterns has shown significant improvements over conventional indexing methods that are based on the detection of individual bands in the EBSD patterns [1,2]. Forward modelling provides superior robustness on poor quality patterns, improved orientation precision, and can resolve common indexing challenges including pseudo-symmetry, non-centrosymmetric point groups (polarity), and overlapping patterns. Furthermore, new GPU implementations of spherical harmonic indexing and real space orientation refinement can both achieve speeds of thousands of patterns per second on modest hardware making its application accessible for routine EBSD analyses.

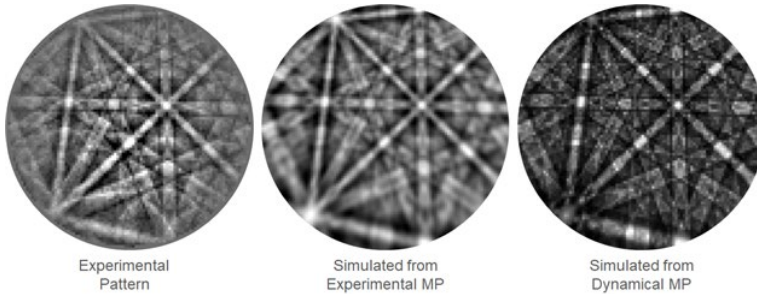
A remaining challenge for these indexing methods, both dictionary indexing and spherical indexing, is that they rely on detailed knowledge of the crystal structure of the phase(s) that are being indexed. The dynamic simulations that are the basis of the forward-model indexing methods are critically dependent on the crystal symmetry, atomic positions, occupancy, and electron scattering parameters. This is especially important in more complex phases such as solid solutions, intermetallic phases, and minerals. In many cases this detailed information is not available.

Alternative master patterns that do not require the same detailed knowledge of the crystal structure can be created using a kinematical model or using actual EBSD patterns. For these methods the information that is already available in the more basic EBSD structure files that are used for Hough transform-based indexing is sufficient. With the lattice parameters, the point group symmetry, a list of expected reflectors or bands, and the relative intensity of the bands in the EBSD patterns a kinematic spherical intensity model can be constructed. Alternatively, Kikuchi spheres may be created using actual EBSD patterns, provided that their phase and orientation is known by conventional EBSD indexing [3]. These spheres can then be applied as experimental master patterns for spherical indexing.

The advantage of using the experimental master patterns is that the required calculation time is less than 1 minute while dynamic simulations may take multiple hours to generate. Experimental patterns will also exhibit the same contrast range as the experimental patterns which may change with specific pattern image processing methods. With a closer match between the experimental patterns and the master pattern, improved indexing results may

be expected. In this presentation the requirements for successful generation of master pattern simulations for pattern matching will be discussed together with application examples.

**Graphic:**



**Keywords:**

EBSD, Forward-model, spherical-indexing, master-pattern

**Reference:**

- [1] Callahan, P. G., & De Graef, M. (2013). Dynamical electron backscatter diffraction patterns. Part I: Pattern simulations. *Microscopy and Microanalysis*, 19(5), 1255-1265
- [2] Lenthe, W. C., Singh, S., & De Graef, M. (2019). A spherical harmonic transform approach to the indexing of electron back-scattered diffraction patterns. *Ultramicroscopy*, 207, 112841
- [3] Day, A. P. "Spherical EBSD." *Journal of microscopy* 230.3 (2008): 472-486