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An algorithm for determining crystal lattices in unknown polycrystalline compounds

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When recovering crystallographic orientations of individual grains in polycrystalline materials both unit cell parameters and Bravais lattice are utilized. These crystallographic properties are normally determined from the radial spectra of diffraction rings by Power Diffraction Indexing programs. Afterwards, grains are located in reciprocal space by identifying replica of the Bravais lattice [1,2].

Here, a new method is presented for determining the crystallographic properties of unknown polycrystalline compounds. Effectively, the method reduces the polycrystalline data set into a single crystal data set. As the Bravais lattice is embedded multiple times in the data set (multiplicity is given by number of grains) the method seeks to recover the base lattice by rotating the whole data set and match it against itself. If, by chance, the rotation is close to the crystallographic mis-orientation between two grains the algorithm identifies the two lattices. A match against previously identified lattice solutions is made. Clearly, the probability of making a false match in either selection step is high. In the algorithm a number of filtering steps ensures that the final estimation of the base lattice is only constructed from high frequency lattice points. The unit cell and Bravais lattice can then be determined from the base lattice by a single crystal indexing program. The algorithm itself is implemented in [2]. The algorithm and results will be presented.

References

- [1] J. Wright, <http://fable.wiki.sourceforge.net/Imaged11>
- [2] S. Schmidt, <http://fable.wiki.sourceforge.net/GrainSpotter>