RIETVELD METHOD FOR BEGINNERS USING THE FULLPROF CODE: TIPS AND TRICKS.

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The Rietveld method [1] is a technique for structure refinement. Initially, it was developed to characterize polycrystalline materials by neutron diffraction. X-rays or neutrons powder diffraction data are recorded as diffraction patterns, typically as intensity plot versus diffraction angle. The Rietveld refinement uses the least squares method to minimize the difference between the experimental and modeled pattern. The height, width and position of these peaks can be used to determine various aspects of the structure of materials. Unlike other methods, it makes it possible to analyze the crystal structures of powders and to obtain reliable results even from patterns in which reflections from several component crystal phases overlap.

For beginners and novice users of Rietveld method a refinement programs may look like a black box. With regard to that, in the presentation the theoretical background of the Rietveld method and the refinement strategy will be presented. The structure of the managing file will be discussed. Illustrative examples of obtaining the outputs with information about structure, bond distances and angles, phase weight percentage and estimation of average crystallite size in the investigated material will be shown.

The examples will be based on the FullProf code [2] (https://www.ill.eu/sites/fullprof/). The atomic structure drawing will be realized by VESTA software [3] (https://jp-minerals.org/vesta/en/).

References

[1] Rietveld HM: A profile refinement method for nuclear and magnetic structures. J. Appl. Crystallogr. 1969;2(2):65

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[3] Momma K, and Izumi F: VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data. J. Appl. Crystallogr. 2011;44:1272