RIETVELD REFINEMENT WITH A MODEL THAT CONSIDERS CRYSTALLITE SIZE DISTRIBUTION AND ANISOTROPIC CRYSTALLITE SHAPE

Oscar Ovalle, Xim Bokhimi

Instituto de Física, Universidad Nacional Autónoma de México, A. P. 20-364, 01000 México D.F., Mexico

In most of the codes to refine crystallite structures using the Rietveld method, the microstructure of any phase is modeled by considering only an average crystallite size. Although this model gives good results, it is important to notice that the real sample has a distribution of crystallite sizes, independently of the synthesis method used to prepare it. In these codes, the most simple of the models for the crystallite size approximates the crystallite shape with a sphere. Some other more complicated models consider a specific morphology of the crystallites; for example, plates of needles. But, the best results for the average crystallite size are obtained by modeling its shape in the reciprocal space with an expansion of symmetrized spherical harmonics; the corresponding crystallite shape obtained in the real space is very similar to that obtained from the analysis of the sample with the electron microscope. The average crystallite obtained using the model of spherical harmonics, however, shows some deformations that could be produced by the fact that the crystallites of a given phase in a sample have a size distribution. Therefore, we have expanded the model of the average crystallite size with spherical harmonics by considering the fact that the size has a distribution. Almost all of the reports in the literature related to the distribution of crystallites size in a sample show that it is well described with a log-normal distribution; therefore, this model was implemented in the code TOPAS used to refine the crystalline structures with the Rietveld method. In the model, we assumed that all crystallites had the same shape. Applying the modified code to refine the crystalline structures of different samples, we show the effect that this distribution has on the refined parameters.