ESTIMATION OF MEAN CRYSTALLITE SIZES OF XRD STANDARD REFERENCE MATERIALS PRODUCED AT IPEN BY XLPA

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Palavras-chave: Standard Reference Materials;Line Profile Analysis;Crystallite Sizes

Resumo:

Standard reference materials (SRM) are used to certify the alignment of diffractometers by calibrating peak positions and its shapes. SRM's are also used in X-ray Line Profile Analysis to correct the instrumental contribution to the experimental line breadth, which permits the determination of mean crystallite sizes and microstrains of materials. For this purpose the SRM must have a large crystallite size (generally greater than 300 nm) and almost zero or none microstrains. Since the profiles of the SRM are usually very narrow, the determination of its size are generally difficult to perform which leads to the application of the simplest XLPA method, the Scherrer method. However this method does not take into account a possible contribution of the microstrains. To overcome this problem the Single-Line method was applied to determine the mean crystallite sizes and microstrains of the SRM's Y_2O_3, CeO_2 and Al_2O_3 produced at IPEN to provide a more refined method to estimate size-strain of these standard reference materials. For this purpose a sample of LaB_6 SRM from NIST was used to correct the instrumental contribution since it presented the narrowest profile among the SRM's. The analysis was performed on synchrotron radiation data measured at the Brazilian Synchrotron Light Source - LNLS.