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Modeling background level of XRD peak profile for the variance method of size-strain analysis

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ABSTRACT

A modified version of the Enzo-Parrish method is introduced, which successfully determines a straight background level with a nonzero gradient. The modeled "true" background levels obtained using both the Enzo-Parrish and modified Enzo-Parrish methods are compared with those obtained using the central moment method. This study proposes a method that uses a scattering vector, $S = 2\cos\theta_0\sin(\theta-\theta_0)/\lambda$, where $2\theta_0$ is the centroid, 2θ is Bragg (scattering) angle, and λ is the wavelength of the X-ray. The proposed method determines the background from the slope of the linear portion of a plot of $I(S)S^2$ versus S^2, where $I(S)$ is the intensity. To the best of the author's knowledge, this is the first time that this method has been used to model and subtract the background level for the variance method of size-strain analysis. The modified Enzo-Parrish method enables modeling and subtracting the background level of an XRD peak of a polymer sample. The accuracy of the method is evaluated based on the linear change of the variance-range curve of the XRD peak of a polymer sample.

Introduction

The X-ray diffractometer (XRD) intensity profile contains information about the size and strain of a polycrystalline material. Before attempting to identify the microstructural parameters, it is important to correct the intensity profile by removing instrumental broadening and subtracting the background level. The central moment method [1] is commonly used to subtract the background level and determine microstructural parameters simultaneously. However, when analyzing XRD patterns with asymmetric background levels with respect to the centroid, it is necessary to determine the background level separately. The Enzo-Parrish method is a useful alternative for determining the background level without considering microstructural parameters [2]. This method successfully avoids the "hook" effect [3] in the Warren–Averbach method of size-strain analysis.

The "true" background level

In studying the variance-range function [4], the "true" background level of an XRD profile pattern is defined

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