Pair Distribution Function and Principal Component Analysis for Structural Discrepancy of Solid

HUA YONGBIAO, 김우식[1,†]

경희대학교 국제캠퍼스;

[1]Department of Chemical Engineering, Functional Crystallization Center, Kyung Hee University

(wskim@khu.ac.kr[†])

This present study aimed to interpret the structure discrepancy of solid using the Pair Distribution Function (PDF) and Principal Component Analysis (PCA). Generally, the Powder X-ray diffraction was the matured method to choose for structure analysis of solid. However, significant, and often sufficient, structure information of complex solid cannot be totally gleaned from the Powder X-ray diffraction this is clearly because the structure information of solid obtaining from powder diffraction was based on the Bragg scattering only. Recently, the Pair Distribution Function, a total diffraction approach, was developed to study the structure of solid. Additionally, Principal Component Analysis (PCA), a multivariate statistical method, can provide an efficient procedure for exploratory data treatment. Thus, PCA can be applied to efficiently evaluate and simplify larger volumes of complex PDF data, as a complementary step in better interpreting the existed discrepancy in the solid. In this study, the structure discrepancy of solid was investigated by a new approach using the Pair Distribution Function and Principal Component Analysis.