

Location of Cation and Water in Zeolites : Combination of Focus and Charge-flipping Algorithms

김택희, 장영배, 선민호, 이 준, 조성준*
전남대학교 신화학소재공학과
(sjcho@chonnam.ac.kr*)

Zeolites are polycrystalline powder materials consisting of infinite tetrahedral units to allow the formation of suitable pore, depending on structure directing agents and hydrothermal synthesis condition and thereby unique structural integrities for adsorption and catalysis. Location of cation and water inside the zeolite's cage play a critical role in hydrothermal stability, catalysis, adsorption etc. Therefore, the determination of these locations has been of special interest. However, it is difficult to obtain the location readily by analyzing the powder XRD patterns with the Rietvelt refinement combined with the fourier difference method even though the data quality is good when the synchrotron radiation is employed as X-ray source. In the present work, the Focus method, a direct method using topology search, has been coupled with the charge-flipping method in which the small electron density was modified to get the final electron density maps, to reveal the location of cation and water, respectively. The combined method has been a successful to elucidate these locations in KL zeolite, Na exchanged modernite, ZSM-22 etc.