Crystal Structure Analysis of $Bi_{4-x}Nd_xTi_3O_{12}$ by Using Neutron Powder Diffraction Data

전민구, 김용일[1], 남승훈[1], 손정민[2], 정창화, 우성일*
한국과학기술원 생명화학공학과 &
초미세 화학공정 시스템 연구센터;
[1]한국표준과학연구원;
[2]전북대학교 자원・에너지공학과
(siwoo@kaist.ac.kr*)

Neutron powder diffraction data was used for crsytal structure analysis of ferroelectric $Bi_{4-x}Nd_xTi_3O_{12}$ (BNT, x = 0, 0.25, 0.5, 0.75 and 1.0). Rietveld refinement was carried out for all samples. Decrease of *a*-axis lattice parameter was observed with an increase in substituted amount of Nd. Orthorhombicity, defined as $2(a-b)/(a+b)$, also decreased with increasing x. Based on the refinement results, spontaneous polarization alogn the *a*-axis was calculated, which decreased from 35.4 to 28.3, 24.8, 22.2 and 7.6 $\mu C/cm^2$ with increasing x from 0 to 0.25, 0.5, 0.75 and 1.0 respectively.