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Structure Refinement of a Sol-gel Derived Pyrochlore Bi₂Ti₂O₇ Using a Neutron Scatterings WON-JEONG KIM, SANG SU KIM, JONG KUK KIM, JUN KI CHUNG, MUN HEUM PARK, TAE GON HA, EUN JIN CHOI, JIN WON KIM, HYUN KYEONG CHO, Dept. of Physics, Changwon National University — Structure of the sol-gel derived pyrochlore Bi₂Ti₂O₇ has been refined by a Rietveld analysis method using neutron and x-ray scattering data. The structure of Bi2Ti2O7 was assumed as Fd-3m (space group number 227). The calculated lattice constant was 10.3735(3) nm. The sample contains a majority Bi₂Ti₂O₇ phase and minor Bi₄Ti₃O₁₂, Bi₁₂TiO₂₀, and TiO₂ phases. After subtracting the secondary phases effect, the total goodness of fit using both scatterings was conversed to χ^2 = 2.6, Rp = 6.5 %, and wRp = 8.6 %, which suggesting that the refined structure of Bi₂Ti₂O₇ is reasonable. Bi atom occupies 96 g site with probability of 0.158(1), while O occupies 8 a site by 0.884(16). Furthermore, Bi₂Ti₂O₇ thin film has been fabricated by a sol-gel method. After depositing electrodes, electrical properties of the thin film have been measured. Interestingly, a ferroelectric characteristics has been observed; electric field dependent dielectric constant. The refined structure information of Bi₂Ti₂O₇ may explain the observed ferroelectricity of the thin films. Details of the structural and electrical properties of Bi₂Ti₂O₇ will be discussed.

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