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Effect of Nonlinear Coupling Between Polarizations and Stresses on the Ferroeletric Properties of $BaTiO_3$

송태권†

창원대학교

(tksong@changwon.ac.kr†)

The effects of lateral stresses in the phase transitions of perovskite ferroelectric materials such as $BaTiO_3$ and $PbTiO_3$ have been studied extensively theoretically and experimentally. Pertsev *et al.* have proposed phase diagrams of BT and PT under 2 dimensional (2D) stresses with the aid of Landau-Devonshire calculations. This 2D clamping condition is compatible with perovskite thin films epitaxially grown on oxide substrates.

With compressive stress or with negative misfit strain, the phase transition temperature (T_3) from paraelectric cubic phase to ferroelectric tetragonal phase (*c*-phase; the direction of polarization is perpendicular to the film surface) was calculated to increase linearly with stress. On the other hand, with tensile stress or with negative misfit strain, the phase transition temperature (T_1) from paraelectric cubic phase to ferroelectric phase (*aa*-phase; the direction of polarization is parallel to the film surface) was also calculated to increase linearly with stress. These theoretically calculated results were realized in the pulsed laser deposited BT thin films with $SrRuO_3$ bottom electrode with $GdScO_3$ or $DyScO_3$ substrates.

Experimentally observed T_3 in $BaTiO_3$ single crystal under two-dimensional pressure, however, showed quadratic increase on external pressure. Similar results were observed in externally stressed $Pb(Zr,Ti)O_3$ thin films and explained by introducing new couplings between σ^2 and P^2.[4] And the fact that the crystal structure below transition temperature is still tetragonal in compressively strained $BaTiO_3$ thin film and observed polarization values are much larger than calculated values asks us more investigation about the character of phase transition.

In this work, the effects of new coupling terms were studied. Polarization values and phase transition temperatures under compressive strains were calculated and compared with previous results.

Keywords: Ferroelectrics, Polarization, Landau-Devonshire theory, Stress

B-6

PEMFC 전극용 CNF의 합성 및 촉매 담지 특성

이원우, 최영민, 류병환†, 신채호*

한국화학연구원 화학소재연구단; *충북대학교 화학공학과

(bhryu@krict.re.kr†)

고분자전해질 연료전지(PEMFC, polymer electrolyte membrane fuel cell)는 작동온도가 낮으면서도 효율이 좋고, 다른 연료전지에 비해 부피를 줄일 수 있다는 장점으로 많은 관심을 받고 있다. 본 실험에서는 PEMFC 전극소재 개발을 위하여 solvothermal 법으로 CNF(carbon nanofiber)를 합성하였다. CNF 성장시간 변화로 길이 조절을 하였으며, CNF를 합성, 정제를 거쳐서 Pt 촉매 담지를 하였다. 이를 PEMFC 전극 소재로의 적용을 위하여 전극 특성을 평가하였다.

전자현미경, XRD, Raman spectra 등의 분석 결과로 성장시간 변화에 의해 합성한 CNF 직경은 약 10nm 이었으며, 길이는 1㎛ 이상까지 제어 가능하였다. 그리고 산처리와 열처리의 정제 과정 후에 Pt 촉매를 담지 하였으며, 담지 여부는 TEM image와 순환전압곡선으로 확인하였다. 이후 전극 특성은 I-V curve로 평가하였다.

Keywords: PEMFC, CNF