Contribution ID : **105** Type : **Oral**

Defect structure-property correlations in Li doped BaTiO3

Friday, 13 November 2020 09:30 (20)

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In the present work we investigate the important issue of the structure and dynamics of smaller ions in oxides and the resulting impact on its functional properties. For this purpose, we selected a 7% Li-doped BaTiO3. Li is a vital ingredient in novel energy storage technologies such as Li-ion batteries. The smaller Li-ion can influence the structural stability, homogeneity, local environment, and dynamic behavior of the host lattice, affecting and optimizing the dielectric and multiferroic properties of novel polar functional materials [1-2]. However, the Li-ion positions and dynamics in functional materials are not completely understood, controversially discussed and are the subject of extensive ongoing research [3]. Furthermore, sample inhomogeneity due to Li migration to the grain boundary and/or development of multiple phases complicates the elucidation of the structure-property correlations that may lead to incorrect interpretations [4]. The selection of BaTiO3 as the host lattice is due to materials based on this being considered as the alternative to the piezoelectric lead zirconate titanate, citing environmental issues [5]. BaTiO3 also crystallizes in a simple perovskite structure and Li ions can be effectively doped into it at lower doping levels. Very recently, field-dependent electric polarization measurements on BaTiO3 exhibited a polarization–electric field double hysteresis loop upon Li doping [4]. These drastic changes to the electric polarization, related to the doping poses a good test case for the investigation of the Li-induced defect structure model and its influence on the functional properties. To elucidate the above structure-property correlations, we combined several techniques, such as neutron powder diffraction electron microprobe associated with the wavelength-dispersive spectroscopy, 7Li nuclear magnetic resonance spectroscopy (NMR), electron paramagnetic resonance (EPR), electric polarization measurement, and theoretical calculations based on density functional theory [6].

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Session Classification : Advanced Materials

Track Classification : Advanced Materials