Point Defects in Lead Titanate : a first-principles study

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Domain Walls have attracted considerable interest recently, for they show enhanced or new properties, such as superconductivity[1] in WO_3, increased conductivity in $BiFeO_3$[2,3], or vortices[4]. Domain walls have also been suggested to trap some point defects. Such property is of crucial interest because it may (i) induce electronic or ionic conductivity in the DW, and (ii) decrease the mobility of the DW. However, these trapping phenomena have not been, to our knowledge, exhaustively investigated in any ferroelectric material. We have chosen $PbTiO_3$ as a prototypical system for modeling the domain walls, and investigated the properties of single vacancies in the domain wall and in the bulk.

In this work, we performed first-principles density-functional calculations, with the ABINIT code, in the Projector-Augmented Wave framework, to simulate Pb, Ti and O vacancies at 180° and 90° domain walls in lead titanate. Here, we focus mainly on 180° DWs, and using the Local Density Approximation in 120-atom (6x2x2) supercells, we show that Pb, Ti and O vacancies preferentially form in the DW, whatever their charge state (formation energies are typically 0.1-0.3 eV lower in the domain wall). Such stabilization is likely to be a consequence of the partial relaxation of the DW elastic energy.

The defect concentration can be tuned by the thermodynamic external conditions (oxygen pressure, Pb and/or Ti chemical potential when the material is formed), and by extrinsic doping (acceptor/donor) to modify the Fermi level. Defect engineering in conjunction with domain engineering could then lead to atomic layer thick 2D conductive pathways, of great interest for new electronic devices.

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References

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