Interactions between Point Defects and Ferroelectric Domain Walls

D.R. Småbråten[1], L. Xia[1], S.H. Skjærvø[1], T. Tybell[2] and S.M. Selbach[1,*]
[1]Department of Materials Science and Engineering,
NTNU Norwegian University of Science and Technology, N7491 Trondheim, Norway
[2]Department of Electronics and Telecommunications,
NTNU Norwegian University of Science and Technology, N7491 Trondheim, Norway
* S.M. Selbach: selbach@ntnu.no

We study interactions between point defects and ferroelectric domain walls by density functional theory (DFT) calculations. Point defects like oxygen vacancies and interstitials, and cation vacancies, change the local strain field and electrostatic environment in the surrounding lattice. Likewise, charged neutral ferroelectric domain walls (e.g. 180º walls) give rise to a local strain field due to the change of ferroelectric displacements across the domain wall. Charged ferroelectric domain walls also, in addition to lattice strain, give rise to electric fields which must be screened. Using the rhombohedral perovskite $BiFeO_3$ as a prototypical ferroelectric and the hexagonal manganite $YMnO_3$ as an example of an improper ferroelectric, we calculate the segregation enthalpy of common point defects in these materials at their respective low-energy ferroelectric domain walls. We suggest general rules for when point defects accumulate or deplete at domain walls, and discuss the influence of point defects on the local ferroelectric polarization and electronic structure at domain walls in relation to recent experimental reports.