Bloch-type Ferroelectric Domain Walls in Rhombohedral $BaTiO_3$

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Ferroelectric domain walls (FDWs) are usually considered to be of Ising type, in which $\mathbf{P}_{\parallel}$, the projection of the polarization vector onto the plane of the domain wall, simply reverses itself by passing through zero along a high-symmetry path as one scans through the domain wall. Ising FDWs tend to be favored because ferroelectrics are generally strongly electrostrictive, so that a rotation of $\mathbf{P}_{\parallel}$ away from this high-symmetry path would entail a significant elastic energy cost. However, there have been some theoretical predictions of the presence of Bloch and even Néel components in some FDWs [1, 2]. Most recently, it has been predicted, in the framework of a phenomenological Ginzburg-Landau-Devonshire (GLD) model, that the 180° FDWs in rhombohedral $BaTiO_3$ are of Bloch type [3].

In the low-temperature rhombohedral phase of $BaTiO_3$, the possible mechanically compatible and electrically neutral FDWs are of three types: R71°, R109°, and R180°, where the angle denotes the rotation relating $\mathbf{P}_1$ and $\mathbf{P}_2$ (the polarizations on either side of the wall). The plane of the domain wall can be either $\{\bar{2}11\}$ or $\{1\bar{1}0\}$ for the 180° FDW, and is normal to $\mathbf{P}_1 + \mathbf{P}_2$ for the other two FDWs. We have investigated the R71°, R109°, and R180°$\{1\bar{1}0\}$ FDWs in $BaTiO_3$ using first-principles calculations within the local-density approximation (LDA).

Our calculations confirm the Bloch nature of the R180°$\{1\bar{1}0\}$ wall, which can be thought of as a combination of Ising R71° and R109° FDWs. Comparison of the first-principles results and the GLD model [3] suggests that a 40% reduction in the gradient term in the GLD model is needed to bring agreement with the first-principles results. The R71° FDW is found to be of Ising type; this is consistent with expectations since the Bloch component for this wall points towards the center of a cube face, which is not one of the preferred directions in the rhombohedral phase. For the R109° FDW, on the other hand, the Bloch component of $\mathbf{P}$ does point toward a rhombohedral polarization direction, making the Bloch configuration competitive with the Ising one in this case. In fact, the Bloch R109° FDW can be considered as a combination of two Ising R71° walls, and the energy difference between this and the Ising R109° FDW is only a few meV.

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