Abstract Submitted
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Bloch-type domain walls in rhombohedral $BaTiO_3$ MARYAM TAHERINEJAD, DAVID VANDERBILT, Rutgers University, PAVEL MARTON, VILGELMINA STEPKOVA, JIRI HLINKA, Academy of Sciences of the Czech Republic — Ferroelectric domain walls (FDWs) are usually considered to be of Ising type, but there have been suggestions in recent years that Bloch-type FDWs, in which the polarization rotates in the plane of the FDW, are also possible. The mechanically compatible and electrically neutral FDWs in rhombohedral $BaTiO_3$ are of 71°, 109°, and 180° type. We have investigated these FDWs based both on first-principles calculations and on a Ginzburg-Landau-Devonshire (GLD) model.[1] The results from both approaches confirm the Ising nature of the 71° FDW and the Bloch nature of the 180° FDW, and predict both Ising-type and Bloch-type FDWs are possible for the 109° case. Considering the relatively small rhombohedral strain in $BaTiO_3$, the competition between the energies of Bloch and Ising FDWs can be discussed in terms of a picture in which a Bloch wall is regarded as being composed of a pair of smaller-angle Ising ones. A reduction by 40% in the parameters describing the gradient term in the GLD model brings it into better agreement with the first-principles results for detailed properties such as the energies and widths of the FDWs.

[1]P. Marton, I. Rychetsky, and J. Hlinka, Phys. Rev. B **81**, 144125 (2010).

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