Zero-temperature Landau-Devonshire Potential for $BiFeO_3$ From the First Principles

P. Marton[1,2,*], A. Klíč[1], M. Paściak[1], and J. Hlinka[1]
[1]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, Praha, Czech Republic, CZ-182 21
[2]Institute of Mechatronics and Computer Engineering,
Technical University of Liberec, Studentská 2, Liberec, Czech Republic, CZ-461 17
*Pavel Marton: marton@fzu.cz

$BiFeO_3$ is a prototypic multiferroic material with rhombohedral ground state, ferroelectric polarization of about $0.9C/m^2$ and oxygen-octahedra tilts of about 14 degree along the rhombohedral [111] axis. The large switchable polarization and possibility to design high-density domain-engineered patterns in bulk crystals and in thin films is indeed favorable for potential applications. Some of them utilize the enhancement of the electromechanical properties due to presence of dense domains, while other focus more on subtle properties related to domain walls and their different electronic structure compared to bulk.

In any case, the domain structure brings yet another level of complexity to understanding of structure-property relationship in this material. The material was recently extensively studied using calculations and simulations at different scales. We focus on the modeling of ferroelectricity in the Ginzburg-Landau-Devonshire framework, which allows to conveniently address some properties of domain walls and, more interestingly, also their behavior in realistic domain patterns. Typically, such task is beyond the actual computational limits of more accurate first-principles and atomistic models. Moreover, parameters of the phenomenological models bear useful information about susceptibilities and couplings between order parameters. Therefore, reliable parametrization for the $BiFeO_3$ is highly desirable. There are already several publications of such potentials [1,2,3], which address particular aspects of the $BiFeO_3$ behavior, but for different reasons they do not seem to be sufficient e.g. for systematic investigation of domain walls.

In contrast to more simple ferroelectrics like $BaTiO_3$ where the important degrees of freedom are polarization and deformation, the $BiFeO_3$ has also rotations of oxygen octahedra and its energy landscape is more complex. Moreover it turns out that there is a strong interplay between polarization, oxygen-octahedra tilting, and strain which determines the structure and properties [4]. In addition, the energetics related to tilting of oxygen octahedra, necessary to parametrize the phenomenological potential, is difficult to address experimentally, and therefore in order to take it into account we rely on outcomes of calculations.

In this work we present our attempt to derive the Landau-Devonshire type potential for $BiFeO_3$ including polarization, tilt and strain degree of freedom, which is based purely on first principles calculations. We use the model to evaluate intrinsic dielectric, piezoelectric and elastic material tensors and compare this prediction with theoretical and experimental data available in the literature. Also, where possible, we compare the obtained parametrization of the Landau potential with other available parametrizations [1,2,3].

[1] F. Xue, Y. Gu, L.Liang, Y. Wang, and L. Q. Chen, "Orientations of low-energy domain walls in perovskites with oxygen octahedral tilts", Phys. Rev. B vol. 90, p. 220101, 2014.
[2] A. F. Popkov, N. E. Kulagin, S. V. Soloviov, K. S. Sukmanova, Z. V. Gareeva, and A. K. Zvezdin, "Electric-field-induced structural and magnetic transformations in BiFeO3 multiferroics", Phys. Rev. B vol. 92, p. 140414, 2015.
[3] N. E. Kulagin, A. F. Popkov, S. V. Soloviov, K. S. Sukmanova, and A. K. Zvezdin, "Electric-field-induced structural and magnetic transformations in BiFeO3 multiferroics", Physics of the Solid State vol. 57, p. 933, 2015.
[4] O. Diéguez, O. González-Váazquez, J. Wojdeł, and J. Íñiguez, "First-principles predictions of low-energy phases of multiferroic BiFeO3", Phys. Rev. B, vol. 83, p. 094105, 2011.