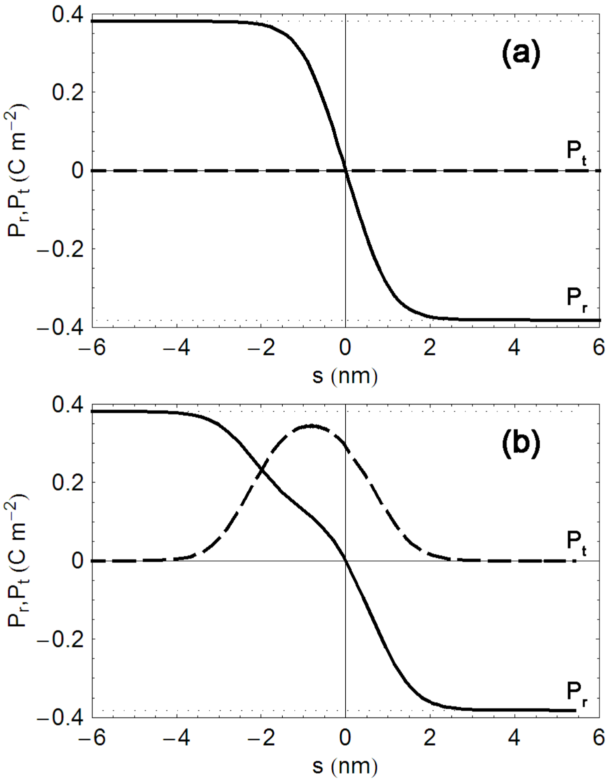

FIG. 9: Profiles of polarization components in R180{1$\bar{1}$0} domain wall showing the SPP stationary trajectory (a) as well as the lower energy Bloch-like solution (b), both for the model parameters corresponding to $T = 118\,\mathrm{K}$. Full line stands for the P_r component of polarization vector, broken line for the P_t one. The bottom panel demonstrates that Bloch solution may considerable modify the domain domain wall profile.

VII. CONCLUSION

The work reports detailed study of mechanically compatible and electrically neutral domain walls in $BaTiO_3$. The investigation was done within the framework of the GLD model. Using the SPP approximation it was possible to compare properties of various kinds of domain wall species from the same perspective.

The phenomenological nature of the GLD model allowed to predict the temperature dependence of the domain wall characteristics in the whole temperature range of ferroelectric phases. Its continuous nature gave us even the opportunity to deal conveniently with the non-crystallographic S-type domain wall, which has a general orientation with respect to the crystal lattice, and which is therefore difficult to cope with in discrete models relying on periodic boundary conditions.

The S-wall in the orthorhombic, as well as the 90° wall in tetragonal phase were both found to be about 4 nm thick and consequently are expected to be mobile, i.e. they could be easily driven by external fields, and they may thus significantly contribute to the dielectric or piezoelectric response of the material.

For several temperatures, we have numerically investigated domain walls allowing for more complicated CPP solutions with non-constant P_t. We have identified solutions, which could be considered as analogues of Bloch walls known from magnetism. Interestingly, in contrast with Ref. 3, our model predicts the Ising-type profile of the O180{1$\bar{1}$0} wall. At the same time the Bloch-like structure of the O180{001} wall is predicted.

We believe that this kind of somewhat exotic walls actually represent important generic examples of ferroelectric domain species, which should be anticipated in all ferroelectrics with several equivalent domain states distinguished simultaneously by the orientation of the spontaneous polarization and strain. They should be certainly taken into account in investigations of domain-wall phenomena in ferroelectric perovskites. At the same time, the energy differences between the Bloch-like and Ising-like solutions are rather subtle here. Therefore, in spite of the fairly good agreement for 180° and 90° domain walls between ab-initio calculations and predictions of this model in the tetragonal phase,[4] the preference for the calculated Bloch-like trajectories may not necessarily reproduced for the domain walls encountered in real $BaTiO_3$ crystal, since there is obviously a considerable uncertainty in the adopted material-specific GLD parameters. In addition, predictions for the domain walls with very small thickness must be considered with a particular caution since the description of the sharp domain wall profiles obviously touches the limits of the applicability of the continuous model.

In conclusion, we have derived a number of qualitative and quantitative predictions for mechanically compatible neutral domain walls of tetragonal, orthorhombic and rhombohedral $BaTiO_3$ on the basis of the previously proposed material-specific GLD model. We believe that the insight into the domain wall properties mediated by the provided analytical and numerical analysis could be helpful for understanding of domain wall phenomena in $BaTiO_3$ as well as in some other intensively investigated members of the ferroelectric perovskite family with same sort of macroscopic ferroelectric phases, for example in $KNbO_3$, $BiFeO_3$, $PbTiO_3$ or even PZT and perovskite relaxor-related materials.

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