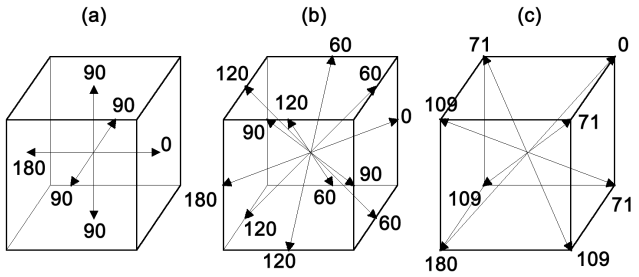

FIG. 1: Directions of spontaneous polarization in the (a) tetragonal, (b) orthorhombic and (c) rhombohedral phase. Angles between polarization direction '0' and its symmetry equivalent ones are indicated.

erties in $BaTiO_3$ are the same as in our preceding work,[4] but for the sake of convenience, the definition and the GLD model and its parameters are resumed in Section III. Section IV. is devoted to the description of the computational scheme and approximations applied here to solve analytically the Euler-Lagrange equations. The main result of our study - systematic numerical evaluation of thicknesses, energies, polarization profiles and other properties for different domain walls, is presented in Section V. Sections VI. and VII. are devoted to the discussion of validity of used approximations and the final conclusion, respectively.

II. MECHANICALLY COMPATIBLE DOMAIN WALLS IN BARIUM TITANATE

The energy-degeneracy of different directions of spontaneous polarization leads to the appearance of ferroelectric domain structure. Individual domains are separated by domain walls, where the polarization changes from one state to another. Here, only planar domain walls are considered. Orientations of mechanically compatible domain walls are determined by the equation for mechanically compatible interfaces separating two domains with the strain tensors $e_{ij}(-\infty)$ and $e_{ij}(\infty)$:

$$\sum_{m,n=1}^{3} [e_{mn}(\infty) - e_{mn}(-\infty)]x_m x_n = 0 \ . \qquad (1)$$

Systematic analysis of this equation using symmetry arguments has been done e.g. in Refs. 10–12. In general, the number N of mechanically compatible domain walls separating two particular domain states can have only one of the three values: $N = 0$, $N = 2$ or $N = \infty$. In case of $N = 2$ there exist two mutually perpendicular domain walls. Each of them is either a crystallographic (W_f-type) wall or non-crystallographic (S-type) wall. Orientation of the W_f-wall is fixed by symmetry of the crystal, while orientation of the S-wall is determined by components of the strain tensor in adjacent domains

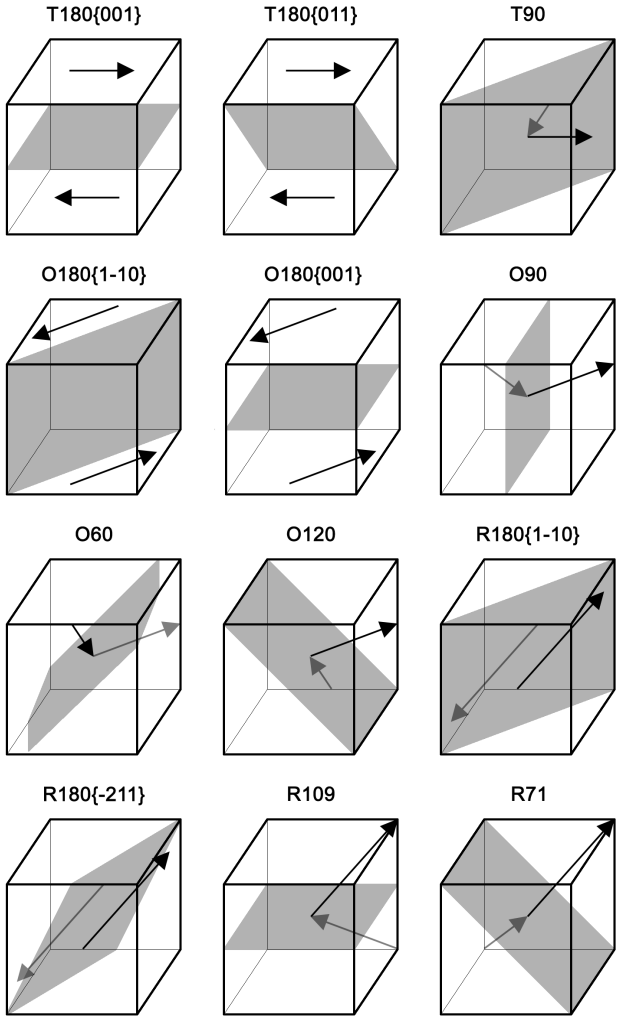

FIG. 2: Set of mechanically compatible and electrically neutral domain walls in the three ferroelectric phases of $BaTiO_3$. In the case of 180° domain walls, where the orientation is not determined by symmetry, walls with the most important crystallographic orientations are displayed.

(and its orientation can be therefore dependent on temperature). For $N = \infty$ there exists infinite number of wall orientations, some of them may be preferred energetically.

Further, the electrically neutral domain walls will be considered.[10] It implies that the difference $\mathbf{P}(\infty) - \mathbf{P}(-\infty)$ between the spontaneous polarizations in the adjacent domains is perpendicular to the unit vector $\mathbf{s}$, normal to the domain wall:

$$(\mathbf{P}(\infty) - \mathbf{P}(-\infty)) \cdot \mathbf{s} = 0 \, . \qquad (2)$$

We also define a unit vector $\mathbf{r} \parallel (\mathbf{P}(\infty) - \mathbf{P}(-\infty))$, which identifies the component of the spontaneous polarization which reverses when crossing the wall. Then the charge neutrality condition (2) can be expressed as $\mathbf{r} \cdot \mathbf{s} = 0$. Finally, let us introduce a third base vector $\mathbf{t} = \mathbf{r} \times \mathbf{s}$,