Macroscopic polarization from antiferrodistortive cycloids in ferroelastic SrTiO$_3$

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Based on a first-principles based multiscale approach, we study the polarity ($P$) of ferroelastic twin walls in SrTiO$_3$. In addition to flexoelectricity, which was pointed out before, we identify two new mechanisms that crucially contribute to $P$: a direct “rotopolar” coupling to the gradients of the antiferrodistortive (AFD) oxygen tilts, and a trilinear coupling that is mediated by the antiferroelectric displacement of the Ti atoms. Remarkably, the rotopolar coupling presents a strong analogy to the mechanism that generates a spontaneous polarization in cycloidal magnets. We show how this similarity allows for a breakdown of macroscopic inversion symmetry (and therefore, a macroscopic polarization) in a periodic sequence of parallel twins. These results open new avenues towards engineering pyroelectricity or piezoelectricity in nominally nonpolar ferroic materials.

Domain walls (DW) in ferroic materials are a recognized source of unusual physical effects, of practical interest for electronic device applications. Such properties are mainly due to the local modification of the crystal structure, which can manifest itself via two distinct mechanisms. First, one or more components of the primary order parameter need to change sign at the DW, and hence it will locally vanish. This implies that latent secondary inabilities, suppressed in the stable bulk phase because of the mutual competition between modes, may in principle become active at the wall. Second, in the domain wall region one or more degrees of freedom undergo a large variation on a short length scale, which means that gradient couplings (e.g., flexoelectricity) can have a strong impact on the physics.

Among all different DWs, ferroelastic twin boundaries seem very promising candidates for emerging functionalities. Indeed, they locally break inversion symmetry, and hence can show a polar behavior, even if the bulk ferroelastic domains are nonpolar. One of the most representative examples is CaTiO$_3$, where the presence of a local polarity at the twin boundaries (TB) was first theoretically predicted via an empirical atomistic model, and later experimentally confirmed by transmission electron microscopy. Interestingly, a recent first-principles analysis has postulated an improper origin of the polarization, which would emerge from trilinear couplings between tilt modes that are enabled in the domain-wall region.

While polarity should, by symmetry, be present at the twin boundaries of SrTiO$_3$ (STO) as well, the available supporting experimental evidence, based on the appearance of electromechanical resonance peaks in the low-temperature regime, is only indirect. Existing phenomenological works emphasize a flexoelectric origin of the polarization at twin boundaries in SrTiO$_3$: A ferroelastic twin wall, by definition, separates two domains with different strain states; thus, a strain gradient must necessarily be present at the boundary. Since flexoelectricity is a universal effect of all insulators, it must produce a net polarization therein. Such an interpretation was recently confirmed by numerical simulations based on a simplified atomistic model, but a first-principles analysis is still missing. Consequently, many fundamental and practical questions are left, to date, unsettled; given the increasing importance of SrTiO$_3$ as a functional oxide material this is a timely moment for clarifying these matters.

The first obvious question concerns the magnitude of the wall polarization: Phenomenological theories or empirical potentials can hardly push their accuracy beyond order-of-magnitude estimates, as many of the relevant coupling coefficients (e.g., the flexoelectric tensor) are difficult to access experimentally. The second, more profound, question concerns the very physical origin of the couplings that may induce a polarization ($P$) at the wall: Is flexoelectricity really the end of the story in SrTiO$_3$? Or is there, similarly to the CaTiO$_3$ case, also an “improper” contribution to $P$, directly related to the tilt pattern? And, if yes, is there a way to write such improper couplings as well-defined bulk properties of the material?

To answer these questions with quantitative accuracy, a sound microscopic analysis, e.g., as provided by density functional theory (DFT), is clearly mandatory. Note that, in the past, DFT has been applied with success to a vast range of complex ferroic systems, e.g., the so-called “hybrid improper” ferroelectrics. Applying the same computational strategies (i.e., of inspecting the energy landscape of the crystal in a vicinity of some high-symmetry reference structure) to a spatially inhomogeneous system such as a domain wall, however, presents considerable methodological challenges. In particular, to correctly describe the local variation of the order parameters near the wall one needs to consider gradient-mediated couplings – these imply a breakdown of translational symmetry, and are therefore difficult to calculate within DFT. As we shall illustrate shortly, recent advances in the first-principles theory of flexoelectricity have now opened the way towards overcoming such lim-
Here we present a novel multiscale theory of emergent polarity at improper ferroelastic walls, which relies on a systematic perturbative approach to bridge the macroscopic and microscopic length scales. In particular, we extract the relevant gradient-mediated terms in the Hamiltonian via a long-wavelength expansion of the linear and nonlinear interatomic force constants (IFCs) of the reference bulk phase. The calculated coupling coefficients are then incorporated in a one-dimensional continuum model, whose solutions yield the relaxed atomic structure of the twin boundary. Application of this method to SrTiO$_3$ reveals that no less than three independent couplings contribute to the polar distortions at a twin wall: (i) the flexoelectric “roto-flexo” coupling that was already considered in earlier works [7,11]; (ii) a new “rotopolar” coupling, involving the tilt amplitude and the gradient of the tilt, which generalizes and provides a formal basis to the “improper” mechanism of Ref. [9] (iii) a trilinear coupling mediated by the antiferroelectric (AFE) displacement of the Ti atoms, which was never reported before, to the best of our knowledge. Our calculations show that contributions (i-iii) are comparable in magnitude, and they all must be included to gain a quantitative, or sometimes even qualitative, insight into the properties of a twinned SrTiO$_3$ sample. Remarkably, the “rotopolar” coupling (ii) has the exact same form as that occurring in spiral magnets [12]; this implies that simple twinned structures can, in close analogy to spin cycloids, produce a measurable macroscopic polarization in ferroelastic SrTiO$_3$. We also find that twin walls in SrTiO$_3$ are much thicker (we find a characteristic length in excess of 5 nm in the low-temperature limit) than previously thought, [13] with a reversed energy ordering between “easy” and “hard” types. [8]

Ferroelastic twins in SrTiO$_3$ occur between tetragonal domains (the tilt pattern is $a^α b^α c^-$ in Glazer notation) whose respective AFE tilt axes are oriented at 90° with respect to each other. Following the usual procedure, [8,13] they can be conveniently represented as a one-dimensional problem, where the relevant vector or tensor quantities are projected along two directions that are either perpendicular (\(\hat{s}\)) or parallel (\(\hat{r}\)) to the wall. (These correspond to the [110] and [110] pseudocubic directions, respectively.) Depending on which component of the AFD pseudovector, \(φ_r\) or \(φ_s\), changes sign at the wall, we have two distinct types of twin boundaries; we shall indicate them as “head-to-tail” (HT) and “head-to-head” (HH) henceforth (see Fig. 4).

With this in mind, we shall expand the energy around the reference cubic phase as follows (\(i = r,s; \partial = ∂/∂s\)),

\[
E = \frac{C_{αβ}}{2} ε_α ε_β + \frac{κ}{2} |φ|^2 + A |φ|^4 + \frac{χ_0}{2} P^2 - R_α φ_α^2 - Q_1 φ_1^2 P^2 - ε_α P^2 ε_α + \frac{Δ_i}{2} (∂φ_i)^2 + \frac{G}{2} (P)^2 - f P η P φ_j - W_{ij} P(∂φ_i)φ_j + \frac{κ_{Ti}^2}{2} (u^{Ti})^2 + NP_u^{Ti} φ_s + S(∂φ_r)u^{Ti},
\]

(1)

where the independent variables (all represented as continuous functions of the \(s\) coordinate) are the tilt amplitudes (\(φ_{r,s}\)), the polarization (\(P\)) along \(\hat{r}\) (we shall neglect the small antisymmetric components of \(P\) that are perpendicular to the wall plane [4]), which we associate with the amplitude of the “soft” zone-center optical phonon, the strain components in Voigt notation (\(ε_α\)) and the amplitude of the antiferroelectric (AFE) displacement of the Ti atoms (\(u^{Ti}\)) along the direction that is orthogonal to both \(\hat{r}\) and \(\hat{s}\). (The motivation for including this latter degree of freedom will become clear shortly.)

The first two lines of Eq. (1) include the well-known couplings that are active in the homogeneous crystalline phase, namely: the elastic energy, the double-well potential associated to the unstable AFD modes (\(κ < 0\) and \(A > 0\)), the susceptibility of the polar mode in the harmonic limit, and the rotostrictive, biquadratic and elec-
trostrictive couplings involving $P$, $\phi$, and $\varepsilon$. The third line contains gradient-mediated couplings, which are directly responsible for the properties of the domain walls. In particular, we have: the correlation term involving either the AFD or the polar mode (these introduce an energy cost associated with spatial variations of the corresponding order parameter), the flexoelectric coupling between gradients of the shear strain and $P$, and the new “rotopolar” term. Finally, the last line contains the terms involving the AFE amplitude: the harmonic restoring force of the mode, a trilinear term involving $P$ and $\phi$, and a further harmonic term that couples $u^{Ti}$ to the gradient of $\phi$. (In 3D, both $S$ and $N$ can be written as third-rank pseudotensors, $S^{ijk}$ and $N^{ijk}$, where $\varepsilon^{ijk}$ is the antisymmetric Levi-Civita symbol.)

Note that $u^{Ti}$ is associated to a zone-boundary (R-point) phonon, i.e. it does not carry any polarization by itself; it is not an active instability of the system either (it is actually quite “hard” – the calculated frequency is $\omega_{Ti} \sim 420$ cm$^{-1}$). Yet, $u^{Ti}$ strongly couples to spatial variations of the AFD modes, which leads to two important consequences: (i) it significantly lowers the cost of tilt gradients, and hence the domain-wall energy (this effect can be understood as an effective rescaling of the coefficient $D_{\varepsilon}$) and (ii) it contributes to the polarization via the trilinear coupling to $\phi$. This clarifies, at a qualitative level, the physical motivation for its explicit consideration; the quantitative impact is rather remarkable, too, as we shall illustrate in the results section.

We calculate the coupling coefficients of Eq. (1) from first-principles, by using the local density approximation to DFT as implemented in the ABINIT code [17]. The homogeneous coupling coefficients are fitted to the energy landscape of the periodic crystal by distorting the lattice along the mode coordinates, following the established practice [10,18]. The harmonic gradient-mediated terms are extracted by loosely following the strategy of Ref. [19] i.e. by first performing a long-wave expansion of the dynamical matrix (calculated via linear-response theory [20]) around either the $\Gamma$- or the R-point of the Brillouin zone, and by subsequently performing the projections onto the relevant mode eigenvectors.

The tricky part consists in the calculation of the non-linear gradient-mediated term, i.e. the rotopolar $W$-coefficients – to the best of our knowledge, there are no reported ab initio calculations of such quantities (or, more generally, of such class of materials properties). We solve this technical obstacle by performing, as above, linear-response calculations of the dynamical matrix as a function of the wavevector $q$. This time, however, we perform the phonon calculations on a 20-atom cell, where we freeze in a small uniform tilt, $\phi_j$, by hand. The two symmetry-allowed $W$-coefficients ($W_{rs}$ and $W_{rs}$) are then calculated by numerically differentiating the dynamical matrix, $D$, with respect to both parameters,

$$W_{ij} = \langle P \rangle \left( \frac{\partial^2 D(\phi_j, q)}{\partial \phi_j \partial q} \right) |_{\phi_j, q=0} |\phi_i\rangle. \quad (2)$$

(|$P$| and $|\phi_i\rangle$ are mode eigenvectors.) More extensive details on the technique will be reported in a forthcoming publication.

Most of our calculated values are in good (sometimes excellent) agreement [17] with earlier experimental and theoretical estimates, [21,22] whenever the latter are available. There are two important exceptions, though, which deserve a separate discussion. The harmonic coefficients that are linked to the polarization and AFD degrees of freedom, respectively $\chi_{0}^{-1}$ and $\kappa$, are notoriously difficult to capture within standard approximations to DFT; as a consequence, the spontaneous tilt angle at zero temperature is severely overestimated ($5 - 6^\circ$ versus the experimental value of $2.1^\circ$), and the reported DFT values for the static dielectric constant of SrTiO$_3$ are remarkably erratic. Luckily, these two coefficients are by far the easiest to estimate from the experimental data (tilt angle and dielectric susceptibility as a function of temperature, respectively); for this reason, we replace their first-principles values with a phenomenological Curie-Weiss function of $T$ [17]. Other coefficients in our model are expected to be quantitatively accurate and to depend only weakly on temperature.

To calculate the two stable domain wall structures by means of Eq. (1), we implement the continuum equations on a discrete 1D mesh, and express the gradient terms as nearest-neighbor interactions; energy minimization proceeds via a steepest-descent algorithm. In Fig. 2 we plot the equilibrium configuration of the primary AFD order parameters at the two types of domain walls. The antisymmetric (with respect to $s \to -s$) AFD component ($\phi_A$) can be very well fitted with a kink-type solution, [2,15] $\phi_A(s) \sim \tanh(s/\xi)$, while the symmet-
We move now to the main result of this work, regarding the induced electrical polarization at either type of domain boundary. To present our findings, we shall work at a reference temperature of $T_{\text{ref}} = 80$ K, where the associated tilt is $1.4^\circ$ \cite{13}. ($T_{\text{ref}}$ is chosen out of convenience, as it is precisely the temperature at which the calculated value of $\chi_0$ matches the experimentally measured \cite{24} dielectric constant of SrTiO$_3$; the main conclusions that will be presented in the following are, nevertheless, valid at any temperature below $T_0=105$ K, where $T_0$ is the ferroelastic transition temperature.)

Looking back at the energy, Eq. (1), one can see that there are three improper (linear in $P$) mechanisms that can induce a polarization at the wall: flexoelectricity, rotopolar coupling, and the trilinear coupling mediated by $u^\text{Ti}$. To quantitatively separate their individual role, we shall start with a simpler Hamiltonian where we artificially set $W_{ij} = S = N = 0$ (i.e., a polarization can only be induced via flexoelectricity), and progressively switch on the new couplings, while monitoring their impact on the total (integrated) polarization, $\langle P \rangle_{HH,HT}$, at either wall. Note that the electrostriction and biquadratic couplings also have an impact on $\langle P \rangle$, although they fall in a different category (they both go like $P^2$); to quantify their importance, we shall perform our computational experiment twice, either with or without the latter two terms.

From our modified Hamiltonian, we obtain (Fig. 3) a points) that the polarity of HH and HT walls is essentially the same. (The small difference is only due to the $P^2$ terms.) This is easily understood: Flexoelectricity is the only mechanism at play here, and therefore the “geometric” field acting on $\langle P \rangle$ can only depend \cite{9} on the total discontinuity in the shear strain component, $\Delta \epsilon_{rs}$. Of course, $\Delta \epsilon_{rs}$ is the same at both types of walls.

Next, we switch on the new rotopolar coupling (B). As we anticipated in the introductory paragraphs, this mechanism clearly distinguishes one type of domain wall from the other: Its contribution to $\langle P \rangle$ is dominated by $W_{rs}$ at HT walls, and by $W_{sr}$ at the HH walls. $W_{sr}$ is very small \cite{17}, so at HH walls the polarization is almost unaffected; conversely, $W_{rs}$ is large and almost cancels the flexoelectric effect at HT walls. Thus, the rotopolar term has a central physical importance: it provides us with the possibility of “engineering” a macroscopic ferrielectric-like polarization, $P_{\text{mac}}$, in a periodic twin wall structure. It suffices to alternate HT and HH wall types, as illustrated in Fig. 3 to obtain $(L$ is the average domain width) $P_{\text{mac}} = (\langle P \rangle_{HH} - \langle P \rangle_{HT})/(2L) \neq 0$. (In absence of this term, $P_{\text{mac}}$ would vanish by symmetry in a sequence of parallel twins. \cite{9}) Interestingly, even without doing the calculations there is an insightful visual proof that such a structure indeed does break macroscopic inversion symmetry. By following the evolution of the AFD pseudovector across the structure, one can easily identify a counterclockwise rotation of $\phi$ for increasing $s$. Such a pattern, in strong analogy to a spin cycloid, \cite{12} does not posses inversion symmetry along $\hat{r}$, which proves our point.

If we stopped our analysis here, we would be forced to conclude that $\langle P \rangle_{HH} > \langle P \rangle_{HT}$. However, as we show in Fig. 3, the trilinear coupling between $u^\text{Ti}$, $P$ and the AFD tilts has a dramatic impact on $\langle P \rangle$, to the point that it reverses (C) the ordering of $\langle P \rangle_{HH}$ and $\langle P \rangle_{HT}$ (and hence the sign of $P_{\text{mac}}$). As expected, the most affected wall type is the HT, where $\phi_r$ changes sign. (The trilinear coupling can be thought as an effective additional contribution to $W_{rs}$, while its contribution to $W_{sr}$ vanishes; note also in Fig. 3 the much larger amplitude of $u^\text{Ti}$ at the HT wall.) Note that, in all cases, the effect of the biquadratic/electrostrictive couplings is a systematic suppression, somewhat stronger at the HT walls, of the
gradient-induced polarization (compare empty and filled symbols in Fig. 3). This observation implies that the $P^2$ terms alone are unlikely to trigger a ferroelectric state at either type of twin boundary, and corroborates improper mechanisms as the main driving force for $P$.

These results open new perspectives for breaking macroscopic inversion symmetry (and hence engineering an effective piezoelectric and/or pyroelectric behavior) via twinning – Ref. 9 explored the potential of defects (kinks, junctions, vortices) in the domain wall topology, while here we demonstrate that a macroscopic $P$ can emerge even in “ideal” ferroelastic structures. These arguments can be readily generalized to other materials systems: For example, the improper mechanism pointed out 5 at CaTiO$_3$ twins can be simply (and quantitatively) rationalized as a rotopolar coupling. More generally, our work open new avenues for materials design via domain wall engineering, an increasingly popular strategy where new functionalities emerge from spatial inhomogeneities, rather than the uniform crystalline phase itself.

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274 (1959).
Ab initio calculations  The ab initio calculations have been performed with norm-conserving pseudopotentials, taking into account explicitly 10 electrons for Sr, 12 for Ti and 6 for O. The pseudopotentials have been generated using the FHI98PP code and the exchange-correlation term has been treated using the local-density approximation (LDA). Finally the energy cut-off used is 70 Ha and in all the first principle simulations we have employed a Monkhorst-Pack mesh equivalent to 8x8x8 grid in the primitive cubic cell.

With these input parameters we get a bulk lattice constant value for the cubic structure of 7.2675 bohr. The phonon dispersion along the directions Γ-M and R-X for this same reference structure is shown in fig. 4. As it is possible to see, we get a polar soft mode which is not unstable. The only instability present in our structure is at R, and it is associated to the AFD of the oxygen atoms.

1D model Both the two types of ferroelastic TBs discussed in the main text have been studied employing a 1D model. This is possible because, by symmetry, it easy to see that the polar component along \( \hat{s} \) is antisymmetric respect to the DW and thus does not contribute to the total polarization. Then the only polar component relevant for a macroscopic polarization at the DW is \( P_r \). Moreover the translational symmetry is preserved along both \( \hat{r} \) and \( \hat{x} \), which is the direction perpendicular to both \( \hat{r} \) and \( \hat{s} \).

As consequence of these symmetries the following mechanical boundary conditions must be imposed: \( \varepsilon_r \) and \( \varepsilon_x \) are fixed to their correspondent value of the bulk AFD phase. Instead \( \varepsilon_s \) and \( \varepsilon_{rs} \) are free to relax during the energy minimization in order accommod the deformation due to the ferroelastic twin walls. A profile of the strain components as function of \( \hat{s} \) is given in fig. 5.

The 1D problem of minimizing eq. 1 of the main text has been solved adopting the steepest descent algorithm. The mesh used to discretize the previous equation has the atomic resolution, i.e. each point of the mesh corresponds to an atomic layer along the direction \( \hat{s} \). The gradient terms have been calculated on the 1D mesh using a symmetric nearest-neighbor formula. Finally we have impose periodic boundary conditions to our 1D problem.

|       | US    | SV    | this work | a.u.   |
|-------|-------|-------|-----------|--------|
| \( \kappa \) | -3.01 | -22.5 | -20.62    | 10\(^{-6}\) Ha/bohr\(^{-3}\) |
| \( A \)     | 5.16  | 4.92  | 5.26      | 10\(^{-5}\) Ha/bohr\(^{-7}\) |
| \( C_{11} \) | 11.43 | 13.02 | 13.14     | 10\(^{-3}\) Ha/bohr\(^{-3}\) |
| \( C_{12} \) | 3.64  | 3.30  | 3.83      | 10\(^{-3}\) Ha/bohr\(^{-3}\) |
| \( C_{44} \) | 4.32  |       | 4.16      | 10\(^{-3}\) Ha/bohr\(^{-3}\) |
| \( R_{11} \) | 1.23  | 1.68  | 1.95      | 10\(^{-4}\) Ha/bohr\(^{-5}\) |
| \( R_{12} \) | -2.37 | -2.70 | -2.74     | 10\(^{-4}\) Ha/bohr\(^{-5}\) |
| \( R_{44} \) | -2.18 |       | -2.42     | 10\(^{-4}\) Ha/bohr\(^{-5}\) |
| \( Q_t \)   |       |       | -0.28     | 10\(^{-1}\) Ha/bohr\(^{-1}\) |
| \( Q_s \)   |       |       | -1.95     | Ha/bohr\(^{-1}\) |
| \( N \)     |       |       | -1.53     | 10\(^{-2}\) Ha/bohr\(^{-3}\) |
| \( \chi_0 \) | 120.00|       |           | Ha/bohr |
| \( \kappa_{Ti} \) | 3.54 | 10\(^{-3}\) | Ha/bohr\(^{-5}\) |
| \( D_r \)   | 1.95  | 10\(^{-3}\) | Ha/bohr\(^{-3}\) |
| \( D_s \)   | 1.00  | 10\(^{-3}\) | Ha/bohr\(^{-3}\) |
| \( S \)     | 1.29  | 10\(^{-3}\) | Ha/bohr\(^{-4}\) |
| \( \varepsilon_s \) | -0.18 | Ha/bohr |
| \( \varepsilon_r \) | 1.31 | Ha/bohr |
| \( \varepsilon_{rs} \) | 1.84 | Ha/bohr |
| \( G \)     | 5.43  |       |           | Ha/bohr\(^{3}\) |
| \( f \)     | -4.70 | 10\(^{-2}\) | Ha |
| \( W_{rs} \) | 2.11  | 10\(^{-3}\) | Ha/bohr\(^{-2}\) |
| \( W_{sr} \) | 0.29  | 10\(^{-3}\) | Ha/bohr\(^{-2}\) |

TABLE I. Calculated model parameters compared with the available literature data (US=Uwe and Sakudo [20], SV=Sai and Vanderbilt [21]). The calculated value of \( \kappa \) is reported in italics, as we replaced it with a phenomenological function of temperature, \( \kappa = \alpha_0(T - T_\varphi) \). (We used \( T_\varphi = 105 \) K, \( \alpha_0 = -0.013 \) Ha/(bohr\(^5\) K).) At 80 K, \( \varphi = 1.4^\circ \), consistent with the experimental value. [11] Note that at 80 K, the measured dielectric constant is approximately consistent with our zero-temperature first-principles calculations, \( 4\pi\chi_0 \sim 1500 \).
FIG. 4. Here we shown the phonon dispersion as function of the wavenumber $q$ in reduced coordinates, where $a_{[110]} = a_0 \sqrt{2}$ and $a_0$ is the cubic lattice parameter of STO. In figure (a) the phonon dispersions are along the $\Gamma$-M direction (as shown by the inset) and they are calculated on one side using the Fourier interpolation of a 3D $q$-mesh (black-solid curves) and on the other side using the two dimensional space defined by the transversal acoustic and center-zone soft polar mode (red dashed and blue dot-dashed), which approximate the ticker black branches, $U_r$ and $P_s$, around $\Gamma$. In particular: the red dashed lines show the phonon bands calculated using only the self-correlation of the acoustic and soft polar mode, which are respectively the elastic constant and the $G$ coupling; the blue dot-dashed lines are calculated taking into account also the ferroelectric interaction term. In a similar way figure (b) shows the phonon dispersion around $R$, in direction [110], of the unstable AFD modes in cubic STO. The labels identify the branch associate to the oxygen octahedron rotation along $\hat{s}$, $\phi_s$, and along $\hat{r}$, $\phi_r$, while the third branch is the dispersion of the AFD with rotational axis perpendicular to both $\hat{s}$ and $\hat{r}$. The red dashed line is calculated using only the AFD self dispersion, $D$, of $\phi_r$ while the blue dot-dashed line takes into account also the trilinear interaction term, $S$. Of this choice in our simulations of ferroelastic domain walls, we have always to take into account at least two opposite walls.
FIG. 5. Cartoons (a) and (b) are sketches of the two ferroelastic twin walls studied in this work, respectively the HH and HT walls. In (c) are shown the strain components across the two DWs. $\varepsilon_r$ and $\varepsilon_x$ do not change across the walls because they are kept fix to their bulk AFD value, in order to satisfy the mechanical boundary conditions for a periodic system. Note that the cartoon (a) and (b) are on top (c) just as reference but they do not have the same scale.