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Ferroelectric Domain Walls as Conductive Channels in Ferroelectric Semiconductors

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ABSTRACT We have studied that ferroelectric domain walls act as conductive channels in ferroelectric semiconductors. The static conductivity of domain walls with different incline angle with respect to the spontaneous polarization vector was calculated numerically in the uniaxial ferroelectric semiconductors of *n* type. The static conductivity drastically increases at the inclined head to head wall by an order of magnitude for small incline angles and by three orders of magnitude for the perpendicular domain wall due to strong accumulation of compensating free charges. We have presented the polarization structure and transport behavior at the domain walls in the multiaxial ferroelectrics like $BiFeO_3$ and $Pb(Zr,Ti)O_3$ determined by the interplay of the strong ferroelectric coupling between polarization components and inhomogeneous elastic strains along the walls. The impact of the ferroelectric coupling, proximity and finite size effect on the polarization vector, potential electric field and carrier redistribution across the thin stripes and cylindrical nanodynamics was analysed. Flexoelectric coupling is high for ferroelectric leads to the appearance of polarization components perpendicular to the wall plane and its strong gradient across the wall and even for unchanged walls. The carrier accumulation effect by the nominally unchanged domain stripes and cylindrical walls appears to be significant and increases upto 10-30 times for domain in $Pb(Zr,Ti)O_3$ for the typical range of flexoelectric coefficients. The charge of accumulated carrier was determined by the sign of the flexoelectric coefficient. We found that the carrier accumulation is highest when the wall plane is perpendicular to the spontaneous polarization direction at wall and it decreases with bound charge decrease and reaches minimum for the parallel domain wall. The obtained results were found in good agreement with previous results.

KEYWORDS Ferroelectric, domain wall, spontaneous, accumulation, coupling, flexoelectric.

INTRODUCTION

For a given ferroelectric material the wall conductivity depend on the wall tilt, local strains due to electrostriction and proximity effects. This inturn determine the possibility for multilevel storage, device size and integration into solid state devices. This effect on wall conductivity is required to analyzing the feasibility of controllable rewritable conductive nanosized design in insulating ferroelectrics. Experimental results in materials such as $BiFeO_3$[1-2], $Pb(Zr,Ti)O_3$ [3], SbSI [4] and $LiNbO_3$ doped with MgO [5] all enabled by the development of scanning probe microscopy techniques capable of probing the conductance on the nanoscale. These results presented the studies of ferroics and low dimensional systems as well as offered new possibilities for oxide nanoelectronics due to nanoscale dimensions of conducting entities and the possibility to control their spatial location by external fields. Theoretical achievements in the field of domain structures in ferroics have been presented by several workers[6-7]. Studies of ferroelectric domain wall was shown by Zhirnov[8] , Cao and Cross [9] who considered 180^o and 90^o domain walls taking into account electrostriction coupling between the spontaneous polarization and strain but considering only electroneutral domain wall. Davind etal[10] considered the case of rhmbohedral symmetry. Orientation of 180^o domain wall was determined by electrostatics. Orientation of 90^o twin domain wall is governed by the strain compatibility [11]. Fridkin etal [12] studied on domains in uniaxial ferroelectrical semiconductors. The studies of Gureev [13] and Wliseev[14] devoted to the perpendicular and inclined domain walls.

METHOD

We have used Laudau-Ginsburg Devonshire model. By using this model the free energy density is given by.

$$G = \Delta G_b + \Delta G_{\text{elast}} + \Delta G_{\text{strict}} + \Delta G_{\text{flexo}} - Pi\frac{E_i^d}{2} + \frac{g_{ijkl}}{2}\frac{\partial P_i}{\partial x_j}\frac{\partial P_k}{\partial x_l}$$

where $P_i\left(i=1-3\right)$ are the ferroelectric polarization vector components, $E_i^d = -\frac{\partial \varphi}{\partial x_i}$ are the components of the depolarization field that is caused by imperfect screening of the inhomogeneous polarization distribution with $\text{div}\left(\text{P}\right) \neq 0$. The symmetrical part of the matrix $\left(\partial P_i / \partial x_j\right)$ contributes to the gradient energy of the bulk system[15]. The polarization dependent density ΔG_b can be written as a Taylor series expansion of the polarization components P_i as[9]

$$\begin{aligned}
\Delta G_b = {} & a_1\left(P_1^2 + P_2^2 + P_3^2\right) + a_{11}\left(P_1^4 + P_2^4 + P_3^4\right) \\
& + a_{12}\left(P_1^2P_2^2 + P_2^2P_3^2 + P_3^2P_1^2\right) + a_{111}\left(P_1^6 + P_2^6 + P_3^6\right) \\
& + a_{112}\left[P_1^4\left(P_2^2 + P_3^2\right) + P_2^4\left(P_3^2 + P_1^2\right)\right. \\
& \left. + P_3^4\left(P_1^2 + P_2^2\right)\right] + a_{123}\left(P_1^2P_2^2P_3^2\right).
\end{aligned}$$

where a_i, a_{ij} and a_{ijk} are the dielectric stiffness and higher order stiffness coefficients at constant stress.

The elastic energy is written as

$$\begin{aligned}
\Delta G_{\text{elast}} = {} & -\frac{1}{2}s_{11}\left(\sigma_1^2 + \sigma_2^2 + \sigma_3^2\right) \\
& - s_{12}\left(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1\right) \\
& - \frac{1}{2}s_{44}\left(\sigma_4^2 + \sigma_5^2 + \sigma_6^2\right).
\end{aligned}$$

where σ_i are the stress tensor components, s_{ij} are the elastic compliances at constant polarization. The coupling energy between polarization and strain ΔG_{strict} is proportional to electrostriction coefficients

$$\Delta G_{strict} = \Big[-Q_{11}\left(\sigma_1 P_1^2 + \sigma_2 P_2^2 + \sigma_3 P_3^2\right) \\ -Q_{44}\left(\sigma_4 P_2 P_3 + \sigma_5 P_3 P_1 + \sigma_6 P_1 P_2\right) \\ -Q_{12}\left\{\sigma_1\left(P_2^2 + P_3^2\right) + \sigma_2\left(P_3^2 + P_1^2\right) + \sigma_3\left(P_1^2 + P_2^2\right)\right\}\Big].$$

Where Q_{ij} is the electrostriction strain tensor.

The electrostatic potential φ satisfies the Poisson equation.

$$\varepsilon_0 \varepsilon_b \Delta\varphi = \operatorname{div}(\mathrm{P}) - e\left(N_d^+(\varphi) + p(\varphi) - n(\varphi) - N_a^-\right)$$

where Δ is the Laplace operator, electron charge $e = 1.60\times10^{-19}\,\mathrm{C}$, $\varepsilon_0 = 8.850\times10^{-12}$ F/m is the universal dielectric constant and ε_b is the backwdard dielectric permittivity of the material. The ferroelectric polarization can be approximated as expansion $P_i = P_i^s + \varepsilon_{ij}^f + \ldots$.

Ionized deep acceptors with field independent concentration N_a^- play the role of a back ground charge. The equilibrium concentration of ionized shallow donors N_d^+ and free electrons *n* and holes *p* are

$$N_d^+(\varphi) = N_{d0}\left(1 - f\left(E_d - E_f - e\varphi\right)\right)$$

$$p(\varphi) = \int_0^\infty d\varepsilon \cdot g_p(\varepsilon) f\left(\varepsilon - E_V + E_F + e\varphi\right)$$

$$n(\varphi) = \int_0^\infty d\varepsilon \cdot g_n(\varepsilon) f\left(\varepsilon + E_C - E_F - e\varphi\right)$$

where N_{d0} is the concentration of donors, $f(x) = 1 + \exp\left(\dfrac{x}{k_B T}\right)^{-1}$ is the Fermi-dirac distribution function. $k_B = 1.38070\times10^{-23}$J/K, *T* is absolute temperature, E_F is the Fermi level, E_d is the donor level, E_C is the bottom of conductive band and E_v is the top of the valence band.

We have assumed a single domain ferroelectric material is electroneutral at zero potential $\varphi = 0$, the condition $N_a^- = N_{d0}^+ + p_0 - n_0$ is valid.

Elastic stresses vanish far from the domain walls where the sytem is mechanically free. Boundary conditions are determined by the configuration of the domain structure in a straight forward way. We have considered only the cases of the quasi one dimensional distribution of polarization for periodic domain, stripes and cylindrical domains.

RESULTS AND DISCUSSION

Figure (1) and (2) show the dependences of the polarization component perpendicular $\tilde{P}_1(\xi) \equiv P_\perp(\xi)$ and parallel $\tilde{P}_{\uparrow\uparrow}(\xi)$ to the wall plane, electric potential $\varphi(\xi)$, ionized donors $N_d^+(\xi)$ and electrons $n(\xi)$ on the distance ξ from the domain wall plane between the neighboring stripes. The dependences were calculated for the domain stripes with different tilt angles $\theta = \frac{\pi}{2}, \frac{\pi}{30}, 0$, negative, zero and positive flexoelectric coupling coefficient *F12*. Without flexoelectric coupling only electrostriction couples polarization and elastic strains. We have found that the flexoelectric coupling leaded to the nontrivial physical responses, including appearance of $P_\perp(\xi)$ and is strong gradient across the nominally unchanged and weakly charged head to head and tail to tail domain walls. The flexoelectric coupling term $F_{12}\tilde{P}_\perp \partial(\tilde{\sigma}_2 + \tilde{\sigma}_3)/\partial\tilde{x}_1$ in the free energy causes the flexoelectric field $F_{12}\frac{\partial(\tilde{\sigma}_2 + \tilde{\sigma}_3)}{\partial\tilde{x}_1}$ that inturn induces the component $P_\perp(\xi)$. From graph (2) it is seen that $P_\perp(\xi) = 0$ for $F_{12} = 0$ and $\theta = 0$. Polarization component $P_{\uparrow\uparrow}(\xi)$ is weakly affected by the presence of the flexoelectric coupling. When tilt is small or zero additional features on the potential, electron and ionized donor distributions appear in vicinity of domain walls due to non zero flexoelectric coupling. The flexoelectric field leads to the carrier redistribution and thus to conductivity changes even across the nominally unchanged parallel domain walls. We found that the compensating electron density is highest for the head to head perpendicular wall when $\theta = \frac{\pi}{2}$ and decreases with decreasing bound charge with decreasing θ. The electron accumulation leaded to the strong increase of the static onductivity across the charged domain stripes up to three orders of magnitude for the perpendicular domain walls. We have considered the 180° periodic domains of half period. The domain walls are parallel when $\theta = 0$ and located close enough to induce proximity effected on the system static conductivity. Calculations showed that the polarization component $\tilde{P}_\perp(\xi)$ leaded to the appearance of lateral depolarization electric field $\tilde{E}_\perp(\xi)$ and carrier redistribution in the vicinity of domain walls. We also found that the carrier accumulation in the domain wall region is caused by the potential barrier $\varphi(\rho)$ that in turn caused by the uncompensated bound charge $\sim div(P_\perp(\rho))$. The potential barrier at the curved domain wall monotonically increases with the domain radius increase and then saturates. The potential barrier in the centre of the domain first increases with radius increases and reaches maximum and then decreases with further increase of radius.

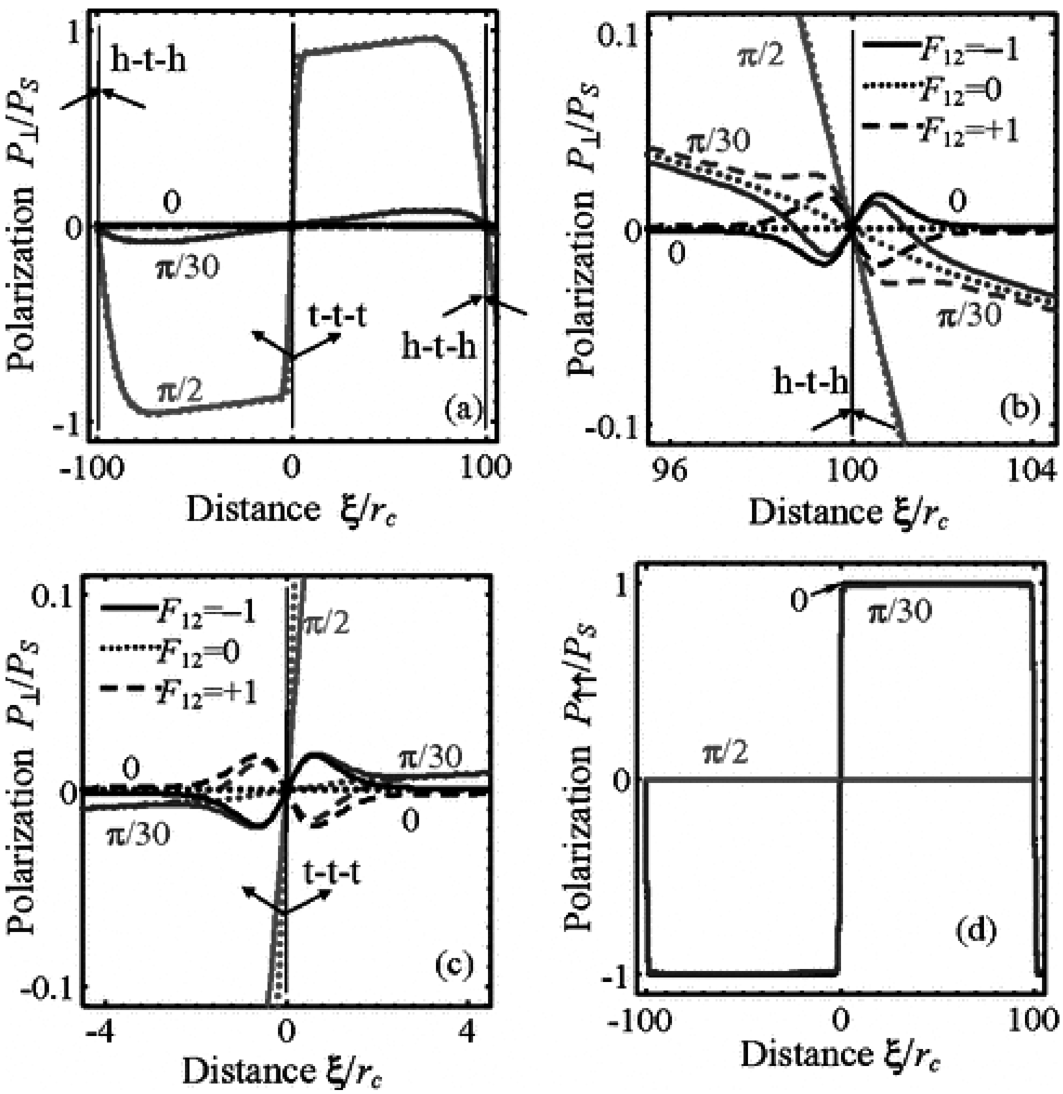

Figure 1: Dependencies of the polarization components $\tilde{P}_{\perp}(\xi)/P_S$ (a), (c), and (d) and $\tilde{P}_{\uparrow\uparrow}(\xi)/P_S$ (b) on the distance ξ from the wall plane between the neighboring stripes with different tilt angle $\theta = \pi/2,\ \pi/30, 0$.

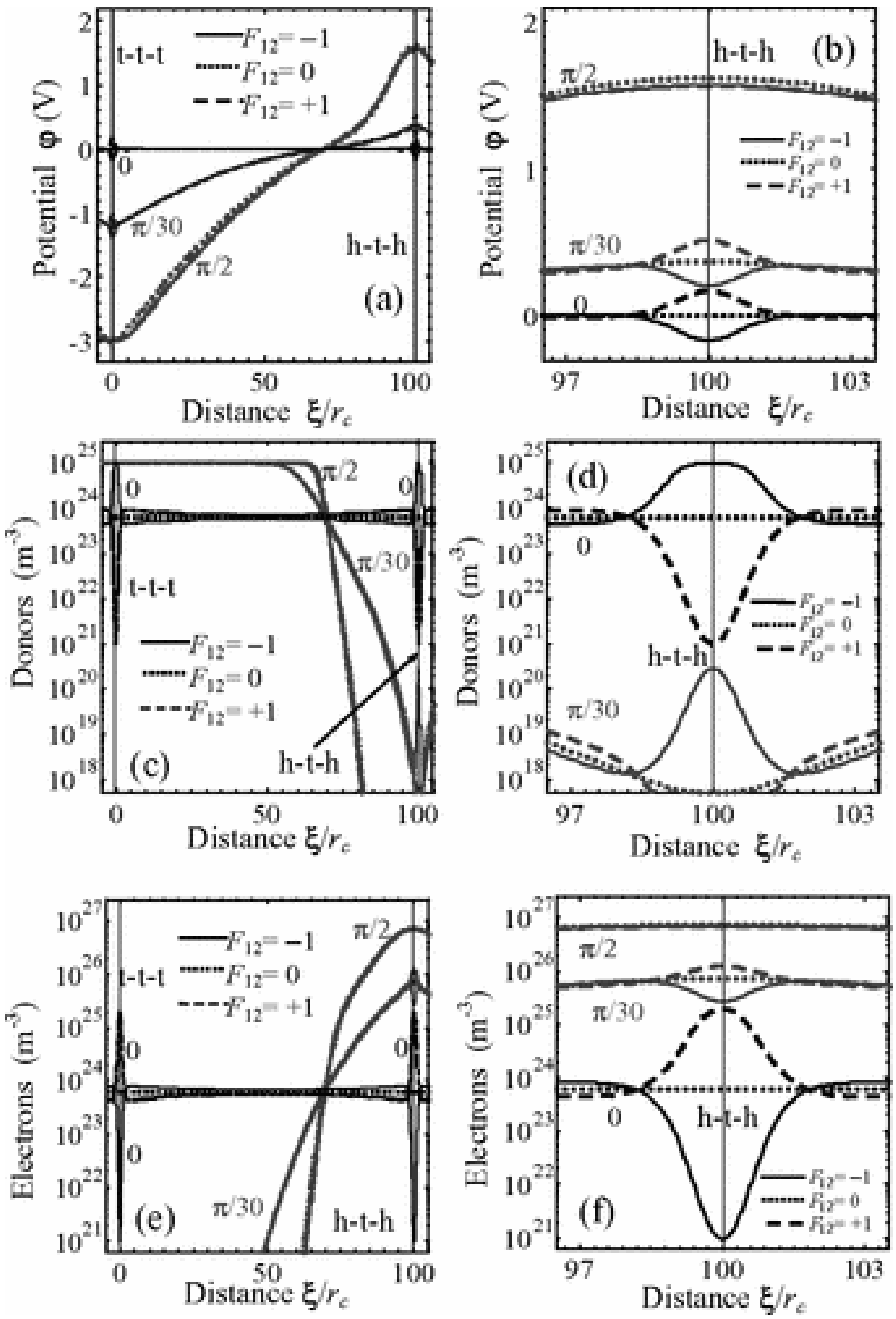

Figure 2: Dependencies of potential $\varphi(\xi)$ (a) and (b), concentration of ionized donors $N_d^+(\xi)$ (c) and (d) and density of electrons $n(\xi)$ (e) and (f) on the distance ξ from the wall plane between the neighboring stripes with different tilt angle $\theta = \pi/2,\ \pi/30, 0$.

CONCLUSION

We have studied the ferroelectric domain walls as conductive channel in ferroelectric semiconductor. Their effects were also studied. The static conductivity of domain walls with different incline angle with respect to the spontaneous polarization vector was calculated numerically in the uniaxial ferro electronics – semiconductor of *n* type. The static conductivity drastically increased at the inclined head to head wall by an order of magnigtude for small incline angles and by three orders of magnitude for the perpendicular domain wall due to strong accumulation of compensating free charge. The impact of flexoelectric coupling and tilt angle on the polarization vector, potential, electric field and carrier redistribution across the stripes domains was analysed. We found that the polarization component normal to the domain wall demonstrated a weak deviation from constant distribution. This leaded to the appearance of an internal electric field and thus to a potential step near the domain walls which is consistent with ab initio calculations. It was also found that the static electronic conductivity increased in the P-type ferroelectric semiconductors across the tail to tail walls. The proximity and size effect of the electron and donor accumulation or depletion by thin stripe domains and cylindrical nanodomains are revealed. The spatial localization of the features induced by the flexoelectric coupling is independent on wall tilt angle but the width increased with decreasing angle. The obtained results were compared with previously obtained results of theoretical and experimental works and were found in good agreement.

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