Tailored Polarization Reversal and Terahertz Frequency Dynamics in Ferrolectric Nanowires

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One promising application of ferroelectric nanowires is for use in ferroelectric memory devices which utilize the binary nature of the reversible polarization to store, read, and write a bit of information.[1] However, the field required to reverse the polarization could be quite large for ferroelectrics.[2] In the interest of energy efficiency, it is desirable to reduce this polarization reversal field (PRF). In this work, we propose one way to achieve such a reduction in ferroelectric nanowires. Our approach is to superimpose a subswitching *dc* electric field with a Gaussian-shaped terahertz electric field pulse. The bias field establishes a preferential direction for the polarization, while the THz pulse provides the energy necessary to raise the nanowire's temperature,[3] thus lowering the PRF in the nanowire.

We developed a computational method which uses classical Molecular Dynamics with the force field derived from the first-principles based effective Hamiltonian.[4] Two nanowires made of $PbTiO_3$ and $Pb(Ti_{0.6}Zr_{0.4})O_3$ with square cross-sections of 21.8 nm^2 were simulated. Below the Curie temperature, each nanowire developed polarization along the axial direction under open-circuit boundary conditions. Next the nanowires were subjected to the electric field

$$E\left(t\right) = E_b + E_0 cos(\omega t) e^{-\left(\frac{t-t_0}{\tau}\right)^2}, \tag{1}$$

where E_b is the subswitching *dc* field applied in the direction opposite to the initial polarization vector. The amplitude of the pulse is given by E_0, while $\omega = 2\pi\nu$ is frequency, t_0 is the time at which the Gaussian envelope is centered, and τ is the pulse half-width.

To achieve polarization reversal in the nanowires, it is essential that the frequency of the THz pulse belongs to the range of frequencies associated with the large imaginary part of the complex electric susceptibility, ϵ_2, of the nanowire. To determine this frequency range, we calculated the complex dielectric response in $PbTiO_3$ and $Pb(Ti_{0.6}Zr_{0.4})O_3$ bulk and nanowires both in the absence and in the presence of bias electric fields. In $PbTiO_3$, the soft mode is underdamped and as a result, its ε_2 exhibits a relatively narrow peak centered at the mode characteristic frequency. The data for the characteristic frequency as a function of temperature for the nanowire is shown in Fig. 1(b). For comparison, we also report computational data for bulk $PbTiO_3$. From Fig. 1(b), we see that the $\nu_0\left(T\right)$ for the nanowire are shifted to the left with respect to the branches for bulk $PbTiO_3$. This is due to the decrease in the Curie point for the nanowires. The complex dielectric response of the nanowire is also affected by the presence of the bias field. In Fig. 1(b), we report the characteristic frequencies of the nanowire subjected to a bias field of 450 kV/cm. The effect of the bias field is to shift the $\nu_0\left(T\right)$ branches further to the left if the field is applied in the direction opposite to the polarization. The field also reduces the degree to which the mode-softening occurs. The dependence of the soft-mode dynamics on the size as well as on the applied electric field could be utilized to enhance the tunability of ferroelectric devices. The frequency response determines the band-width of a device, so by applying bias fields of various strengths, the sensitivity of a ferroelectric device can be tuned to a specific frequency.

We investigated the possibility of controllable polarization reversal through tailoring the parameters of the electric field, E_b, E_0, ν, and τ. By varying the parameters we found

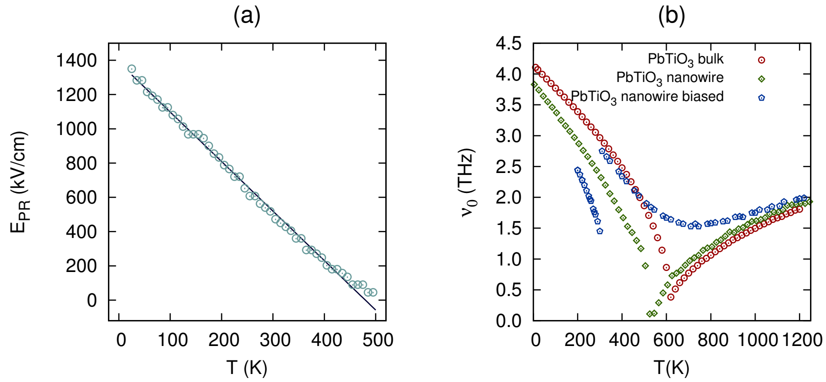

FIG. 1. Panel (a) shows the dependence of the polarization reversal field in the $PbTiO_3$ nanowire on the temperature. Panel (b) summarizes the dependence of the characteristic frequency on the temperature in bulk $PbTiO_3$, biased and unbiased $PbTiO_3$ nanowire. The bias field is 450 kV/cm.

that their certain combinations lead to polarization reversal in the nanowire. Briefly, for polarization reversal to occur, the pulse needs to supply the energy sufficient to elevate the nanowire's temperature by $\Delta T \approx \frac{dT}{dE_{PR}}\left(E_b + E_0 - E_{PR}\left(T_{init}\right)\right)$, where $\frac{dT}{dE_{PR}}$ is the slope in the $T\left(E_{PR}\right)$ dependence in Fig. 1(a), while $E_{PR}\left(T_{init}\right)$ is the PRF associated with the initial temperature. The change in the nanowire's temperature due to the interaction with the THz pulse is given by $\Delta T \approx \sqrt{\frac{\pi}{8}}\frac{\varepsilon_2(\omega)\varepsilon_0 E_0^2 \tau\omega}{C_P}$ [3], where C_P is the heat capacity at constant pressure. Combining these two expressions, we obtain a relationship between the parameters of the electric field associated with polarization reversal in the nanowire

$$\sqrt{\frac{\pi}{8}}\varepsilon_2\left(\omega, T, E_b\right) E_0^2 \tau\omega = C_P\left(E_b + E_0 - E_{PR}\left(T_{init}\right)\right). \quad (2)$$

The set of parameters which satisfies Eq. (2) is expected to reverse the polarization in the nanowire. We tested the validity of Eq. (2) and will report our results for both $PbTiO_3$ and $Pb(Ti_{0.6}Zr_{0.4})O_3$ nanowires.[5]

Acknowledgments: The present work is supported by the Army Research Office under contract 57787-EL (polarization reversal studies) and by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award DE-SC0005245 (soft mode dynamics studies).

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