FLEXOELECTRIC EFFECT IN PEROVSKITE FERROELECTRICS: A PHASE-FIELD MODEL

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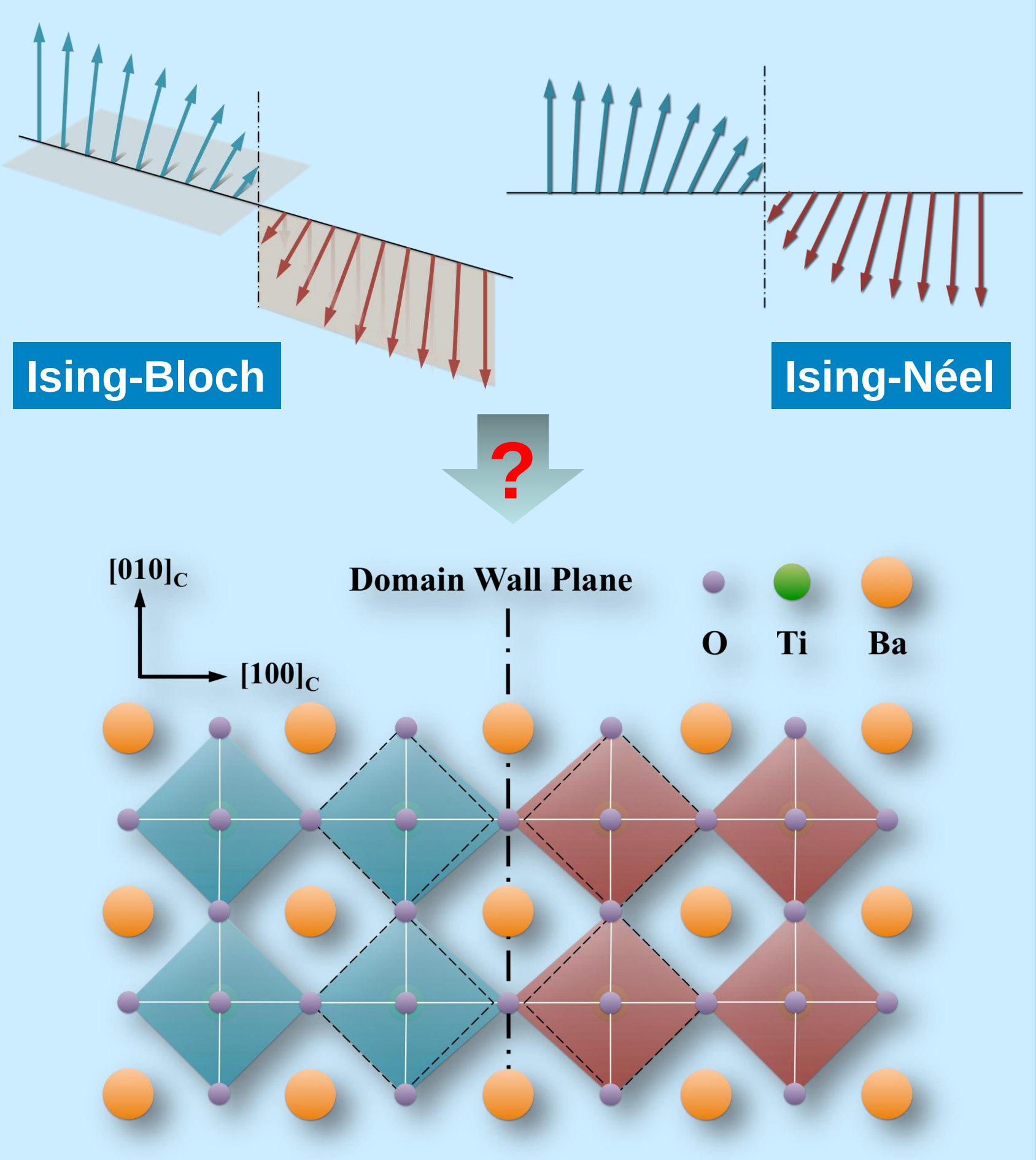
ABSTRACT

The phase-field model of ferroelectric domains is extended to include the contribution of flexoelectricity by introducing the strain gradient – polarization coupling. we first apply our model to study the domain walls of perovskite ferroelectrics. It is shown that even the classic Ising 180° ferroelectric domain wall contains both Bloch and Néel types of polarization components due to the flexoelectric effect. Secondly, the nanoscale mechanical switching of ferroelectric domains via flexoelectricity is analyzed using the extended phase-field model. Our simulation results show good agreement with experimental observations.



The schematic of 180˚ domain wall in tetragonal $BaTiO_3$. The blue and red oxygen octahedra indicate positive and negative out-of-plane polarizations, respectively. Additional characteristics (Bloch and Néel) was found by theoretical calculations.

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INTRODUCTION

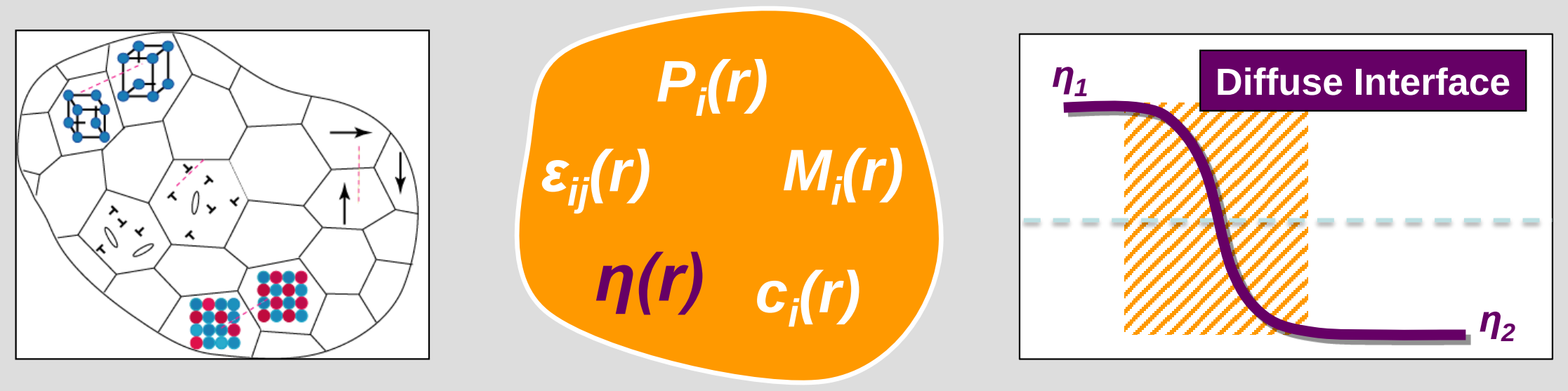
Stress → Polarization

$$P_i = d_{ijk}\varepsilon_{jk} + \mu_{ijkl}\frac{\partial \varepsilon_{kl}}{\partial x_j}$$

Piezoelectricity **Flexoelectricity**

Phenomenologically, polarization can be related to the mechanical deformation through the expression above. To be specific, the piezoelectric effect and the flexoelectric effect contribute. Even though the flexoelectric coefficients are very small, the flexoelectric effect may still dominate the behavior of the ferroelectrics at the ***nano*** scale.

PHASE-FIELD MODEL



The evolution of polarization is governed by the time-dependent Ginzburg-Landau equation,

$$\frac{\partial \eta_p}{\partial T} = -L\left(\frac{\delta F}{\delta \eta_p}\right)$$

where

$$F = \int_V [f_B(P_i) + f_G(\nabla_j P_i) + f_{Elec}(P_i) + f_{Elast}(P_i, \varepsilon_{ij}) + f_F(P_i, \varepsilon_{ij}, \nabla_j P, \nabla_k \varepsilon_{ij})]dV$$

the bulk energy

$$f_B(P_i) = \alpha_{ij}P_iP_j + \alpha_{ijkl}P_iP_jP_kP_l + \alpha_{ijklmn}P_iP_jP_kP_lP_mP_n$$

the gradient energy

$$f_G(\nabla_j P_i) = \frac{1}{2} g_{ijkl}\frac{\partial P_i}{\partial x_j}\frac{\partial P_k}{\partial x_l}$$

the elastic energy

$$f_{Elast}(P_i, \varepsilon_{ij}) = \frac{1}{2} c_{ijkl}\varepsilon_{ij}\varepsilon_{kl} - q_{ijkl}\varepsilon_{ij}P_kP_l$$

the electrostatic energy

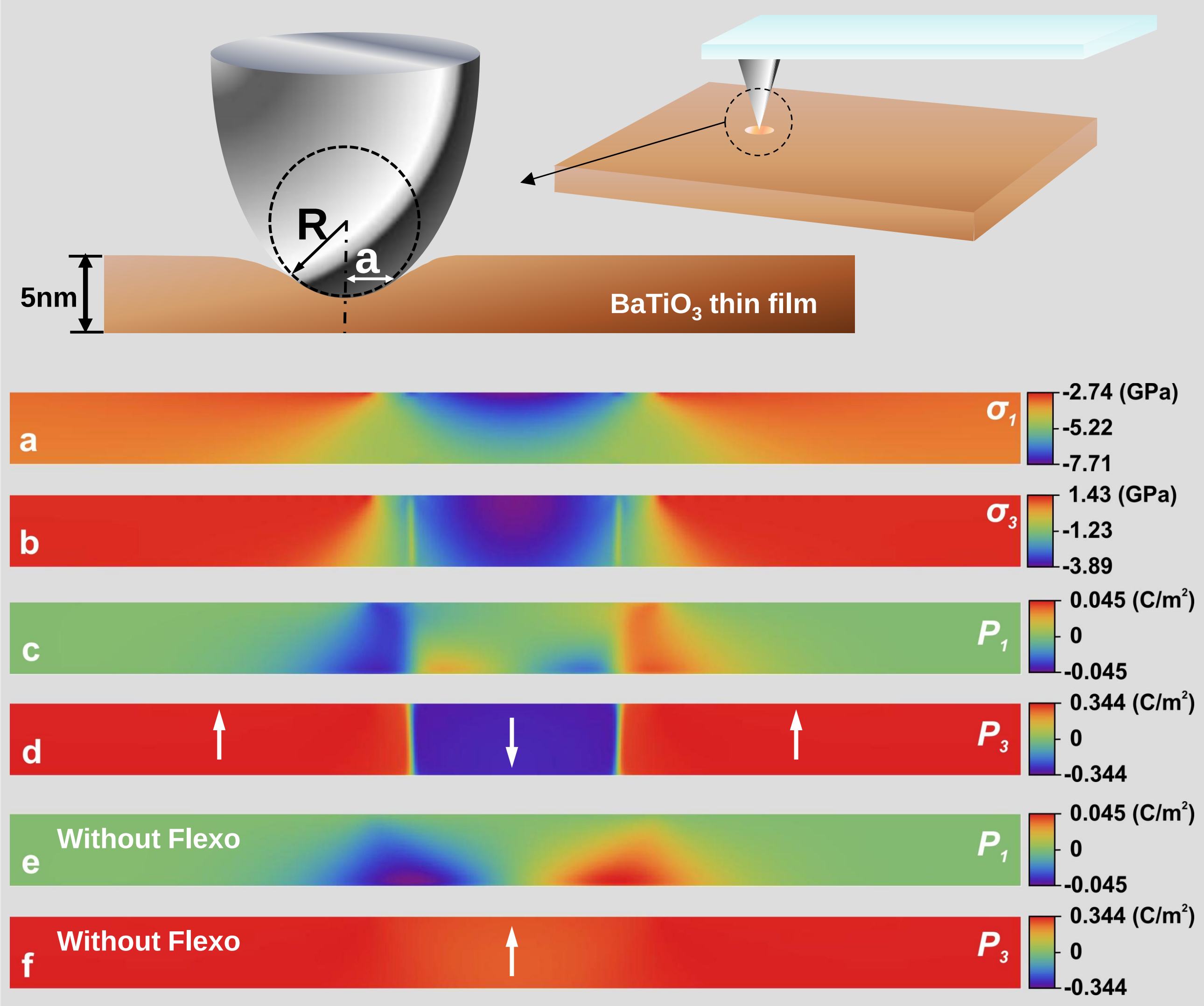
$$f_{Elec}(P_i) = -P_i(E_i + \frac{E_i^d}{2})$$

the flexoelectric contribution

$$f_F(P_i, \varepsilon_{ij}, \nabla_j P, \nabla_k \varepsilon_{ij}) = \frac{f_{ijkl}}{2}(\frac{\partial P_k}{\partial x_l}\varepsilon_{ij} - \frac{\partial \varepsilon_{ij}}{\partial x_l}P_k)$$

MECHANICAL SWITCHING VIA FLEXO

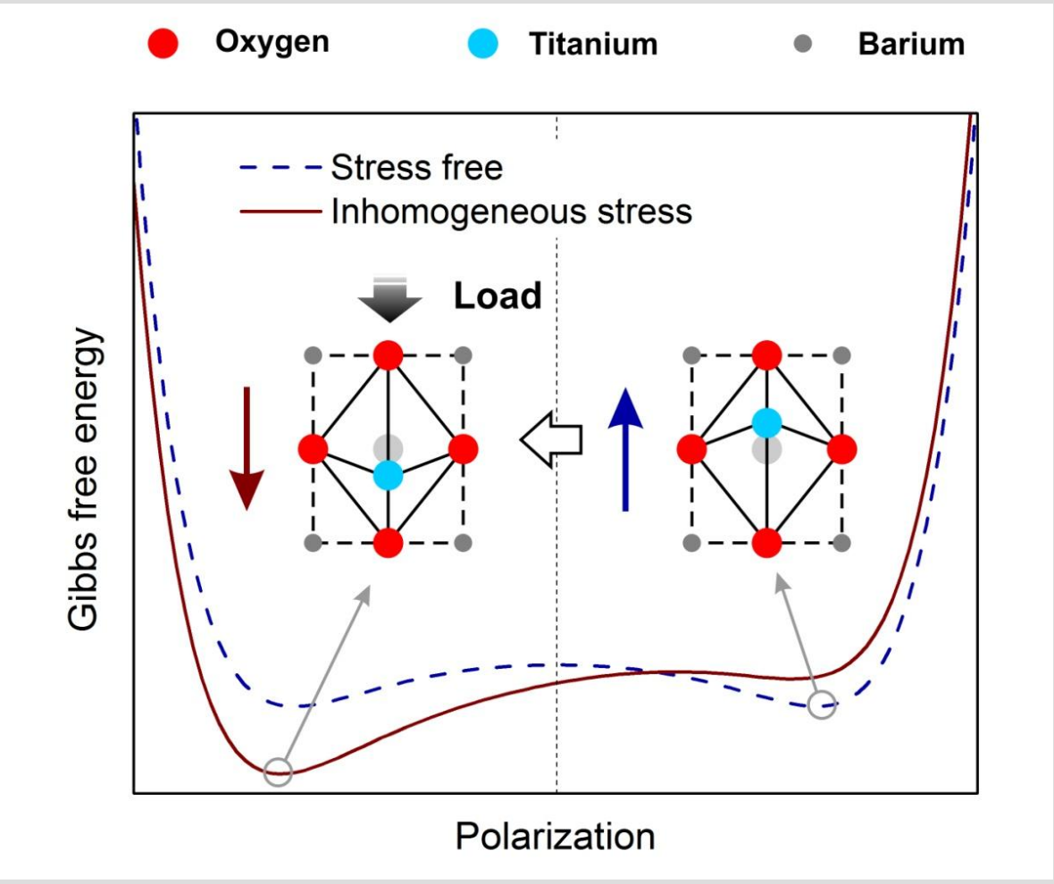
Phase-Field Simulation



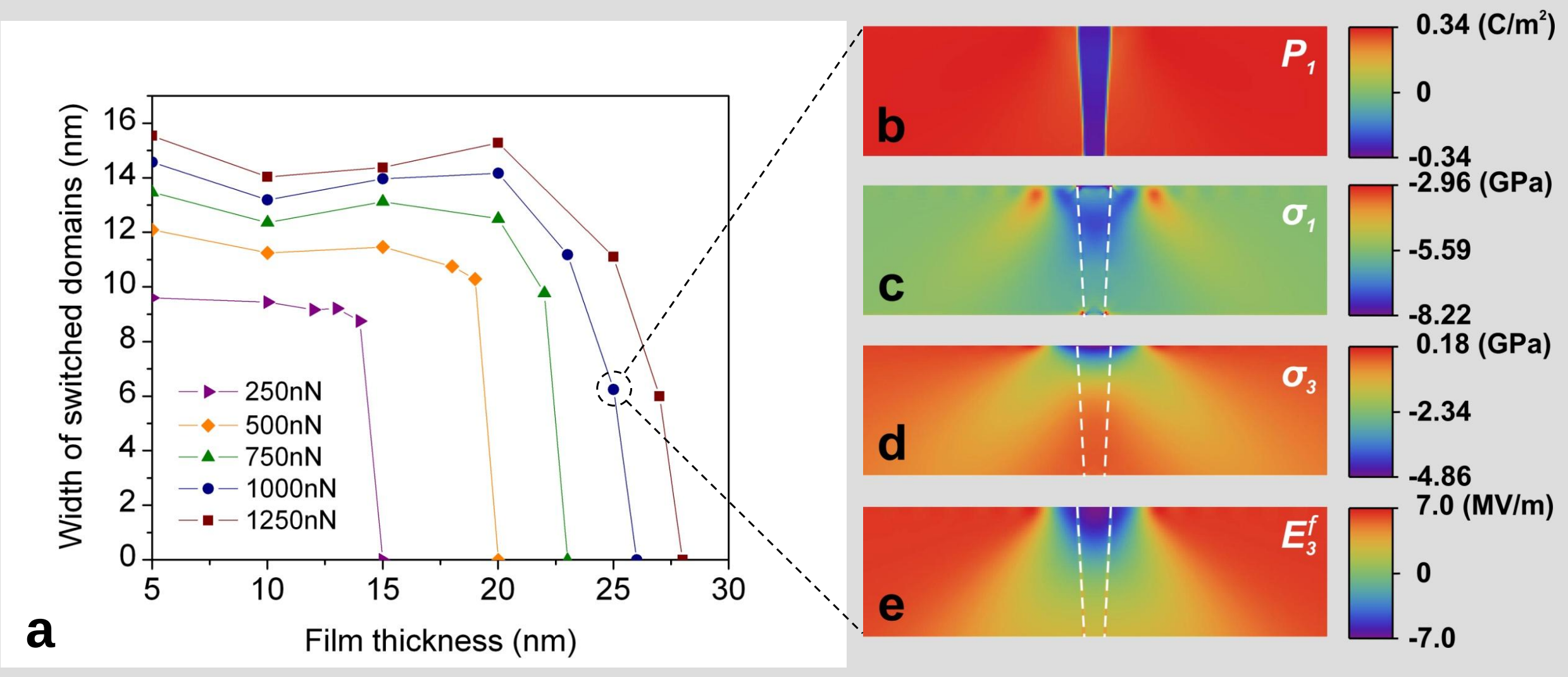
Phase-field simulation of mechanical switching via flexoelectric effect. The calculated distribution of stress components σ_1(a) and σ_3(b), polarization components P_1(c) and P_3(a). Clearly, the domain beneath the AFM tip is switched. However, as shown in the polarization profile (e) and (f), without flexoelectric effect the domain cannot be switched.

Switching Mechanism

As shown in the energy profile on the right, the flexoelectric effect can asymmetrically modify the energy landscape. Hence, the polarization can be switched. And the switched domains are thermodynamically stable even after unloading (they are already in the other energy well). This is quite different from the conventional mechanical switching through piezoelectricity.



Thickness Dependence



By varying the load and the film thickness, we calculated the dependence of switched domain width on these two factors, as shown in (a). (b - e) show the polarization, stress components and flexoelectric effect of 1000nN load on 25 nm film. The switched domain is well inside the contact area, because the flexoelectric effect is weak at the film bottom.

UNIAXIAL 180° DOMAIN WALL

Flexoelectricity induced new features

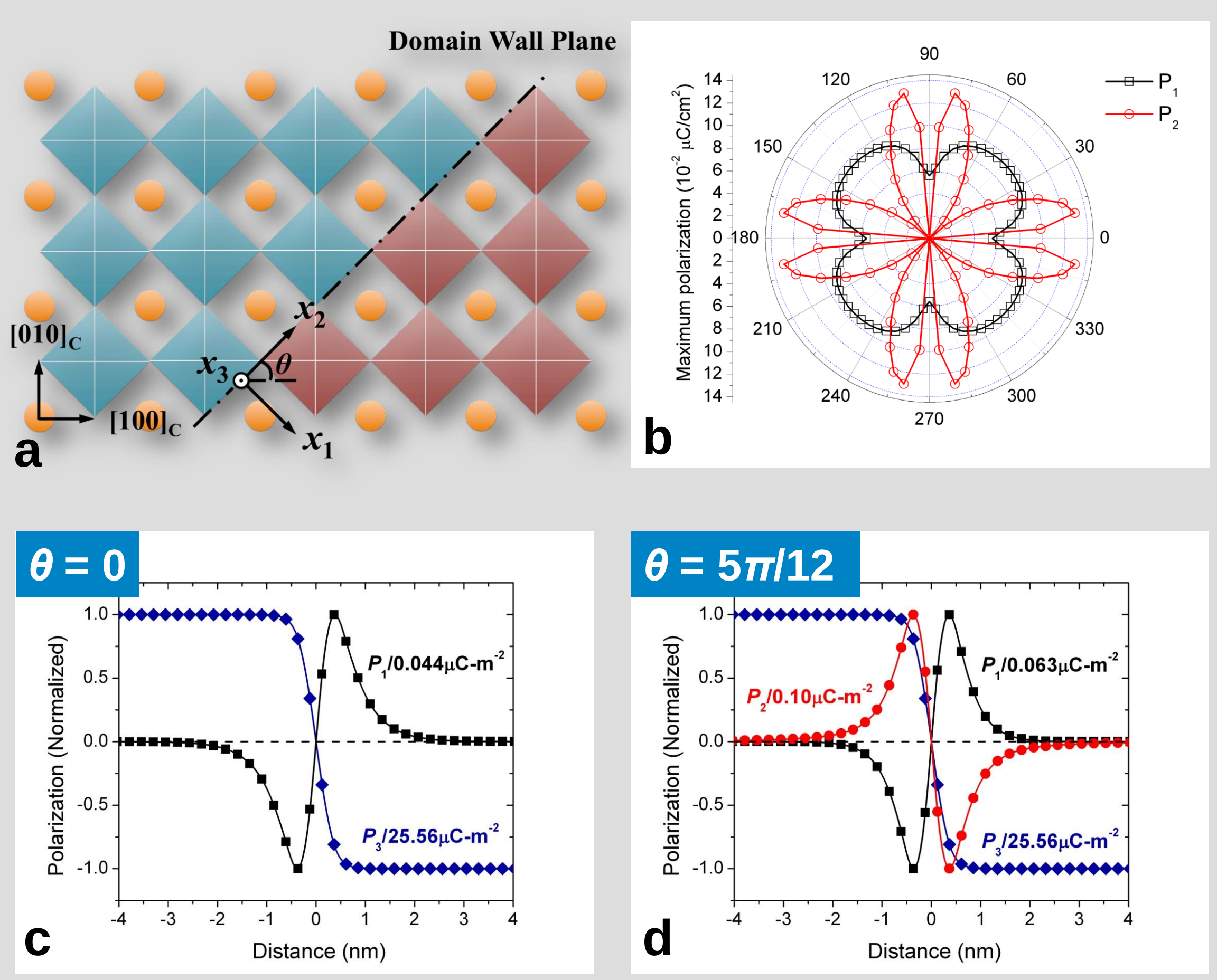


Figure (a) shows the setup of the simulation system with the angle θ representing the angle between the wall and the [100] direction. Figure (b) shows the maximum values of the induced Bloch and Néel components as a function of θ. When $\theta = n\pi/4$ (n is integer), the 180 domain wall is Ising – Néel like (Figure c); while for the other angles the wall is Ising – Néel – Bloch like (Figure d). We found the new features are entirely due to the flexoelectric effect, by comparing the results with and without flexoelectric effect.

CONCLUSIONS

- A phase-field model of ferroelectric domains with flexoelectric effects was developed
- The classical Ising ferroelectric domain walls also possess both Néel-like and Bloch-like features, which are induced by the flexoelectric effect
- The mechanical switching process with AFM was successfully simulated by our phase filed model
- The mechanism mechanical switching via flexoelectric effect was revealed, and the thickness dependence was analyzed

REFERENCES

1. Y. Gu, M. Li, A.N. Morozovska, Y. Wang, E.A. Eliseev, V. Gopalan, and L.-Q. Chen, *Flexoelectricity and Ferroelectric Domain Wall Structures: Phase-field Modeling and DFT Calculcatons,* **Phys. Rev. B 89**, 174111 (2014)
2. Y. Gu, J. Britason and L.-Q. Chen, *Mechanical switching via flexoelectric effect*, to be submitted (2014)