Ionic corrugation makes sliding ferroelectric switching easier

Ziwen Wang(王子文) and Shuai Dong(董帅)*

Key Laboratory of Quantum Materials and Devices of Ministry of Education, School of Physics, Southeast University, Nanjing 211189, China

Email: sdong@seu.edu.cn

Abstract: Research reveals that in van der Waals sliding ferroelectrics, the electric field induced ionic corrugation plays an important role in polarization switching.

Keywords：sliding ferroelectrics, ionic corrugation, Born effective charge, domain walls

Developing novel ferroelectric materials is essential for advancing low-power, high-speed, nonvolatile memory technologies. Traditional ferroelectric devices rely on perovskite-type ferroelectrics containing lead or titanium atoms. In these materials, ferroelectric polarization typically arises from small ionic displacements away from centrosymmetric positions [Fig. 1(a)], originating from the polar phonon mode instability. In recent years, however, a growing variety of unconventional ferroelectrics have been proposed and experimentally demonstrated, which exhibits exotic properties. Among them, van der Waals (vdW) interfacial ferroelectrics, also known as sliding ferroelectrics, have attracted considerable attention [1–4]. Unlike conventional ferroelectrics, sliding ferroelectrics derive their polarization from the stacking-dependent breaking of spatial inversion symmetry. Although an individual layer is nonpolar, a specific vdW stacking arrangement in a bilayer (or multilayer) can induce a net polarization through interlayer charge redistribution, as illustrated in Fig. 1(b). As a general mechanism for realizing ferroelectricity, interlayer sliding has substantially expanded the range of low-dimensional ferroelectrics and opened new opportunities for exploring connections with other areas of physics, including multiferroicity and magnetoelectric coupling, topological phenomena, and nonlinear optoelectronic effects, as illustrated in Fig. 1(c).

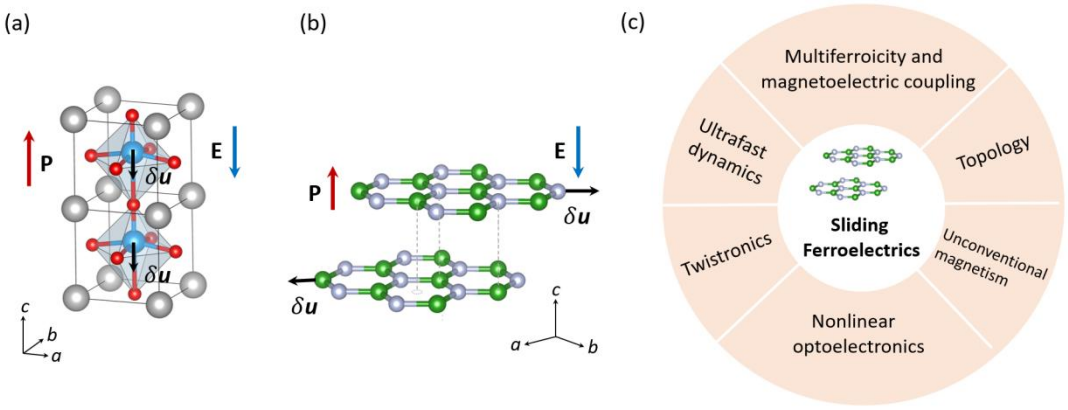

Fig. 1. ***Comparison between the conventional perovskite ferroelectric $BaTiO_3$ and sliding ferroelectric BN bilayer.*** *(a) Conventional perovskite ferroelectric. Polarization mainly (represented by the red arrow) arises from off-center*

displacements of Ti^{4+} (denoted by blue spheres) within the oxygen octahedra. Upon an applied electric field (blue arrow), the ions shift along the field direction (black arrows). (b) Sliding ferroelectric. Under the electric field, the two layers undergo in-plane relative sliding perpendicular to the field direction. (c) Sub-areas of physics connected with the sliding ferroelectricity.

The different origins of ferroelectricity give rise to distinct polarization switching mechanisms. In conventional perovskite ferroelectrics, applying an electric field opposite to the polarization direction drives the central ion to move along the field direction (the central ion has a positive Born effective charge), as shown in Fig. 1(a). In sliding ferroelectrics, by contrast, the ionic motions are not along the external electric field. Instead, ions move via the in-plane sliding mode, perpendicular to the electric field direction, as shown in Fig. 1b. Phenomenally, this perpendicular relationship is somewhat similar to the Hall effect of electronic transport under magnetic field. This unconventional switching mechanism is believed to originate from nonzero off-diagonal elements of the Born effective charge tensor induced by external factors (e.g., domain walls, twist angles) [5-7], and enables ultrafast polarization switching [6,8,9].

Now, writing in *Chinese Physics Letters*, Xu, Duan, and Tong report that the ionic corrugation plays a non-negligible role in polarization switching of sliding ferroelectrics [10]. Through large-scale molecular dynamics (MD) simulations, they emphasize that during polarization switching, the field-enhanced ionic corrugation induced by the diagonal element of the Born effective charge tensor can substantially increase the domain-wall velocity, rather than being a negligible structural response, as shown in Fig. 2. The markedly enhanced domain-wall velocity arises from the in-plane driving force increasing linearly with ionic corrugation. Furthermore, they show that in the presence of domain walls, even without off-diagonal elements of Born effective charge tensor, the ionic corrugation induced by the diagonal element can also act as an independent factor driving the domain wall motion, a view that goes beyond the previous understanding of polarization switching within the off-diagonal elements framework.

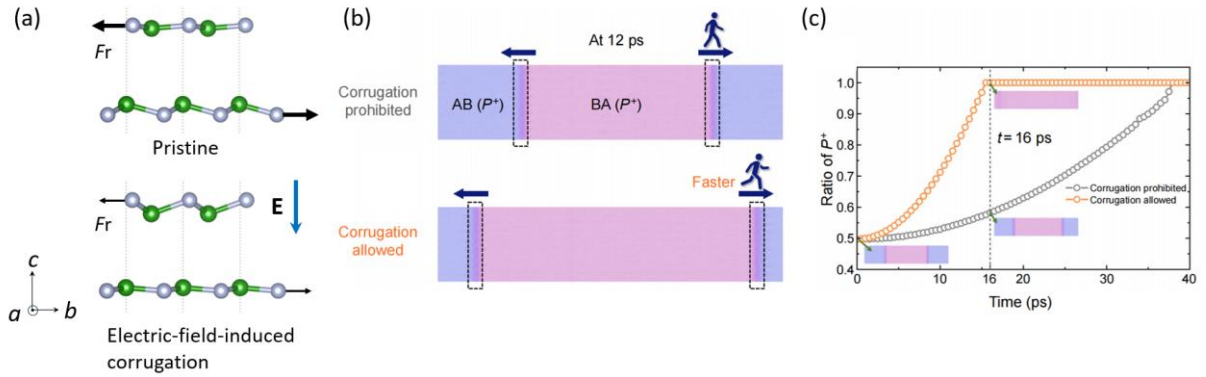

Fig. 2. ***Comparison of switching dynamics with and without the ionic corrugation.*** *(a) Side views of the pristine and electric-field-induced corrugated structures. For clarity, the corrugations in the figure are exaggerated. The*

induced corrugation reduces the restoring force (Fr), leading to faster polarization switching. (b) Snapshots of the domain wall motion at 12 ps from the same initial configuration during the MD simulations. Top: corrugation prohibited case. Bottom: corrugation allowed case. The faster growth of the BA (P+) domain in (b) demonstrates that ionic corrugation accelerates the polarization switching process. The dashed boxes indicate the areas of domain walls. (c) Evolution of the BA (P+) domain fraction during the MD simulations. (b-c) Reprinted with permission from Ref. [10]. Copyright 2026 Chinese Physical Society.

Since polarization switching driven by ionic corrugation also requires the presence of domain walls, its contribution may be intertwined with that arising from the off-diagonal elements of the Born effective charge tensor, potentially causing challenges for experimental verification of this mechanism. Nevertheless, this important advance introduces a new degree of freedom for understanding polarization switching in sliding ferroelectrics and may offer valuable insights into the design of novel ferroelectric materials and the optimization of their functional properties.

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