

Tip-based proximity ferroelectric switching and piezoelectric response in wurtzite multilayers

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Proximity ferroelectricity is a paradigm for inducing ferroelectricity when a nonferroelectric polar material (such as AlN), which is unswitchable with an external field below the dielectric breakdown field, becomes a practically switchable ferroelectric in direct contact with a thin switchable ferroelectric layer (such as $\text{Al}_{1-x}\text{Sc}_x\text{N}$). Here, we develop a Landau-Ginzburg-Devonshire approach to study the proximity effect of local piezoelectric response and polarization reversal in wurtzite ferroelectric multilayers under a sharp electrically biased tip. Using finite-element modeling, we analyze the probe-induced nucleation of nanodomains, the features of local polarization hysteresis loops and coercive fields in the $\text{Al}_{1-x}\text{Sc}_x\text{N}/\text{AlN}$ bilayers and three-layers. Similar to the wurtzite multilayers sandwiched between two parallel electrodes, the regimes of “proximity switching” (when all layers collectively switch) and the regime of “proximity suppression” (when they collectively do not switch) are the only two possible regimes in the probe-electrode geometry. However, the parameters and asymmetry of the local piezoresponse and polarization hysteresis loops depend significantly on the sequence of the layers with respect to the probe. The physical mechanism of proximity ferroelectricity in the local probe geometry is a depolarizing electric field determined by the polarization of the layers and their relative thickness. The field, whose direction is opposite to the polarization vector in the layer(s) with the larger spontaneous polarization (such as AlN), renormalizes the double-well ferroelectric potential to lower the steepness of the switching barrier in the “otherwise unswitchable” polar layers. Tip-based control of domains in otherwise nonferroelectric layers using proximity ferroelectricity can provide nanoscale control of domain reversal in memory, actuation, sensing, and optical applications. The ability of the tip-induced proximity switching to differentially switch multilayers, based on the order of the layers, provides a powerful tool for selective domain engineering.

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I. INTRODUCTION

“Proximity ferroelectricity” was recently reported by Skidmore *et al.* [1] who define this phenomenon

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as follows: “Proximity ferroelectricity is an interface-associated phenomenon, where electric field driven polarization reversal in a non-ferroelectric polar material is induced by one or more adjacent ferroelectric materials.” The proximity ferroelectricity was revealed experimentally in the nonferroelectric layers (such as AlN and ZnO) coupled with the ferroelectric layers (such as $\text{Al}_{1-x}\text{B}_x\text{N}$, $\text{Al}_{1-x}\text{Sc}_x\text{N}$ and $\text{Zn}_{1-x}\text{Mg}_x\text{O}$) in nitride-nitride, oxide-oxide, and nitride-oxide multilayers. The layered structures, whose thicknesses varied from tens to hundreds of nanometers, included two-layer (asymmetric, e.g., $\text{Al}_{1-x}\text{Sc}_x\text{N}/\text{AlN}$, $\text{Al}_{1-x}\text{B}_x\text{N}/\text{AlN}$, $\text{ZnO}/\text{Al}_{1-x}\text{B}_x\text{N}$) and three-layer (symmetric, e.g., $\text{Al}_{1-x}\text{B}_x\text{N}/\text{AlN}/\text{Al}_{1-x}\text{B}_x\text{N}$, $\text{AlN}/\text{Al}_{1-x}\text{B}_x\text{N}/\text{AlN}$, $\text{Zn}_{1-x}\text{Mg}_x\text{O}/\text{ZnO}/\text{Zn}_{1-x}\text{Mg}_x\text{O}$)

configurations [1]. The tip-based proximity ferroelectric reversal will potentially provide local control of domain structures, which is important for memory, piezoelectric and optical applications.

We note that the ferroelectric layers such as $\text{Zn}_{1-x}\text{Mg}_x\text{O}$, $\text{Al}_{x-1}\text{Sc}_x\text{N}$ and $\text{Al}_{x-1}\text{B}_x\text{N}$ in the examples above, as well as others such as $\text{Hf}_x\text{Zr}_{1-x}\text{O}_2$, rely on doping-induced chemical stress to turn a nonferroelectric layer into a ferroelectric layer: Zr doping of HfO_2 , Mg doping of polar but unswitchable ZnO, and Sc or B doping of the polar but unswitchable AlN) [2–5]. The local lattice distortions and charged defects around chemical dopants can locally allow for polarization switching to create domain nuclei, which then propagate through long-range electrostatic forces [6,7]. These materials have become promising candidates for the next generation of Si-compatible electronic memory elements such as ferroelectric random-access memories, steep-slope field-effect transistors, and other logic devices [8–12]. However, the parent phases (AlN and ZnO) are not switchable with practical electric fields unless the proximity effect is exploited in a multilayer film stack.

The goal of this work is to develop the theoretical formalism for proximity switching and piezoelectric response in ferroelectric/nonferroelectric multilayers under a sharp, electrically biased tip such as those used in scanning probe microscopes. Theoretical calculations of the polar properties and polarization switching in alternating ferroelectric and paraelectric (or dielectric) bilayers, multilayers, and superlattices, placed in the capacitor geometry, were performed using the Landau-Ginzburg-Devonshire (LGD) phenomenological approach [13–16], first principles [17, 18], combination of the LGD approach with the phase-field method [19], and/or direct variational methods [20–22]. These works, like many others, consider perovskite-perovskite bilayers, multilayers, and superlattices, such as $\text{BaTiO}_3/\text{SrTiO}_3$, $\text{PbTiO}_3/\text{SrTiO}_3$, $\text{CaTiO}_3/\text{BaTiO}_3$, and $\text{BiFeO}_3/\text{SmFeO}_3$.

Eliseev *et al.* [23] have developed a Landau-Ginzburg theory of proximity ferroelectricity in wurtzite multilayers of nonferroelectrics and ferroelectrics to analyze their switchability and coercive fields. The theory predicts regimes of both “proximity switching,” where the multilayers collectively switch, and “proximity suppression,” where they collectively do not switch. The mechanism of proximity ferroelectricity is an internal electric field determined by the polarization of the layers and their relative thickness in a self-consistent manner that renormalizes the double-well ferroelectric potential to lower the steepness of the switching barrier. Further reduction in the coercive field emerges from charged defects in the bulk that act as nucleation centers, since correlated nucleation of the spikelike domains in the vicinity of sign-alternating randomly distributed electric charge sources [24], as well as correlated polarization switching in the proximity of

ferroelectric domain walls [25], have a significant influence on the coercive field reduction.

This theoretical work tests the hypothesis that a biased piezoelectric force microscope (PFM) probe can be considered as the strong external charged defect, and so a strong reduction of the coercive field can be expected in the case of local polarization reversal under the probe. The local piezoelectric response (PFM signal) can be simulated in the semianalytical linear decoupling approximation [26–28], partial coupling between the ferroelectric polarization and elastic fields [29], or by solving the fully coupled problem numerically [30,31]. The simulation results obtained in the decoupling approximation well describe the results of PFM experiments (see, for example, the topical review in [32] and references therein).

There are several methods for simulations of probe-induced nucleation of nanodomains, which include the semianalytical approach proposed by Prof. M. Molotskii’s group [33–35], the phase-field simulations performed by Prof. L.-Q. Chen’s group [36–38], and the hybrid mesoscopic-microscopic approach created by Prof. A. Rappe’s group [39–41]. The full list, of course, is by no means limited to these works.

In this work we develop the LGD approach to study the proximity effect of local polarization reversal and piezoelectric response in wurtzite ferroelectric multilayers. Using finite-element modeling (FEM), we analyze the probe-induced nucleation of nanodomains, the features of local polarization hysteresis loops and coercive fields in the $\text{Al}_{1-x}\text{Sc}_x\text{N}/\text{AlN}$ bilayers and three-layers. We reveal that the parameters and asymmetry of the local piezoelectric response and polarization hysteresis loops depend significantly on the sequence of the layers with respect to the probe (e.g., whether the ferroelectric $\text{Al}_{1-x}\text{Sc}_x\text{N}$ or the nonferroelectric AlN layer is directly in contact with the probe).

II. PROBLEM STATEMENT

Figures 1(a)–1(d) depict the geometries of asymmetric bilayers and symmetric three-layers considered, which consist of AlN and $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layers placed between the PFM probe apex and the bottom flat electrode. The total thickness of $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layers is h_1 and the total thickness of the AlN layers is h_2 . The total thickness of the multilayer stack, h , is the same for all geometries considered.

The tip-surface contact is considered using the “shielded probe” model [42,43] that allows one to fix the electric potential φ at the unperturbed surface $z = h$. Within the model, the PFM probe apex is approximated by a biased disk of radius R . The free surface of the wurtzite layer outside the disk electrode is covered by a layer of screening charge, which is capable of providing the condition $\varphi = 0$ outside the probe-surface contact. The model is mostly realistic and accurate, because “squashed” tips are widely used, being such as prepared or become squashed during

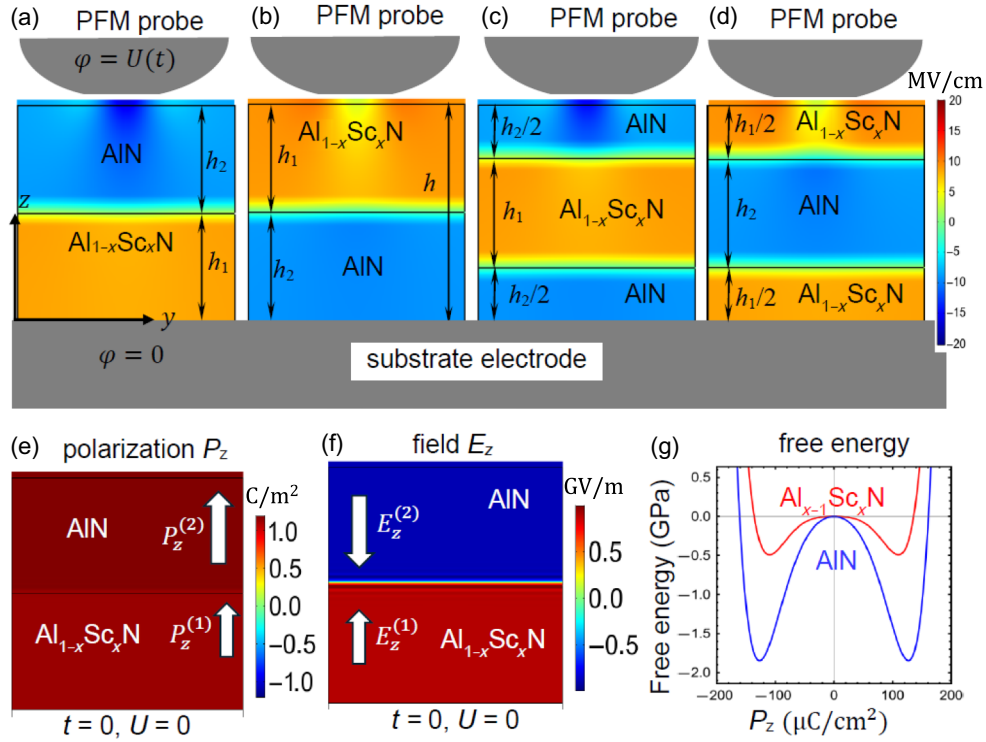


FIG. 1. Geometries of heterostructures considered: (a) probe/AlN/Al_{1-x}Sc_xN/electrode; (b) probe/Al_{1-x}Sc_xN/AlN/electrode; (c) probe/AlN/Al_{1-x}Sc_xN/AlN/electrode; (d) probe/Al_{1-x}Sc_xN/AlN/Al_{1-x}Sc_xN/electrode. The sample coordinates (x, y, z) form a right-handed coordinate system. The thickness of Al_{1-x}Sc_xN layer is h_1 and the thickness of the AlN layer is h_2 . Color maps show the electric field distributions for the considered geometries of single-domain multilayers for the bias $U \approx -7.5$ V. The right scale corresponds to the electric field. The total thickness of the multilayer stack, $h = 40$ nm, is the same for all heterostructures considered. Initial distributions of (e) the spontaneous polarization and (f) depolarization electric field in the probe/AlN/Al_{1-x}Sc_xN/electrode heterostructure. (g) Free energy wells of Al_{0.73}Sc_{0.27}N (red curve) and AlN (blue curve) bulk materials.

the exploitation. The accuracy of the approximation for a truncated-conical shape probe, in which electric potential can be rigorously represented by the charged disk (tip part) and the linear charge (conical part), is analyzed in Ref. [43]. The shielded probe model is well applicable for the squashed tips, if the surface screening of the ferroelectric polarization is present outside the tip-surface contact. Since the screening outside the tip-contact area is provided by the ambient charges, which may be fast or retarding depending on the ambient conditions (e.g., humidity), on the relaxation time of polarization changes, and on the sweep frequency, the natural limitation of the shielded probe model is the fast switching of polarization at high bias voltages, when the lateral size of the tip-induced domain well exceeds the radius R , and the ambient charges outside the tip-contact area do not have enough time to screen the bias-induced changes of the ferroelectric polarization. We do not consider such situations further.

A time-dependent electric voltage $U(t)$ is applied to the shielded probe. The voltage pulse is sinusoidally modulated and its amplitude increasing linearly in time from zero to $U_{\max}$, namely $U(t) = U_{\max}(t/t_{\max})\sin(\omega t)$, where ω is the pulse frequency and $t_{\max}$ is the pulse duration.

We performed the FEM for $2 \text{ nm} \leq R \leq 10 \text{ nm}$, which is significantly less than $h \sim 40 \text{ nm}$. The free surface of the wurtzite layer outside the disk electrode is covered by a layer of screening charges (not shown in Fig. 1), which is capable of providing the condition $\varphi = 0$ outside the probe-surface contact. The smooth transition between the edge of the biased disk probe and the screened surface is modeled by a Gaussian function.

Importantly, the shielded probe is regarded as “elastically soft” in order not to perturb the local piezoelectric response of the wurtzite layers. The substrate electrode is regarded as electrically grounded ($\varphi = 0$ at $z = 0$) and “elastically rigid”. The elastic and electric boundary conditions are periodic at the side boundaries of the computational cell.

The time-dependent LGD equations for the Al_{1-x}Sc_xN layer (subscripts and superscript “1”) and the AlN layer (subscripts and superscript “2”) are the following [23]:

$$\Gamma_1 \frac{\partial P_z^{(1)}}{\partial t} + \tilde{\alpha}_1 P_z^{(1)} + \beta_1 (P_z^{(1)})^3 + \gamma_1 (P_z^{(1)})^5 - g_z^{(1)} \frac{\partial^2 P_z^{(1)}}{\partial z^2} - g_{\perp}^{(1)} \left(\frac{\partial^2 P_z^{(1)}}{\partial x^2} + \frac{\partial^2 P_z^{(1)}}{\partial y^2} \right) = E_z^{(1)}, \quad (1a)$$

TABLE I. LGD model parameters.^a

Compound	α_i , m/F	β_i , m ⁵ /(F C ²)	γ_i , m ⁷ /(F C ⁴)	$g_z^{(i)}$, m ³ /F	$g_\perp^{(i)}$, m ³ /F	$\varepsilon_b^{(i)}$
Al _{0.73} Sc _{0.27} N	$-2.792 \cdot 10^8$ ^b	$-3.155 \cdot 10^9$	$2.788 \cdot 10^9$	$5 \cdot 10^{-10}$	$1 \cdot 10^{-10}$	3 ^b
AlN	$-2.164 \cdot 10^9$	$-3.155 \cdot 10^9$	$2.788 \cdot 10^9$	$5 \cdot 10^{-10}$	$1 \cdot 10^{-10}$	4

^aParameters are taken from Table CII in the Supplemental Material [55], given in the supplemental to Ref. [23], except those marked “^b”.

^bThe parameter α_1 is refined in this work allowing for the electrostriction energy contribution; the background permittivity $\varepsilon_b^{(1)}$ is not equal to $\varepsilon_b^{(2)}$, because the approximation $\varepsilon_b^{(1)} \approx \varepsilon_b^{(2)}$, used in Ref. [23], is not used hereinafter.

$$\Gamma_2 \frac{\partial P_z^{(2)}}{\partial t} + \tilde{\alpha}_2 P_z^{(2)} + \beta_2 (P_z^{(2)})^3 + \gamma_2 (P_z^{(2)})^5 - g_z^{(2)} \frac{\partial^2 P_z^{(2)}}{\partial z^2} - g_\perp^{(2)} \left(\frac{\partial^2 P_z^{(2)}}{\partial x^2} + \frac{\partial^2 P_z^{(2)}}{\partial y^2} \right) = E_z^{(2)}. \quad (1b)$$

Here Γ_i is the Landau-Khalatnikov relaxation coefficient of layer i , and we consider $\Gamma_1 = \Gamma_2$ for the sake of simplicity. The coefficients $\tilde{\alpha}_i$, β_i , and γ_i are the Landau expansion coefficients for Al_{1-x}Sc_xN and AlN layers, and the $E_z^{(i)}$ are the z -components of the electric field acting inside the layers. Hereafter, $i = 1$ corresponds to Al_{1-x}Sc_xN layer(s) and $i = 2$ corresponds to AlN layer(s). The LGD parameters of Al_{1-x}Sc_xN and AlN used in our calculations are listed in Table I. These were determined from the experimentally measured spontaneous polarization [3,44] and linear dielectric permittivity [45] as described in Refs. [46] and [23]. Free energy wells of Al_{0.73}Sc_{0.27}N and AlN bulk materials are shown in Fig. 1(g).

The boundary conditions for the polarization at the top surface, interfaces, and bottom surface of the multilayer stack are of the third type [47,48] in general [i.e., a function plus its derivative is a constant; see Eq. (3) in Ref. [23] for details]. Below, for the sake of simplicity, we consider the polarization components and their derivatives continuous at the interfaces between AlN and Al_{1-x}Sc_xN layers. The boundary conditions at the top and bottom surfaces are regarded as “natural,” namely $(\partial P_z^{(i)}/\partial z) = 0|_{z=0}$ and $(\partial P_z^{(i)}/\partial z) = 0|_{z=h}$. The initial distribution of polarization is either a single-domain or a multidomain state with randomly small fluctuations.

The coefficients $\tilde{\alpha}_i$ in Eqs. (1) are renormalized by elastic stresses $\sigma_{kl}^{(i)}$ as $\tilde{\alpha}_i = \alpha_i - Q_{12}^{(i)}(\sigma_{22}^{(i)} + \sigma_{33}^{(i)}) - Q_{11}^{(i)}\sigma_{11}^{(i)}$,

where the $Q_{kl}^{(i)}$ are electrostriction coefficients of the layers, which are listed in Table II. Elastic stresses satisfy the equation of mechanical equilibrium in the layers.

$$\frac{\partial \sigma_{jk}^{(i)}}{\partial x_j} = 0. \quad (2a)$$

Elastic equations of state follow from the variation of the free energy with respect to elastic stress, namely,

$$s_{jklm}^{(i)} \sigma_{lm}^{(i)} + Q_{jklm}^{(i)} P_l^{(i)} P_m^{(i)} = u_{jk}^{(i)}. \quad (2b)$$

Here the $u_{jk}^{(i)}$ are elastic strains, and $s_{jklm}^{(i)}$ are elastic compliances (also listed in Table II).

Elastic boundary conditions correspond to the absence of normal stresses at the top surface $z = h$, elastic displacement continuity at the AlN-Al_{1-x}Sc_xN interface (or interfaces), and zero elastic displacement in the rigid substrate, $z = 0$. Hereafter, we neglect the influence of the flexoelectric coupling for the sake of simplicity.

Electric field in the layers, $E_z^{(i)} = -(\partial \varphi^{(i)}/\partial z)$, obeys the Poisson equations for the electric potential $\varphi^{(i)}$ inside the layers:

$$\varepsilon_0 \varepsilon_b^{(i)} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \varphi^{(i)} = \frac{\partial^2 P_z^{(i)}}{\partial z^2}. \quad (3)$$

Here $\varepsilon_b^{(i)}$ is the background dielectric permittivity [50, 51] of layer i . The electric boundary conditions are the continuity of $\varphi^{(i)}$ and electric displacement component $D_z^{(i)}$ at the AlN-Al_{1-x}Sc_xN interfaces, and the fixed

TABLE II. Electrostriction coefficients Q_{ij} and elastic stiffness c_{ij} .

Parameters	Q_{ij} , m ⁴ /C ²	Ref.	c_{ij} , GPa	Ref.
AlN	$Q_{13} = -0.0087$, $Q_{33} = 0.0203$	[46]	$c_{11} = 396$, $c_{12} = 137$, $c_{13} = 108$, $c_{33} = 373$, $c_{44} = 116$, $c_{66} = 130$	[49]
Al _{0.73} Sc _{0.27} N	$Q_{13} = -0.0152$, $Q_{33} = 0.0406$	[46]	$c_{11} = 319$, $c_{12} = 151$, $c_{13} = 127$, $c_{33} = 249$, $c_{44} = 101$, $c_{66} = 84$	[49]

potential at the electrodes, for example, $\varphi^{(1)} = 0|_{z=0}$, $\varphi^{(2)} = U(t)\exp(-(x^2 + y^2/R^2))|_{z=h}$.

Despite the fact that the bias applied between the tip and the flat bottom electrode is the same ($U = -7.5$ V) in all four cases shown in Figs. 1(a)–1(d), and the spontaneous polarization of the single-domain layers is directed upward [see, for example, Fig. 1(e)], the sign of electric field is opposite in the AlN and $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layers due to the dominant depolarization field effect, which is “inverted” in the AlN layer [see, for example, Fig. 1(f)].

The effect of the field “inversion” can be described analytically when domains are absent, and the polarization is almost constant inside each layer. Indeed, when $(\partial P_z^{(i)}/\partial z) = 0$, the depolarization field inside the multilayer, whose top and bottom surfaces are covered by conducting electrodes, is given by the analytical expression derived in Ref. [23]. These expressions allow us to estimate the electric field in the shielded probe geometry if $2R \sim h$. The approximate expressions for the electric field inside the bilayer are

$$E_z^{(1)}(x, y, z, t) \approx -\frac{P_z^{(1)} - \bar{D}}{\varepsilon_0 \varepsilon_b^{(1)}} + \frac{U(t)\exp(-(x^2 + y^2/R^2))R^2}{\varepsilon_b^{(1)}[(h_1/\varepsilon_b^{(1)}) + (h_2/\varepsilon_b^{(2)})](R + z/\chi_b^{(1)})^2}, \quad (3a)$$

$$E_z^{(2)}(x, y, z, t) \approx -\frac{P_z^{(2)} - \bar{D}}{\varepsilon_0 \varepsilon_b^{(2)}} + \frac{U(t)\exp(-(x^2 + y^2/R^2))R^2}{\varepsilon_b^{(2)}[(h_1/\varepsilon_b^{(1)}) + (h_2/\varepsilon_b^{(2)})](R + z/\chi_b^{(2)})^2}. \quad (3b)$$

The first term in Eqs. (3), $-(P_z^{(i)} - \bar{D})/\varepsilon_0 \varepsilon_b^{(i)}$, is the internal depolarization field $E_{dz}^{(i)}$ [52,53]. The second term in Eqs. (3) is the external field proportional to the probe bias $U(t)$ [27]. The values $\chi_b^{(i)}$ are dielectric anisotropy factor of the layers. $\bar{D}$ is the average displacement of the multilayer, which is equal to [54]

$$\bar{D} = \frac{1}{(h_1/\varepsilon_b^{(1)}) + (h_2/\varepsilon_b^{(2)})} \left(\frac{h_1}{\varepsilon_b^{(1)}} \bar{P}_z^{(1)} + \frac{h_2}{\varepsilon_b^{(2)}} \bar{P}_z^{(2)} \right), \quad (4)$$

where $\bar{P}_z^{(i)}$ is the average polarization of layer i . Note that the average displacement $\bar{D}$ coincides with the average polarization $\bar{P}$ when $\varepsilon_b^{(i)}$ is the same for both layers. From Eqs. (3) and (4), the depolarization fields are opposite,

namely,

$$E_{dz}^{(1)} = -E_{dz}^{(2)} = -\frac{P_z^{(1)} - P_z^{(2)}}{2\varepsilon_0 \varepsilon_b},$$

$$\text{for } h_1 = h_2 = \frac{h}{2} \text{ and } \varepsilon_b^{(1)} = \varepsilon_b^{(2)} = \varepsilon_b.$$

Since the depolarization field is much higher than the probe field at small biases, the simple estimate explains the field inversion effect shown in Fig. 1(f). From Fig. 1(f), the depolarization field of the AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ bilayer with polarization directed upward in both layers [as shown in Fig. 1(e)] is directed downward in the AlN layer and upward in the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer.

Below we will show that the opposite direction of the field in the AlN and $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layers, as well as its strong inhomogeneity under the biased probe, are the main reasons for the dependence of local polarization reversal and piezoelectric response on the sequence of the layers. The depolarization field, whose direction is opposite in the layer(s) with the larger spontaneous polarization (i.e., in the AlN), renormalizes the double-well ferroelectric potential to lower the steepness of the switching barrier in the otherwise “unswitchable” polar layers. Note that this effect is intrinsic to the multilayer structure and is independent of any additional reduction in coercive field due to the presence of defects.

The vertical surface displacement $u_z(x, y, t)$ is measured by the PFM, being directly related with the local piezoelectric response signal d_{33}^{eff} as $d_{33}^{\text{eff}} = (du_z/dU) \sim (u_z/U)$ [28]. The linear relation $d_{33}^{\text{eff}} \sim (u_z/U)$ allows us to analyze the peculiarities of d_{33}^{eff} using the FEM results for u_z .

III. RESULTS AND DISCUSSION

A. Peculiarities of local polarization switching and piezoelectric response in bilayers and three-layers

Due to the inhomogeneous electric field distribution in the probe-electrode geometries considered [shown in Figs. 1(a)–1(d)], the average polarization and local piezoelectric response depend on the sequence of the layers, being different for AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ (Fig. 2) and $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN (Fig. 3) bilayers, as well as for AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN (Fig. 4) and $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ (Fig. 5) three-layers, where either the AlN or $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer is in contact with the probe tip. Results, shown in various panels of Figs. 2–5, are calculated in the case of a single-domain initial distribution of polarization in all layers. Specifically, the initial state was an upward-directed spontaneous polarization with random small fluctuations in all layers. We waited until the initial relaxed to a single-domain upward-directed spontaneous polarization without any fluctuations [such as that shown in Fig. 1(e)] and then applied the bias according to the same timing protocol shown in panels (a) in Figs. 2–5. Note that

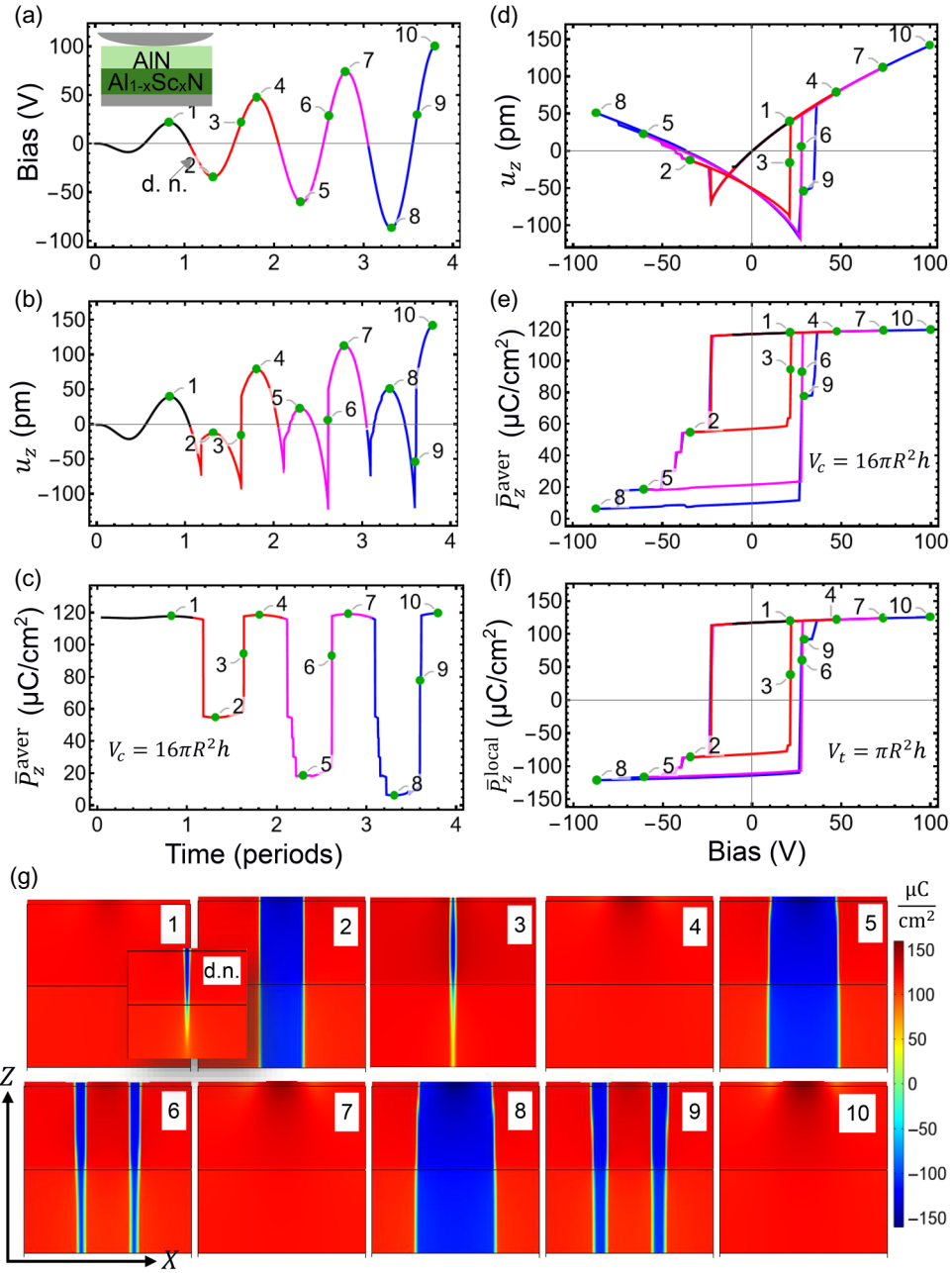


FIG. 2. Time dependences of (a) the bias applied between the PFM probe and the bottom electrode, (b) the vertical displacement u_z of the surface below the probe tip, and (c) the average polarization P_z^{aver} in the probe/AlN/Al_{0.73}Sc_{0.27}N bilayer/bottom electrode heterostructure. Bias dependences of (d) the surface displacement u_z , (e) the polarization P_z averaged over a larger volume V_c and (f) over a smaller volume V_t . (g) The distribution of polarization in the cross section of the bilayer at moments of time numbered from 1 to 10 shown by the pointers in (a)–(f). The abbreviation “d.n.” denotes domain nucleation. The distribution of electric field at moments 1–10 is shown in Fig. S1 in the Supplemental Material [55]. The thickness of the AlN and Al_{0.73}Sc_{0.27}N layers is 20 nm, the tip-surface contact radius $R = 5$ nm. LGD parameters and elastic constants are listed in Tables I–II. The averaging volumes $V_c = 16\pi R^2 h$ and $V_t = \pi R^2 h$; the initial distribution of polarization is a single-domain state with randomly small fluctuations.

the single-domain state of the spontaneous polarization is the ground state of the layered structure, since the surface screening is regarded as ideal, and the boundary condition $\varphi = 0$ is valid at both surfaces.

The bias amplitude linearly increases in time as shown in panels (a) in Figs. 2–5. The time sweeps of the vertical surface displacement $u_z(0, 0, t)$ under the PFM tip, which correspond to the bias sweep, are shown in panels (b). The

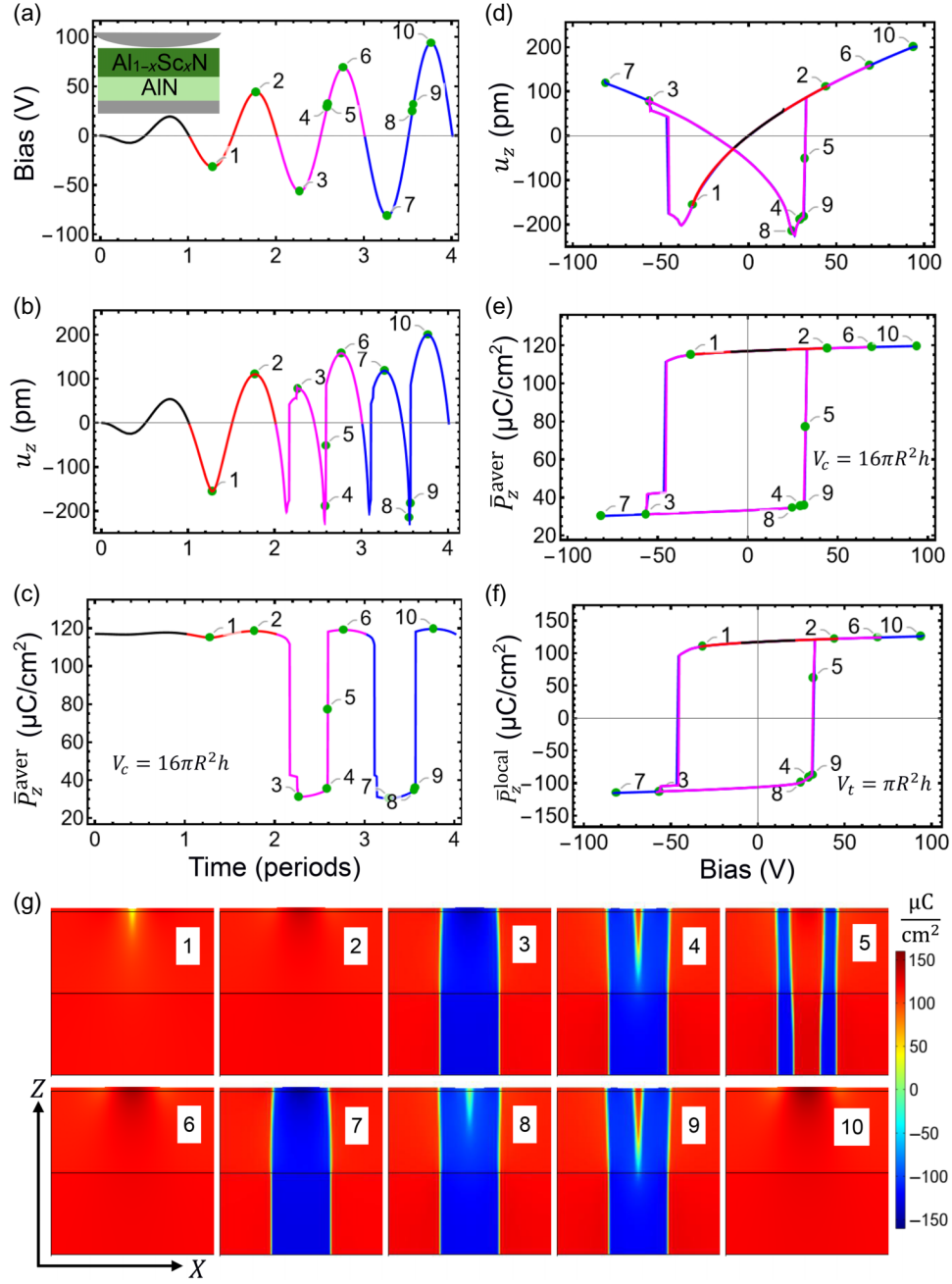


FIG. 3. Time dependences of (a) the bias applied between the PFM probe and the bottom electrode, (b) the vertical displacement u_z of the surface below the probe apex, and (c) the average polarization $\bar{P}_z^{\text{aver}}$ in the probe/ $\text{Al}_{0.73}\text{Sc}_{0.27}\text{N}$ /AlN bilayer/bottom electrode heterostructure. Bias dependences of (d) the surface displacement u_z , (e) the polarization P_z averaged over a larger volume V_c and (f) over a smaller volume V_t . (g) The distribution of polarization in the cross section of the bilayer at moments of time numbered from 1 to 10 shown by the pointers in (a)–(f). The distribution of electric field at moments 1–10 is shown in Fig. S2 in the Supplemental Material [55]. Other parameters and conditions are the same as in Fig. 2.

time sweeps of the polarization z -component $\bar{P}_z^{\text{aver}}$ averaged over the volume of the computation cell, namely in the cylinder $\{0 \leq \sqrt{x^2 + y^2} < 4R, \quad 0 \leq z \leq h\}$ with the volume $V_c \cong 16\pi R^2 h$, are shown in panels (c). The butterflylike loops of $u_z(0, 0, t)$ are shown in panels (d). The ferroelectric hysteresis loops of the “average”

polarization $\bar{P}_z^{\text{aver}}$, averaged over the cell volume V_c , are shown in panels (e). The ferroelectric hysteresis loops of the “local” polarization $\bar{P}_z^{\text{local}}$ averaged over a small region under the tip, namely in the cylinder $\{0 \leq \sqrt{x^2 + y^2} < R, \quad 0 \leq z \leq h\}$ with the volume $V_t \cong \pi R^2 h$, are shown in panels (f). The distribution of

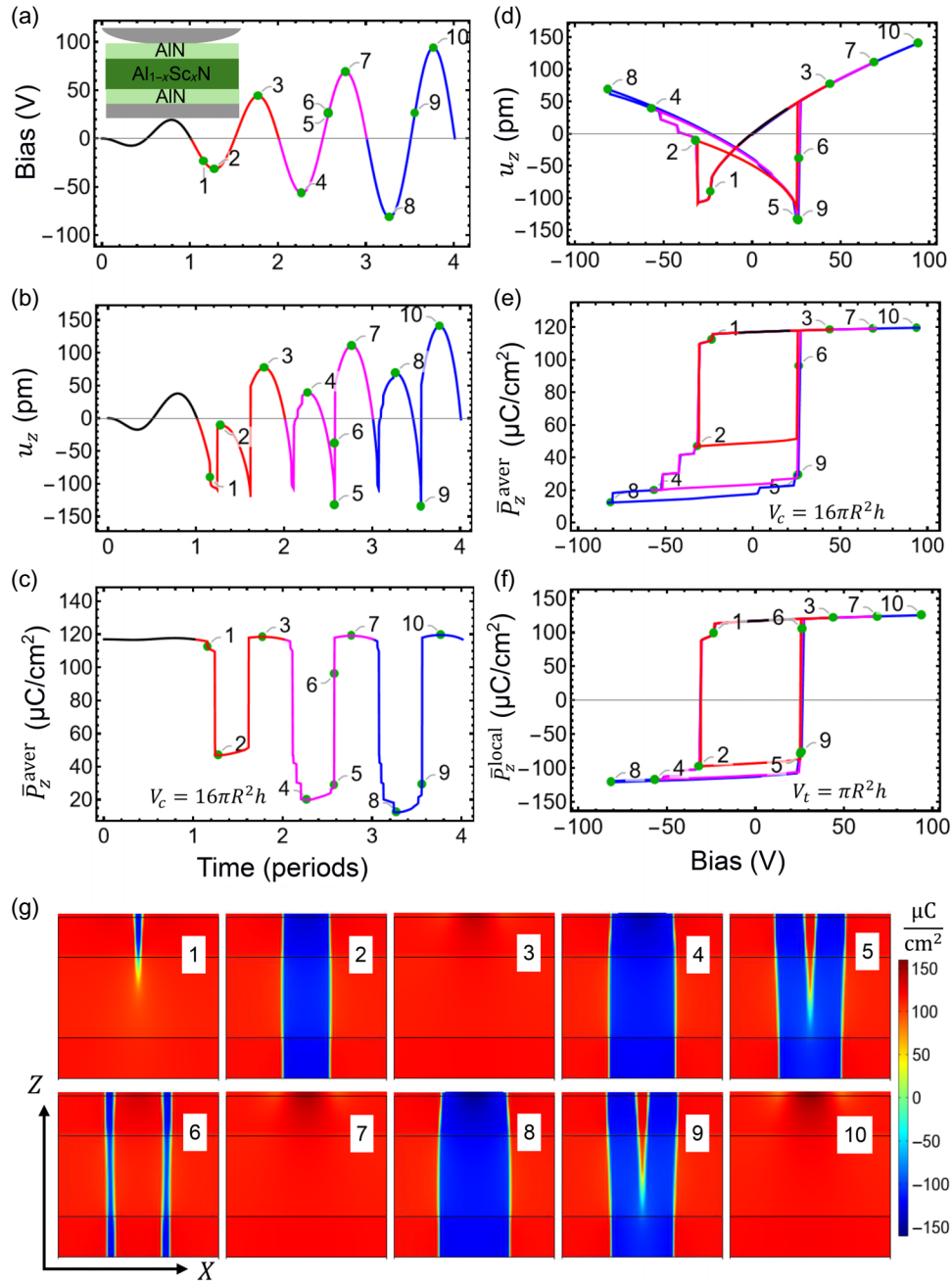


FIG. 4. Time dependences of (a) the bias applied between the PFM probe and the bottom electrode, (b) the vertical displacement u_z of the surface below the probe apex, and (c) the average polarization $\bar{P}_z^{\text{aver}}$ in the probe/AlN/Al_{0.73}Sc_{0.27}N/AlN three-layer/bottom electrode heterostructure. Bias dependences of (d) the surface displacement u_z , (e) the polarization $\bar{P}_z$ averaged over a larger volume V_c and (f) over a smaller volume V_t . (g) The distribution of polarization in the cross section of the three-layer at moments of time numbered from 1 to 10 shown by the pointers in (a)–(f). The thickness of the Al_{0.73}Sc_{0.27}N layer is 20 nm and the thickness of AlN layers is 10 nm. Other parameters and conditions are the same as in Fig. 2.

polarization z -component P_z in the cross section of the bilayers and three-layers at the moments of time numbered from 1 to 10 in panels (a) are shown in panels (g). The distribution of electric field at the moments 1–10 in the bilayers are shown in Figs. S1 and S2 in the Supplemental Material [55].

The local polarization reversal in bilayer and three-layer structures has several features, such as different positive and negative coercive bias, steplike features at the hysteresis loops, and proximity switching in the AlN layer(s), which are listed in Table III and discussed in detail below.

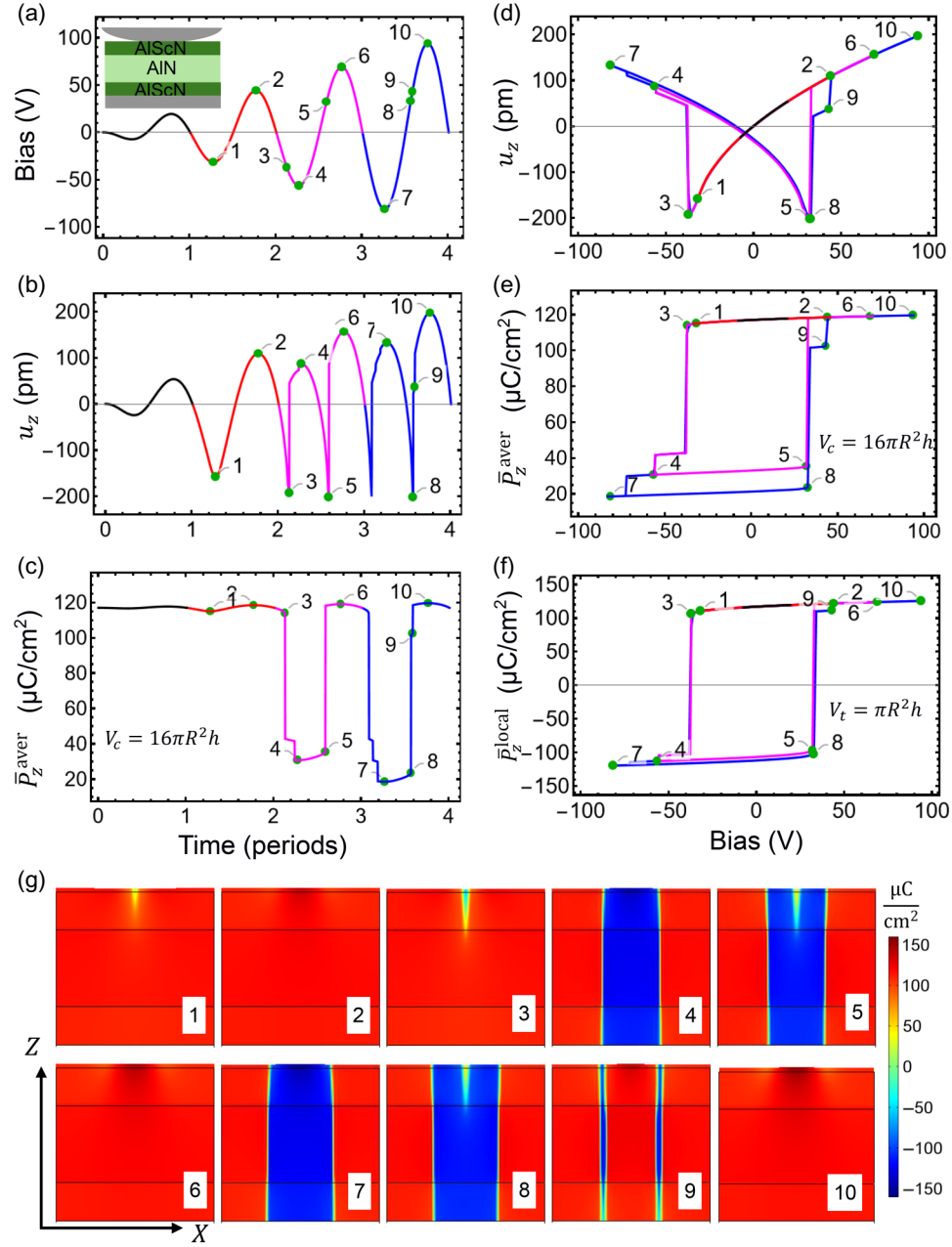


FIG. 5. Time dependences of (a) the bias applied between the PFM probe and the bottom electrode, (b) the vertical displacement u_z of the surface below the probe apex, (c) and the average polarization $\bar{P}_z^{\text{aver}}$ in the probe/ $\text{Al}_{1-x}\text{Sc}_x\text{N}/\text{AlN}/\text{Al}_{1-x}\text{Sc}_x\text{N}$ three-layer/bottom electrode heterostructure. Bias dependences of (d) the surface displacement u_z , (e) the polarization P_z averaged over a larger volume V_c and (f) over a smaller volume V_t . (G) The distribution of polarization in the cross section of the three-layer at moments of time numbered from 1 to 10 shown by the pointers in (a)–(f). The thickness of the $\text{Al}_{0.73}\text{Sc}_{0.27}\text{N}$ layers is 10 nm and the thickness of AlN layer is 20 nm. Other parameters and conditions are the same as in Fig. 2.

The small bias amplitude (below the coercive voltage) is insufficient to induce the local polarization reversal under the probe [see the black curves in panels (e) and (f) in Figs. 2–5]. Since the biased probe acts as a strong external charged defect, the switching of polarization is multidomain even in the absence of point charge or elastic defects, which are not considered in this work. When the probe

field overcomes the coercive field, the domain nucleus emerges under the probe and rapidly grows through the multilayer, leading to the switching within the smallest red loop nested inside the larger magenta and blue loops. The polarization loop opens with an increase in the bias amplitude [see magenta and blue loops in panels (e) and (f)]. When the probe bias increases further, the domain walls

TABLE III. Features of local polarization reversal in wurtzite multilayers.

Multilayer structure (figure number)	Positive and negative coercive biases (U_c^- and U_c^+) ^a ; loop width	Steplike features (observed in the bias range 0–100 V) ^b	Proximity switching effect in the AlN layer(s) (in dynamics)
AlN/Al _{1-x} Sc _x N $h_{\text{AlN}} = h_{\text{AlScN}} = 20$ nm (see Fig. 2)	$U_c^- \approx -23$ V, $U_c^+ \approx 21$ V, loop width ≈ 44 V	multiple steplike features are observed at negative bias	domain nucleation in the AlN layer and its vertical growth through the bilayer
Al _{1-x} Sc _x N/AlN $h_{\text{AlN}} = h_{\text{AlScN}} = 20$ nm (see Fig. 3)	$U_c^- \approx -45$ V, $U_c^+ \approx 32$ V, loop width ≈ 79 V	a single steplike features is observed	domain nucleation in the Al _{1-x} Sc _x N layer and its vertical growth through the bilayer
AlN/Al _{1-x} Sc _x N/AlN $2h_{\text{AlN}} = h_{\text{AlScN}} = 20$ nm (see Fig. 4)	$U_c^- \approx -31$ V, $U_c^+ \approx 25$ V, loop width ≈ 56 V	multiple steplike features are observed at negative bias	domain nucleation in the AlN layer under the probe and its vertical growth through the layers
Al _{1-x} Sc _x N/AlN/Al _{1-x} Sc _x N $h_{\text{AlN}} = 2h_{\text{AlScN}} = 20$ nm (see Fig. 5)	$U_c^- \approx -38$ V, $U_c^+ \approx 32$ V, loop width ≈ 70 V	several steplike features are observed at negative bias	domain nucleation in the Al _{1-x} Sc _x N layer under the probe and its vertical growth through the layers

^a U_c^- and U_c^+ are the negative and positive coercive biases corresponding to the red loops in Figs. 2–5.

^bThe direction of the spontaneous polarization in the layers determines the sign of the bias for which the pronounced steplike polarization response is observed. In the case considered the spontaneous polarization was directed upward in all layers when the bias was absent [see, for example, Fig. 1(e)].

start to move in the transverse direction; when the bias changes the sign, an oppositely polarized domain starts to grow inside the existing domain [see panels (g)]. We would like to emphasize that the upshift of $\bar{P}_z^{\text{aver}}$ loops, shown in panels (e), is conditioned by the polarization averaging over the large area $S_c \gg \pi R^2$; and the shift virtually disappears when the averaging is performed over the small tip-surface contact area $S_t \cong \pi R^2$ [see the loops of $\bar{P}_z^{\text{local}}$ in panels (f)]. Thus, the averaging of polarization over the whole computation cell V_c underestimates significantly the complete switching of polarization, which occurs under the probe tip [as shown by blue domains in panels (g)]. After the averaging over $V_c \gg \pi R^2 h$, it looks like the switching of polarization is always partial [see panels (e)], which is not the case under the probe [see panels (f)]. However, for the purposes of this work we also consider the polarization $\bar{P}_z^{\text{aver}}$ because it determines the charge density stored at the electrodes (since the latter is proportional to the volume-averaged electric displacement), as well as correlating with the behavior of the local piezoelectric response recorded by the PFM.

Indeed, the vertical surface displacement $u_z(0, 0, t)$ under the PFM tip, calculated at the point $x = y = 0$ without any averaging and shown in panels (d) in Figs. 2–5, responds to the changes of polarization in the area larger than $0 \leq \sqrt{x^2 + y^2} < R$, because elastic fields are very long range (as was shown using the decoupling approximation for PFM response [38]). The loops of u_z are strongly

asymmetric with respect to the initial state $u_z = 0$ (vertical asymmetry) as well as to the bias axis $U = 0$ (horizontal asymmetry). The asymmetry and steplike features of u_z [shown in panels (d)] correlate well with the asymmetry and features of the polarization hysteresis loops $\bar{P}_z^{\text{aver}}$ and $\bar{P}_z^{\text{local}}$ [shown in panels (e) and (f), respectively]. It is seen that the steplike features are the most pronounced at the hysteresis loops of $\bar{P}_z^{\text{aver}}$.

The steplike features at the hysteresis loops of u_z , $\bar{P}_z^{\text{aver}}$, and $\bar{P}_z^{\text{local}}$ are associated with the pairwise “annihilation” of domain walls being similar to Barkhausen jumps in ferromagnets [56] and Barkhausen pulses in ferroelectric-ferroelastics [57]. As can be seen from panels (g) in Figs. 2–5, the steplike features appear at the loops when the small domain, which grows inside the larger domain, reaches the boundaries of the larger domain. The steplike features are present at the loops independent of the initial polarization state, but the amount and position of the features depend on the initial state.

Note that the direction of the spontaneous polarization in the layers determines the sign of the bias for which the pronounced steplike polarization response is observed. In the case considered the ground-state spontaneous polarization was directed upward in all layers when the bias was switched off [see Fig. 1(e)]. Then the pronounced steplike polarization response was observed when a negative bias was applied. When the spontaneous polarization was directed downward in all layers, the pronounced steplike

polarization response was observed after a positive bias was applied. When the initial distribution of spontaneous polarization is a multidomain state with randomly small fluctuations, the steps can occur for positive and negative biases [compare Figs. S3(c) and S4(c) in the Supplemental Material [55]]. However, the multidomain state can be the ground state for incomplete screening conditions only.

Sometimes strongly up- or downshifted loops of local piezoresponse are observed experimentally (see, for example, Fig. 3 in Ref. [5]). It is worth noting that the character (upward or downward shift) and magnitude (large or small shift) of the vertical asymmetry of the $\bar{P}_z^{\text{aver}}$ hysteresis loops depend also on the initial state (single-domain or multidomain) of polarization in the layers and its direction (upward or downward) under the probe. For example, the $\bar{P}_z^{\text{aver}}$ loops are shifted upward when the initial state of polarization is single-domain, and the initial polarization is directed upward. The vertical shift becomes downward for the multidomain initial state of the polarization [compare Figs. 2(e) and 3(e) with Fig. S3(c) in the Supplemental Material [55]]. It is seen from Fig. S4(c) in the Supplemental Material [55] that it is possible to minimize the vertical and horizontal asymmetry of $\bar{P}_z^{\text{aver}}$ hysteresis loops by the appropriate choice of the initial multidomain polarization state. This result can be explained by considering that new domains may not arise from the multidomain initial state during the switching, since the switching occurs via the growth of existing domains. In addition, the internal depolarization field is suppressed due to the presence of domains [48,53], and, accordingly, the electric interaction between the layers is weaker.

B. Proximity effect of polarization switching in the wurtzite bilayers and three-layers

It is very important to note that we observe the proximity effect of the hysteresis loops shown in panels (f) in Figs. 2–5, discovered earlier by Skidmore *et al.* [1] for electroded films, including AlN/Al_{1-x}Sc_xN bilayers and three-layers. Indeed, the “otherwise irreversible” polarization of the AlN layer(s) switches simultaneously with the ferroelectric polarization of the Al_{1-x}Sc_xN layer(s). As can be seen from the images 1–10 in panels (g), proximity switching is observed in the AlN layers, where the ferroelectric nanodomains emerge and/or sprout.

Note that the proximity effect of polarization switching occurs via the nanodomain nucleation for the probe-electrode geometry, because the external electric field is localized under the biased PFM probe in the case considered. To understand the features of the proximity switching in the AlN/Al_{1-x}Sc_xN multilayers studied, one should consider that the local switching of polarization (as well as corresponding vertical displacement of the surface under the probe) occurs in six stages, which are described below using an example of the AlN/Al_{1-x}Sc_xN bilayer:

- *Pre-nucleation stage I.* The polarization switching does not occur at low voltages, only small local changes in polarization and surface displacement are observed [see image 1 in Fig. 2(g)]. The images labeled 4, 7, and 10 in Fig. 2(g) correspond to the same stage but for increasing applied bias.
- *Nucleation stage II.* When the bias exceeds the coercive value, a nanodomain nucleation appears between time moments 1 and 2, shown by the inset labeled “d.n.” in Fig. 2(g). Notably, the small nucleus rapidly transforms into the next stage. The time between moments 4 and 5 corresponds to the same nucleation stage as between 1 and 2, but realized for a larger applied bias. Note that the domain nucleus appears near the surface of the AlN layer under the probe, because the probe electric field is maximal in the spatial region [see Fig. 1(a)] and the direction of depolarization field favors the domain formation in this case [see Fig. 1(f)]. It should be emphasized that the domain nucleation becomes possible in the unswitchable AlN layer because its “effective” double-well ferroelectric potential is renormalized to lower the steepness of the switching barrier due to the proximity of the switchable Al_{1-x}Sc_xN layer [23]. The “agent” of the renormalization is the depolarization field, which is codirected with the spontaneous polarization of the Al_{1-x}Sc_xN layer and counterdirected with the spontaneous polarization of the AlN layer [see Fig. 1(f)], as thus the field favors the domain formation in the AlN layer.
- *Vertical growth stage III.* The nanodomain elongates, rapidly grows vertically through both layers, reaches the bottom electrode, and forms a cylindrical domain with uncharged domain walls [see images 2, 5, and 8 in Fig. 2(g)]. The stage is rapid, lasting for times comparable with a very small Landau-Khalatnikov (LK) relaxation time, due to the proximity effect. Note that the period of applied voltage is four orders of magnitude higher than the LK relaxation time in the considered case.
- *Lateral growth stage IV.* The cylindrical domain grows in the transversal direction with the bias increase [after time moments 2, 5, and 8 in Fig. 2(g)]. The transverse growth is very slow (comparable to hundreds of LK times) in comparison with the rapid vertical growth.
- *Back-switching stage V.* When the probe bias decreases, the domain size does not decrease at once due to the pinning effect associated with the finiteness of the numerical grid. Only when the bias changes sign and overcomes the critical value does a new domain nucleus appear inside the existing cylindrical domain [see images 6 and 9 in Fig. 2(g)].

- *Complete switching stage VI.* When the magnitude of the bias increases further, the walls of the “nested” domain collapse and complete switching occurs under the probe [see images 7 and 10 in Fig. 2(g)].

When changing the sequence of the layers, for instance when swapping the AlN and $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layers, the width of the hysteresis loop increases significantly (compare Fig. 3 with Fig. 2). Looking at the free energy form shown in Fig. 1(g), one might expect that the negative and positive coercive fields should be much higher for the AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ bilayer than the fields for the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN bilayer for the following reasons. The nucleus of a new domain arises under the surface of the layer that is in direct contact with the charged probe (because the probe electric field is maximal under the surface), which is the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer in the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN bilayer [see Fig. 3(g)] and the AlN layer in the AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ bilayer [see Fig. 2(g)]. Since the potential wells of the AlN are much deeper than that of $\text{Al}_{1-x}\text{Sc}_x\text{N}$, the nucleation threshold bias is expected to be smaller for $\text{Al}_{1-x}\text{Sc}_x\text{N}$. However, our calculations showed the opposite trend: we reveal that a significantly larger external probe bias is needed for domains nucleation in the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN bilayer in comparison with the bias for the AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ bilayer [see Table III and compare Figs. 2(e)–2(f) with Figs. 3(e)–3(f)].

This opposite trend is explained by the proximity effect [1] in the multilayers, being a direct consequence of the field inversion effect [such as shown in Fig. 1(f)]. Namely, the internal electric field depolarizes the “strong” nonferroelectric AlN layer with a large spontaneous polarization and polarizes the “weaker” ferroelectric $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer with a smaller spontaneous polarization [23]. When the z -component of the PFM probe electric field is opposite to the direction of the spontaneous polarization in the layers, the internal depolarization field will be either subtracted (in the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer) or added (in the AlN layer) to the external field. In conclusion, the coercive bias is smaller for the AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ bilayer than those in the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN bilayer. Note that the effective double-well LGD potential is changed by a proximity effect in both layers [23], and that the physical reason for the LGD potential change is the counterdirected depolarization field induced by the difference of the layer spontaneous polarizations.

This conclusion maintains its validity for the three-layers, AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN and $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$, whose local polarization reversal and effective piezoelectric response are shown in Figs. 4 and 5, respectively. The larger coercive biases and the wider polarization loop correspond to the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ three-layer (see Table III). Moreover, the features of the local polarization reversal and surface displacement

under the probe are very similar for the AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ bilayers and the AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN three-layers, as well as for the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN bilayers and the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ three-layers. This observation is valid because the total thickness of the AlN and $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layers is the same for the bilayer and three-layer structures (e.g., for the $h_1 = h_2 = 20$ nm for the cases shown in Figs. 1–5). However, the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ three-layer exhibits lower coercive biases compared to the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN bilayer (see Table III). This happens because the thickness of the top $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer in the three-layer is half that in the bilayer. Thus, the spikelike nanodomain, which nucleates under the probe apex, sprouts the half as thick layer of $\text{Al}_{1-x}\text{Sc}_x\text{N}$, where the direction of the “net” depolarization field precludes its growth. Then it penetrates to the thicker central AlN layer, where the depolarization field helps its further growth. When the nanodomain reaches the bottom $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer, where the depolarization field counteracts its growth again, its sizes are sufficiently large for the domain breakdown effect [38], and the lateral growth starts rapidly. Therefore, the coercive bias is mostly determined by the thickness of the top $\text{Al}_{1-x}\text{Sc}_x\text{N}$ and AlN layers. For the same reason the AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /AlN three-layers show higher coercive biases than the AlN/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ bilayers (see Table III). Here the thickness of the top AlN layer in the three-layer is half that in the bilayer. Thus, the nanodomain, that nucleates under the probe apex, sprout half of the thickness of AlN layer, where the direction of the “net” depolarization field stimulates its growth, then it penetrates to the thicker central $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer, where the depolarization field counteracts its further growth. Again, the coercive bias is mostly determined by the thickness of the top AlN and $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layers. Moreover, it can be shown that the “net” depolarization fields calculated in the ground state (at $U = 0$) are the same for the three-layers and bilayers [see Supplement S1 in the Supplemental Material [55]].

C. Size effect of the proximity switching in wurtzite multilayers

Figure 6 shows the hysteresis loops of local polarization $\bar{P}_z^{\text{local}}$, average polarization $\bar{P}_z^{\text{aver}}$, and surface vertical displacement u_z calculated when h_2 changes from 0 ($\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer) to h (AlN layer); recall that the condition of constant sum $h_1 + h_2 = h$ (e.g., for $h = 40$ nm) is valid. It is seen from the figure that the coercive bias increases from 20 to 30 V with increase in h_2 from 0 to 40 nm.

It is interesting that the steplike features, which are almost absent (for $h_1 \leq 10$ nm) or relatively small (for $10 \text{ nm} < h_1 \leq 20$ nm) at the hysteresis loops of $\bar{P}_z^{\text{local}}$, are much larger and/or more pronounced at the hysteresis loops of $\bar{P}_z^{\text{aver}}$. The position and size of the steplike features

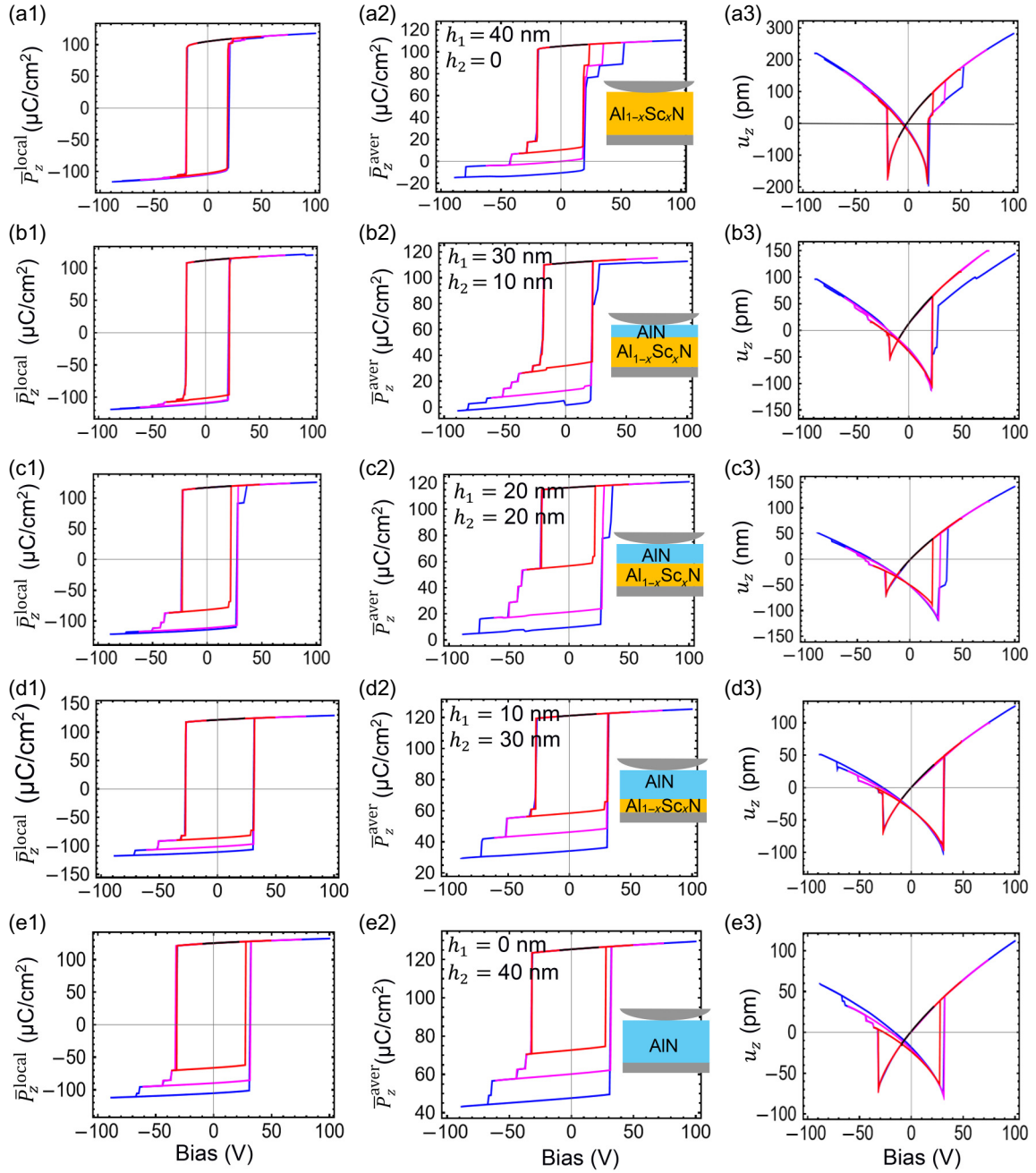


FIG. 6. Bias dependences of (a1)–(e1) the local polarization $\bar{P}_z^{\text{local}}$, (a2)–(e2) averaged polarization $\bar{P}_z^{\text{aver}}$, and (a3)–(e3) vertical surface displacement u_z in the probe/AlN/Al_{0.73}Sc_{0.27}N bilayer/bottom electrode heterostructure. Thicknesses h_1 of the Al_{0.73}Sc_{0.27}N layer and h_2 of the AlN layer are indicated on the plots (a2)–(e2). Other parameters and conditions are the same as in Fig. 2.

of $\bar{P}_z^{\text{aver}}$ and u_z correlate at positive biases. At the same time the position and size of the steplike features of $\bar{P}_z^{\text{local}}$ and u_z correlate at negative biases. This observation underscores the urgency to consider both polarizations, $\bar{P}_z^{\text{local}}$ and $\bar{P}_z^{\text{aver}}$, for the explanation of the u_z behavior.

It is worth noting that the negative and positive coercive biases are indifferent to the method of averaging, being the same for $\bar{P}_z^{\text{local}}$, $\bar{P}_z^{\text{aver}}$, and u_z loops (compare the first, second, and third columns in Fig. 6).

The coercive field of the 40-nm-thick AlN layer (about 7.5 MV/cm) is stronger than the field of electric breakdown (about 6 MV/cm). The average coercive field of the 40-nm-thick Al_{1-x}Sc_xN layer (about 5 MV/cm) is weaker than the breakdown field. Remarkably, both coercive fields calculated in the probe-electrode geometry are much weaker than the thermodynamic coercive fields in the capacitor geometry, which are 26 MV/cm for the AlN and 9.5 MV/cm for Al_{1-x}Sc_xN [23]. The coercive

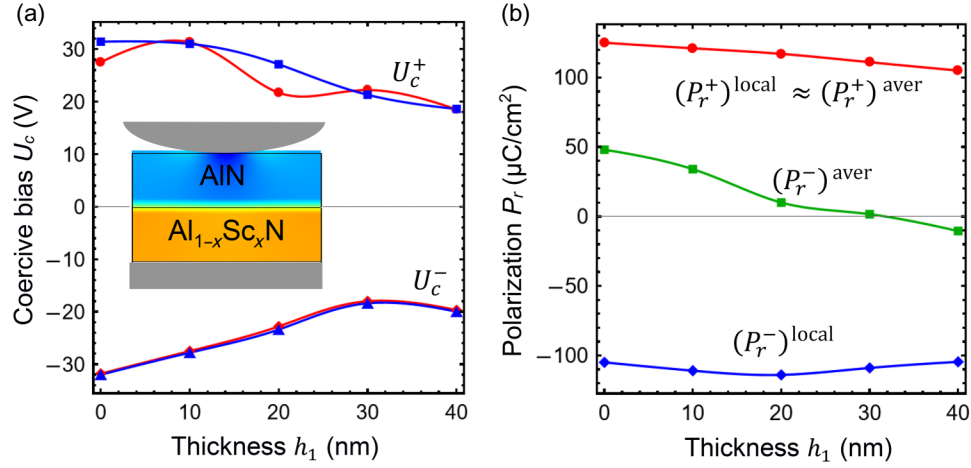


FIG. 7. (a) The thickness dependences of the left (U_c^-) and right (U_c^+) coercive biases in the probe/AlN/Al_{1-x}Sc_xN bilayer/bottom electrode heterostructure. Red and blue curves correspond to the red and blue loops in Fig. 6, respectively. Note that the coercive biases are the same for $\bar{P}_z^{local}$, $\bar{P}_z^{aver}$, and u_z . (b) The minimal (P_r^-) and maximal (P_r^+) values of remanent polarization in the same heterostructure. Red and blue curves correspond to the red and blue loops of $\bar{P}_z^{local}$, respectively, shown in Figs. 6(a1)–(e1). The green curve corresponds to the blue loops of $\bar{P}_z^{aver}$, shown in Figs. 6(a2)–(e2). The thickness h_1 of the Al_{0.73}Sc_{0.27}N layer changes from 0 to 40 nm; and the thickness h_2 of the AlN layer is $40 - h_1$. Other parameters and conditions are the same as in Fig. 2.

fields of the Al_{1-x}Sc_xN/AlN multilayers vary in the range 5–7.5 MV/cm depending on the layer thickness ratio h_1/h_2 for the fixed probe size ($R = 5$ nm in the case considered). The strong reduction of the coercive fields occurs in the probe-electrode geometry because the biased probe acts as an external charged defect. The external charged defect appeared strong in comparison with a point charged defects in the bulk (considered in Ref. [23]).

It is interesting that the coercive bias of the AlN/Al_{1-x}Sc_xN bilayers with $h_1 \geq 20$ nm is still about 20 V for the red hysteresis loops, which corresponds to a coercive field of about 5 MV/cm [see Figs. 6(a1)–6(c3)]. A visible increase in the coercive bias is observed at $h_1 \leq 10$ nm [see Figs. 6(d1)–6(e3)]. This observation allows us to conclude that the coercive biases (as well as other features of the local polarization reversal) depend nonlinearly on the thickness ratio h_1/h_2 . The nonlinear dependence of the loop parameters on layer thickness reflects the nonlinear origin of the proximity effect.

The dependences of the negative (U_c^-) and positive (U_c^+) coercive biases on the thickness h_1 can be analyzed from Fig. 7(a). Red and blue curves in the plot correspond to the red and blue loops in Fig. 6, respectively. Note that the coercive biases are almost the same for the loops of $\bar{P}_z^{local}$, $\bar{P}_z^{aver}$, and u_z . The dependences are nonlinear and tend to saturate at $h_1 > 30$ nm. The asymmetry of coercive biases and insignificant oscillations of the red curves originate from the steplike features at the hysteresis loops related with the jumplike changes in the domain structure under the probe. The negative coercive bias U_c^- is the same for red, magenta, and blue loops, while the positive coercive bias U_c^+ is a bit larger for the blue loop.

The thickness dependences of the minimal (P_r^-) and maximal (P_r^+) values of remanent polarization are shown in Fig. 7(b). Red and blue curves in the plot correspond to the red and blue loops of $\bar{P}_z^{local}$, and the green curve corresponds to the blue loops of $\bar{P}_z^{aver}$ in Fig. 6, respectively. The dependence of $(P_r^+)^{local}$ and $(P_r^-)^{local}$ on the thickness h_1 is relatively weak, while the dependence of $(P_r^-)^{aver}$ on the thickness h_1 is relatively strong. The difference in the thickness dependences of $(P_r^+)^{local}$ and $(P_r^-)^{aver}$ can be explained as follows: the magnitude of $(P_r^\pm)^{local}$ is mainly determined by the polarization distribution under the probe, and the magnitude of $(P_r^-)^{aver}$ is mainly determined by the polarization distribution far from the probe.

Above we considered bilayers and three-layers only. We expect that proximity ferroelectricity should exist in multilayers with the total thickness of otherwise nonswitchable layers comparable to or smaller than the total thickness of switchable layers. In this case the size effect of proximity switching depends on the thickness ratio of the individual layers h_1/h_2 , on the total thickness h , and on the tip-surface contact radius R . In particular, if the total thickness of the four-layer system is fixed (e.g., 40 nm as above), and one considers four alternating 10-nm layers, the behavior of local and average polarization will look very similar to those of three-layer system, but the horizontal asymmetry of the loops and the dependence of coercive biases on the sequence of the layers under the probe will be smaller. This happens because the probe field in the second and third layers of the four-layer system is larger than in the case of three-layer system. Next, if we consider, for example, an ten-layer system with total thickness $h = 40$ nm and

4-nm-thick alternating AlN and AlScN layers, the dependence of coercive biases on the sequence of the layers under the probe becomes very small for $R = 5$ nm, because $h_i < R$ and the difference in the probe field is small in the two upper layers. The conditions $h_i \ll R$ and $h \gg R$ lead to symmetric proximity-induced polarization switching in the multilayer, and we postpone consideration of this case to further study.

IV. SUMMARY

Using the LGD thermodynamic approach, we explored the proximity effect of local piezoelectric response and polarization reversal in wurtzite ferroelectric multilayers. We analyze the probe-induced nucleation of nanodomains, the features of local polarization hysteresis loops, and coercive fields in the $\text{Al}_{1-x}\text{Sc}_x\text{N}/\text{AlN}$ bilayers and three-layers. The regimes of “proximity switching” (where the multilayers collectively switch) and “proximity suppression” (where they collectively do not switch) are the only possible regimes in the probe-electrode geometry. This result is reminiscent of the case of wurtzite multilayers sandwiched between flat electrodes.

We predict that the coercive bias, horizontal asymmetry, and steplike features of the local polarization and piezoresponse hysteresis loops depend significantly on the sequence of the layers with respect to the probe. We find that the negative and positive coercive biases (and hence the loop width) are significantly smaller when the AlN layer is under the probe. This result is explained by the proximity effect in the multilayers, being a direct consequence of the field inversion effect. The physical mechanism of the proximity ferroelectricity in the local probe geometry is a depolarizing electric field determined by the polarization of the layers and their relative thickness in a self-consistent manner. Namely, the internal electric field, whose direction is “inverted” in the layer(s) with the larger spontaneous polarization, depolarizes the nonferroelectric AlN layer with a large spontaneous polarization and polarizes the ferroelectric $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer with a smaller spontaneous polarization. Thus, the depolarization field renormalizes the double-well ferroelectric potential to lower the steepness of the switching barrier in the nominally “unswitchable” polar layers and hence reduces the coercive field.

The coercive fields calculated by FEM in this work in the probe-electrode geometry, are much smaller than the thermodynamic coercive fields calculated earlier in the capacitor geometry [23]. In accordance with our calculations, the coercive field of the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer (about 5 MV/cm) is weaker than the breakdown field. The coercive field of the AlN layer (about 7.5 MV/cm) is stronger than the field of electric breakdown (about 6 MV/cm). The coercive fields of the $\text{Al}_{1-x}\text{Sc}_x\text{N}/\text{AlN}$ multilayers vary in the range 5–7.5 MV/cm, dependent on the layer thickness

ratio h_1/h_2 for the fixed probe size of approximately 5 nm. The strong reduction of the coercive fields occurs in the probe-electrode geometry because the biased probe acts as an external charged defect, whose strength, with an increase in bias increase, is comparable to or higher than that of the point charge defects located in the bulk of the layers. The ability of the tip-based proximity switching to differentially switch multilayers, based on the order of the layers, provides a powerful tool for selective domain engineering. The ability to locally pattern domain structures in previously unswitchable ferroelectrics such as AlN by exploiting the proximity effect in combination tip-based switching techniques opens up avenues for domain-based nanoengineered ferroelectric devices for memory, actuation, and nonlinear optics.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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