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In-Plane Ferroelectric Tunnel Junction

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Ferroelectric materials are an important platform for the realization of nonvolatile memories. So far, existing ferroelectric memory devices have utilized out-of-plane polarization in ferroelectric thin films. In this paper, we propose a type of random-access memory (RAM) based on ferroelectric thin films with in-plane polarization, called an “in-plane ferroelectric tunnel junction.” Apart from nonvolatility, lower power usage, and a faster writing operation compared with traditional dynamic RAMs, our proposal has the advantage of a faster reading operation and a nondestructive reading process, thus overcoming the write-after-read problem that exists widely in current ferroelectric RAMs. The recent discovered room-temperature ferroelectric IV-VI semiconductor thin films are a promising material platform for the realization of our proposal.

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I. INTRODUCTION

To meet the daily increasing demands of modern electronic devices, especially those of portable devices, memories with a low energy consumption and high performance are highly desirable. The current commercial dynamic random-access memories (DRAMs) are volatile and consume a large amount of energy to refresh the stored data in order to prevent leakage from the capacitor. To reduce the energy consumption, a nonvolatile memory might be the ultimate solution [1,2].

Ferroelectric materials have been proposed as ideal candidates for nonvolatile memories due to their electric switchable bistable ground states since 1952 [3] and ferroelectricity-based nonvolatile memories have been developed rapidly over recent decades [4,5].

Depending on the readout mechanism, ferroelectric nonvolatile memories can be roughly classified into two generations. The first generation of ferroelectric RAM (FERAM) uses polarized charges in the ferroelectric capacitor to represent the data [6–8]. As a result, discharging the capacitor to measure the polarized charge destroys the stored data and the capacitor needs to be recharged after the reading operation. Limited by the destructive reading process, the ferroelectric size effects [9,10], and various practical issues such as fatigue [11] and imprint [12], the market for FERAMs remains relatively small.

To overcome the destructive readout problem, a second generation of ferroelectric tunnel junctions (FTJs) has been proposed to probe the ferroelectric polarization using the tunneling-electroresistance effect [13–15]. The basic structure of the FTJ is a metal-ferroelectric-metal junction, where the tunneling potential barrier is determined by the out-of-plane polarization in the ferroelectric layer. In this way, the FTJ realizes bistable resistance states. The major challenge of realizing an FTJ is to fabricate ultrathin ferroelectric films so that the tunneling current surpasses the threshold of the peripheral amplifiers. The depolarization field induced by the out-of-plane polarization dramatically suppresses the ferroelectric critical temperature or even destroys the ferroelectricity when the films are too thin [16–19].

In this work, we propose a type of ferroelectric memory that we call an “in-plane ferroelectric tunnel junction.” Unlike FERAMs or FTJs, which employ bistable states of out-of-plane ferroelectric polarization to represent “on” and “off”, our proposal is based on the in-plane polarization of ferroelectric thin films. Due to the insufficient screening in two dimensions, the in-plane polarization could induce strong band bending around an interface such as the material edge or the ferroelectric-domain wall. Depending on the polarization direction, the upward or downward band bending could be used to represent the on or off state respectively. By measuring the out-of-plane tunneling current through ferroelectric thin films, the bending direction can be detected and hence the stored information can be read nondestructively. Moreover, our design enjoys great tunability. By choosing proper layer sizes and the insulator-layer band gap, the tunneling current and the on:off current ratio can be tuned simultaneously. In principle, all ferroelectric thin films with in-plane polarization can be used as the material platform to realize our
The paper is organized as follows. We first introduce in-plane ferroelectric polarizations and the induced robust band bending. We then demonstrate the device design and explain its reading and writing mechanism in detail. The demonstration is supported by the quantum-mechanical tunneling-current simulation. Finally, we discuss the advantage of our design over conventional ferroelectricity-based memories.

II. IN-PLANE POLARIZATION

Ferroelectricity as a symmetry-breaking state is generally destabilized by the finite-size effect. The out-of-plane ferroelectric polarization is found in perovskite ultrathin films, in which imperfect charge screening, substrate strain, and chemical bonding play important roles in stabilizing the ferroelectricity [31–36]. As already mentioned in Sec. I, the critical temperature of these perovskite ferroelectric materials decreases with the film thickness. On the other hand, in-plane polarization in perovskite thin films [20–23] and even liquid crystals [24] has been studied. Although it is predicted that in-plane polarization will survive in the two-dimensional (2D) limit [19], it is currently hard to prepare free-standing 2D perovskite ferroelectrics.

Surprisingly, the recently discovered in-plane polarization in 2D ferroelectrics is enhanced instead of reduced in thin films [25,27–30]. For example, in SnTe, compared with the bulk-ferroelectric transition temperature of 98 K, the one-monolayer (ML) thin film has a critical temperature of 270 K, and thicker 3-ML films show robust spontaneous polarization even at room temperature [25,26]. Moreover, the weak van der Waals interlayer coupling enables more freedom in device design as, in principle, 2D materials can be stacked freely without the constraint of lattice mismatching.

An important signature of in-plane polarization is the band bending near an interface such as the material edge [25] or the ferroelectric-domain wall [37]. Taking the material edge as an example, without screening, the bound charges induced by the in-plane ferroelectric polarization \( \sigma_b = P \cdot n \) are of opposite signs at the two boundaries, where \( P \) is the polarization vector and \( n \) is the normal vector of the boundary. The resulting electric field leads to a linear band tilting in three dimensions and a logarithmic one in two dimensions, where the energy decreases from the negatively charged boundary to the positively charged boundary. When free charge carriers are present, which could be contributed by the substrate or could arise from defects in the ferroelectric material, the screening effect cancels the boundary charge, so that only the band bending near the boundary remains. In the following, we consider ferroelectric materials with a large band gap, so that the free charge carriers are from the metallic substrate. Due to the insufficient screening in two dimensions, the band bending can extend over quite a region (typically several nanometers) near the interface. For example, the scanning-tunneling-microscopy-measured band bending near the boundary of 1-ML SnTe film can be fitted nicely by an exponential function \( V = a e^{-y/\lambda} + c \) [25], which is sketched in Fig. 1. SnTe thin films with an odd number of monolayers all share similar band-bending profiles. We emphasize that this band bending near the interface generally exists for all ferroelectric thin films with in-plane polarization and does not depend crucially on material details.

III. DEVICE DESIGN

The robust band bending induced by in-plane polarization motivates us to propose a type of nonvolatile memory. The schematic of the device is shown in Fig. 2(a). The core of the design is a ferroelectric thin film sandwiched by a metallic substrate and a wide-band-gap insulator. The writing and reading electrodes are deposited at two different edges of the top insulator, which is (mostly) parallel to the polarization direction. In the figure, the in-plane polarization is assumed to be along the \(+y\) direction, which will induce opposite net charges at different boundaries. Depending on the polarization direction (\(+y\) or \(−y\)), the band bending near the reading electrode could be upward or downward, the mechanism for which has already been discussed in the previous paragraph. The band diagrams near one of the electrodes are shown in Figs. 2(b) and 2(c), where the chemical potential is set to be near the valence band.

To write the information or manipulate the polarization direction, one can apply a writing voltage \( \pm V_{\text{w}} \) on the
To read the information or measure the polarization direction, one can apply a reading voltage $V_R$ on the reading electrode with reference to the metallic substrate and measure the tunneling current. The tunneling current depends on the band bending and hence the polarization direction. More specifically, if the chemical potential is near the valence or the conduction band, respectively, the charge carriers can be holes or electrons. In the case of hole charge carriers, the tunneling current in the “on” state $I_{on}$, where the band bends upward near the reading electrode, is significantly larger than that in the “off” state $I_{off}$, where the band bends downward. This is illustrated in Figs. 1(a)–1(c). In the case of electron charge carriers, the downward bending represents the “on” state and the upward bending represents the “off” state, as shown in Fig. 1(b). Since the electric field generated by the reading voltage is perpendicular to the polarization, the reading process is nondestructive. Note that no capacitor discharge is involved in this process: the time cost of the reading operation is almost solely determined by the peripheral-current-measurement device.

IV. THE TUNNELING CURRENT

We now turn to a detailed study of the tunneling-electroresistance effect between the metallic substrate and the reading electrode. Without loss of generality, we assume that the Fermi level of the metal is close to the valence band of the ferroelectric film. If the band bending is upward and sufficiently strong, the valence-band edge will be higher than the Fermi level of the metal, making the ferroelectric thin film conducting. In this case (the “on” state), the tunneling happens between the metallic substrate and the ferroelectric thin film and the reading electrode [Fig. 2(b)]. It is worth noting that the above discussion also works for the scenario of downward band bending if the Fermi level in the metal is close to the conduction band of the ferroelectric film and a parallel computation is presented in Ref. [42]. On the other hand (the “off” state), downward band bending makes the ferroelectric thin film insulating. The tunneling then happens between the metallic substrate and the reading electrode [Fig. 2(c)]. In this way, the threshold voltage for the “on” state is determined by the band gap and the thickness of the insulator, while the on/off ratio $I_{on}/I_{off}$ is determined by the band bending and the thickness of the ferroelectric thin film.

To make the above intuitive argument more concrete, we compute the tunneling current in a metal-ferroelectric-insulator-metal junction using the two-terminal Landauer formula:

$$I = \frac{2e}{h} \int_{-\infty}^{\infty} T(E) \left[ f_L(E) - f_R(E) \right] dE = \frac{2e}{h} \int_{0}^{U} T(E) dE,$$

(1)

where $T(E)$ is the transmission coefficient of the tunnel junction, and $f_L(E)$ and $f_R(E)$ are the Fermi-Dirac distribution functions at the left and right terminals, respectively.
where \( T(E) \) is the transmission probability and \( f_{L/R}(E) = \left[ e^{-(E-\mu_{L/R})/k_B T} + 1 \right]^{-1} \) is the Fermi-Dirac distribution function. \( \mu_L \) and \( \mu_R \) are the chemical potentials of the left and the right electrodes, respectively. In the following, we always set \( \mu_L = 0 \) as the reference. At zero temperature, \( f_{L/R}(E) \) becomes the step function and Eq. (1) reduces to its final form, where \( U \equiv \mu_R - \mu_L \) is the voltage bias.

The geometry of the system is taken to be the same as the device design in Fig. 2, where from the \(-z\) to \(+z\) there are, in order, the left metal electrode (substrate), the ferroelectric, the insulator, and the right metal electrode (reading electrode). The dimensions are \( X \times Y \times Z \). Here, \( Z = d_{FE} + d_f \), where \( d_{FE} \) and \( d_f \) are the thicknesses of the ferroelectric and the insulator film, respectively.

Inside the junction, the electrons and the holes are governed by the Schrödinger equation:

\[
\left[ -\frac{\hbar^2}{2m^*} \nabla^2 + V(x,y,z) \right] \psi = E \psi. \tag{2}
\]

The potential barrier of the ferroelectric \( V(x,y,z) \) is modeled by the fitted potential of 1-ML SnTe thin film [25,43]. The potential of the insulator \( V(x,y,d_{FE} \leq z < d_{FE} + d_f) \) is modeled by a square potential of monolayer hexagonal boron nitride [44]. All of the calculation details, including the parameters, can be found in Ref. [42].

Due to the complicated shape of the potential, the transmission probability in Eq. (1) is computed numerically using the Kwant software package [45], based on the discretized version given in Eq. (2). Both of the tunneling-current contributions from the electrons and the holes are taken into account. The results are summarized in Fig. 3. Since the magnitude of the tunneling current and the on:off ratio are two quantities that determine the sensitivity and the accuracy of the peripheral-current-measuring device, we mostly focus on them.

We first discuss the voltage-current characteristics [Fig. 3(a)]. When the reading voltage is very small, the current of the “on” state and that of the “off” state both come from the tunneling. With an increase in the voltage, there is first a threshold in the “on” state, after which \( V > V_{on} \) and Ohm’s law \( I \propto U \) governs. The threshold voltage of the “off” state \( V_{off} \) is larger than that of the “on” state. In Fig. 3(a), \( V_{on} \approx 0.1 \) V and \( V_{off} \approx 0.4 \) V. When the voltage is in between the two threshold voltages, i.e., \( V_{on} < V < V_{off} \), a very large on:off ratio decreases exponentially with an increase in the voltage. In order to maximize the on:off ratio, it is important for the bias voltage to be within this “sweet spot.”

From a device design point of view, the on:off ratio and the size of the “sweet spot” \( V_{off}/V_{on} \) can be enhanced by increasing the \( d_{FE}/d_f \) ratio, as shown in Fig. 3(b). This can be understood from our intuitive argument before—the difference between the tunneling region of the “on” state and that of the “off” state is the ferroelectric film. This result suggests that the thickness of the insulator film \( d_f \) should be small, but still large enough to prevent the electric discharge between the electrodes. Note that for a fixed total thickness, increasing \( d_{FE}/d_f \) also increases the magnitude of the “on”-state current significantly. The on:off ratio can be as large as about 1000 for \( d_{FE}/d_f = 6/1 \).

The magnitude of the “on”-state current after the threshold \( V > V_{on} \) can be enhanced simply by increasing the width of the device in the \( x \) direction. As shown in Fig. 3(c), \( I_{on} \) increases linearly with \( X \) because the number of modes per unit energy in the electrode also grows linearly. It is also possible to increase the current magnitude by decreasing the band gap of the insulator layer \( \Delta_t \) [Fig. 3(d)]. Note that for both approaches, the on:off ratio is almost unaffected, implying an independent control of the “on”-state current and the on:off ratio.

We emphasize that although Fig. 3 is computed using the parameter of SnTe, the qualitative conclusion is independent of the material. The device design and the transport model are completely general and are applicable to any nanoplates or even nanodots with in-plane ferroelectricity, where the band bending can be both upward or downward, located at the material edge or the ferroelectric-domain wall, and the charge carrier can be both electrons or holes.

V. CONCLUSION

In conclusion, we propose a type of ferroelectric memory based on in-plane polarization. Compared with the DRAM or the out-of-plane-polarization-based FERAM, our design has advantages including nonvolatility, a nondestructive reading operation, a faster reading and writing operation, and greater tunability of the tunneling current.
and the on:off ratio. Our design is based on a ferroelectric thin film with an in-plane polarization component that is switchable by an external electric field. Compared with FTJs, in thin films the in-plane polarization is much more robust. The 2D nature of the material, i.e., the weak van der Waals interlayer coupling, makes the device easy to fabricate. In particular, boundary effects caused by lattice mismatching can be reduced greatly if the device is fabricated by stacking 2D materials [46,47].

A wide family of materials, for example, the IV-VI semiconductors \(XY\), where \(X = Ge, Sn, Pb\) and \(Y = S, Se, Te\), along with their alloys (e.g., \(Pb_xSn_{1-x}Te\) and \(Pb_xSn_{1-x}Se\)) and superlattices (e.g., \(PbTe/SnTe\)), are ideal candidates for the realization of our proposal [25,48–52]. Although \(SnTe\) nanoplates grown by molecular-beam epitaxy (MBE) are not scalable at the moment, we believe that as more 2D ferroelectrics are being discovered, 2D ferroelectrics that can grow with uniform crystalline orientations will soon be found. For example, it has already been found that \(In_2Se_3\) has in-plane polarization and can be grown by both MBE and chemical-vapor deposition (CVD) [27–30]. We hope that our design can open up a new direction for ferroelectric nonvolatile memories.

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