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## Effect of ferroelectric parameters on ferroelectric diodes

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We investigate the effect of various ferroelectric parameters, such as the doping density, the permittivity, and the thickness, on ferroelectric diodes based on the proposed self-consistent numerical model. Our calculations clarify the dependence of the band diagrams, the charge density distributions, and the  $I$ - $V$  curves on these important ferroelectric parameters in metal/ferroelectrics/metal structures. The calculated results reveal that the ON/OFF ratio of the ferroelectric diodes decreases with the increase of the doping density, the permittivity, and the thickness in the ferroelectric film, respectively. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.3692769>]

### I. INTRODUCTION

The nonvolatile random access memory based on resistive switching is one of the most promising candidates to replace the conventional memory devices and has recently sparked considerable physical and engineering interests.<sup>1</sup> Nevertheless, various recent investigations prove that the possible underlying physical origin of the resistive switching in non-ferroelectric oxides is associated to the migration of the oxygen vacancies under an applied large enough electric field,<sup>2</sup> indicating the potential disadvantages for the precise control of conduction properties.<sup>3</sup> On the contrary, ferroelectric diodes are on the basis of the reversible spontaneous polarization, where the ferroelectric thin film is sandwiched between two electrodes to form a simple metal/ferroelectrics/metal structure (MFM),<sup>4</sup> surmounting undesirable disadvantages of ferroelectric capacitive memories.<sup>5</sup> They might thus have the higher potential to develop as the next generation of nonvolatile memory devices,<sup>6</sup> making researches in this field more than intriguing.

In the past decades, great efforts have been devoted to the ferroelectric diodes due to their potential device applications.<sup>7–10</sup> Recently, Choi *et al.* reported a novel switchable diode effect in the BiFeO<sub>3</sub> (BFO) bulk ferroelectric diode.<sup>11</sup> Many further studies on the BFO film ferroelectric diodes have confirmed that the forward conduction direction in ferroelectric diodes is completely governed by the polarization direction and the polarization dominates the switchable diode effect.<sup>3,12,13</sup> In our recent work, we have proposed a self-consistent numerical model, which can well describe the switchable diode effect in ferroelectric diodes.<sup>14</sup> Then we theoretically revealed the important role played by the polarization-modulated barrier, and clarified the influence of the electrodes on ferroelectric diodes.<sup>14</sup> However, it is important to reveal the effect of some important ferroelectric parameters on the switchable diode effect, to further understand the switchable diode effect and improve the performance of ferroelectric diodes. In this paper, we perform numerical calculations based on our self-consistent model,

and focus on the effect of the doping density, the permittivity and the thickness in the ferroelectrics. It is highly expected that our calculations will be helpful in giving insight into the underlying physical origins in the switchable diode effect and promoting the further designing of ferroelectric memory devices.

### II. MODEL AND METHOD

We consider a one-dimensional MFM structure as shown in the schematic diagram Fig. 1, where NP, RP, and LP denote the states of non-polarization, right polarization, and left polarization, respectively. It is appropriate to treat ferroelectric thin films as semiconductors with a large bandgap instead of good insulators, in order to quantitatively describe the characteristics of ferroelectric devices.<sup>15</sup> For simplicity, we treat the ferroelectrics as a single domain structure and only consider the electron transport. The fundamental equations are as follows<sup>14</sup>:

$$\frac{d^2\phi(x)}{dx^2} = -\frac{e}{\varepsilon(x)}\rho(x), \quad (1)$$

$$\frac{1}{e} \frac{dj(x)}{dx} - R(x) = 0, \quad (2)$$

$$j(x) = \frac{\sigma(x)}{e} \frac{d\kappa(x)}{dx}, \quad (3)$$

$$\sigma(x) = e\mu(x)n(x), \quad (4)$$

where  $x$  is the spatial coordinate,  $e$  denotes the elementary charge.  $\phi(x)$ ,  $\varepsilon(x)$ ,  $\rho(x)$ ,  $j(x)$ ,  $R(x)$ ,  $\sigma(x)$ ,  $\kappa(x)$ ,  $\mu(x)$ , and  $n(x)$  represent the electrostatic potential, the dielectric constant, the charge density, the current density, the recombination rate, the conductivity, the electrochemical potential, the mobility and the electron density, respectively. For metals, we employ the well-known free electron model and Thomas–Fermi approximation.<sup>16</sup> Then, the electrochemical potential of the metal  $\kappa_m(x)$  is given by<sup>17</sup>

$$\kappa_m(x) = \frac{\hbar^2}{2m} [3\pi^2 n_m(x)]^{2/3} - e\phi(x), \quad (5)$$

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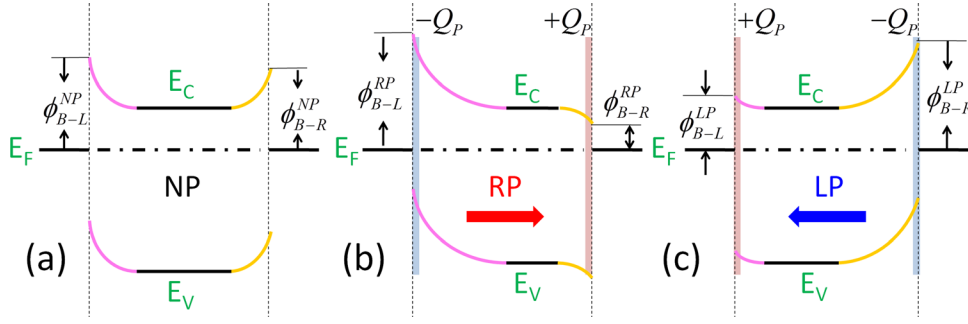


FIG. 1. (Color online) The schematic band diagrams of ferroelectric diodes under short circuit conditions in the case of non-polarization (NP) (a), right polarization (RP) (b), and left polarization (LP) (c). The arrow denotes the direction of the polarization.  $Q_P$  is the polarization charge;  $\phi_{B-L}$  and  $\phi_{B-R}$  are the left and right barrier heights, respectively.

where  $\hbar$  is the reduced Planck's constant, and  $m$  denotes the effective electron mass. For ferroelectrics, the electrochemical potential  $\kappa_f(x)$  reads as

$$\kappa_f(x) = kT \ln \left[ \frac{n_f(x)}{N_c} \right] + E_c - e\phi(x), \quad (6)$$

where  $k$ ,  $T$ , and  $E_c$  is Boltzmann constant, temperature, and the bottom of conduction band, respectively. The effective density of states  $N_c$  is expressed as  $N_c = 2(m_f kT / 2\pi\hbar^2)^{3/2}$ , where  $m_f$  represents the electron effective mass of the ferroelectrics.

For the modeling of the transport property, appropriate boundary conditions have to be defined. In our model a simple approach is adopted in which the ferroelectric polarization is regarded as an infinite thin sheet of charges located at the interfaces. Thus, the electrostatic properties at the interface can be characterized by the interface charge density  $\sigma$ , induced by the ferroelectric polarization  $P$ <sup>18</sup>:

$$\epsilon_f \epsilon_0 \frac{d\phi(x)}{dx} \Big|_{X_l^+} - \epsilon_m \epsilon_0 \frac{d\phi(x)}{dx} \Big|_{X_l^-} = -\sigma(X_l) = P, \quad (7)$$

$$\epsilon_m \epsilon_0 \frac{d\phi(x)}{dx} \Big|_{X_r^+} - \epsilon_f \epsilon_0 \frac{d\phi(x)}{dx} \Big|_{X_r^-} = -\sigma(X_r) = -P, \quad (8)$$

where  $X_l$  and  $X_r$  denote the positions of the left and right interfaces, respectively. A simple boundary condition is employed to solve the continuity equation<sup>17</sup>:

$$\kappa(x) = \text{continuous}. \quad (9)$$

An analytical solution to the set of Eqs. (1)–(6) is hardly obtained coupled with the boundary conditions Eqs. (7)–(9). Hence, we solve these equations self-consistently using the numerical method. For doing that, the standard finite difference method<sup>19</sup> is applied to discretizing these equations. The system is solved for the primary variables the electric potential  $\phi(x)$  and the electrochemical potential  $\kappa(x)$  by the iterative technique.

### III. RESULTS AND DISCUSSION

As an example, we consider a model system under short-circuit conditions as exhibited in Fig. 1. The length of the whole system is set as 300 nm, and the thickness of the metal electrode is taken as 30 nm. A forward bias is defined

as the positive voltage applying to the left electrode. Here the left and right metals are taken the same. The static dielectric constants contributed by bound electrons in metals are on the order of 1–10,<sup>20,21</sup> and a small dielectric constant 2.3 is taken in our calculations. According to Ref. 16 typical values of the electron concentration and mobility for metals are of the order of  $10^{22} \text{ cm}^{-3}$  and dozens of  $\text{cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ , respectively. Without loss of generality,  $10^{22} \text{ cm}^{-3}$  and  $60 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  are assumed as the electron density and mobility for the electrodes. It is assumed that the doping density  $N_d = 1 \times 10^{17} \text{ cm}^{-3}$ , the mobility  $\mu_s = 5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ , the permittivity  $\epsilon_f = 50$ , and the polarization  $P = \pm 30 \text{ } \mu\text{C}/\text{cm}^2$  in the ferroelectrics. In this paper, the positive and negative polarization values are defined to be RP and LP, respectively. The electrochemical potential of the metal without external bias is set as the zero point of the energy band, and the electrochemical potential of the ferroelectrics is  $\sim 0.1 \text{ eV}$ .

Figure 2 shows the calculated band structures, electron density distributions, and  $I$ – $V$  curves under NP, RP, and LP.<sup>14</sup> In the case of NP, electrons will flow into metals once the semiconductor is connected with the metal, then Schottky barriers will be built up. In the case of RP, positive polarization charges exist at the right interface, giving rise to the band bending toward the electrochemical potential, whereas negative polarization charges emerge at the left interface, inducing the band bending away from the electrochemical potential. In the case of LP, the band structure will be reversed compared with that of RP. Therefore, the polarization can modulate the interface barrier, and the forward conduction of ferroelectric diodes can be reversed with the polarization reversal.<sup>14</sup> Then, two resistance states “ON” and “OFF” are acquired. To put it differently, the two binary states of the intrinsic switchable ferroelectric polarization can be probed by a change in resistance, which is the operating principle of ferroelectric resistive memories.

Moreover, we study the dependence of the band structures, the electron density distributions and the  $I$ – $V$  curves on the doping density in the ferroelectrics under RP. As shown in Fig. 3(b), an electron accumulation layer can be formed at the right interface, whereas an electron depletion region can be formed at the left interface for  $10^{17} \text{ cm}^{-3}$  under RP. With the decrease of the donor doping density, for  $10^{16} \text{ cm}^{-3}$ , the band diagram is rather like that of insulators as illustrated in Fig. 3(a). The depletion region length in the ferroelectrics is longer than that of  $10^{17} \text{ cm}^{-3}$ . The current is smaller than that of  $10^{17} \text{ cm}^{-3}$  as shown in

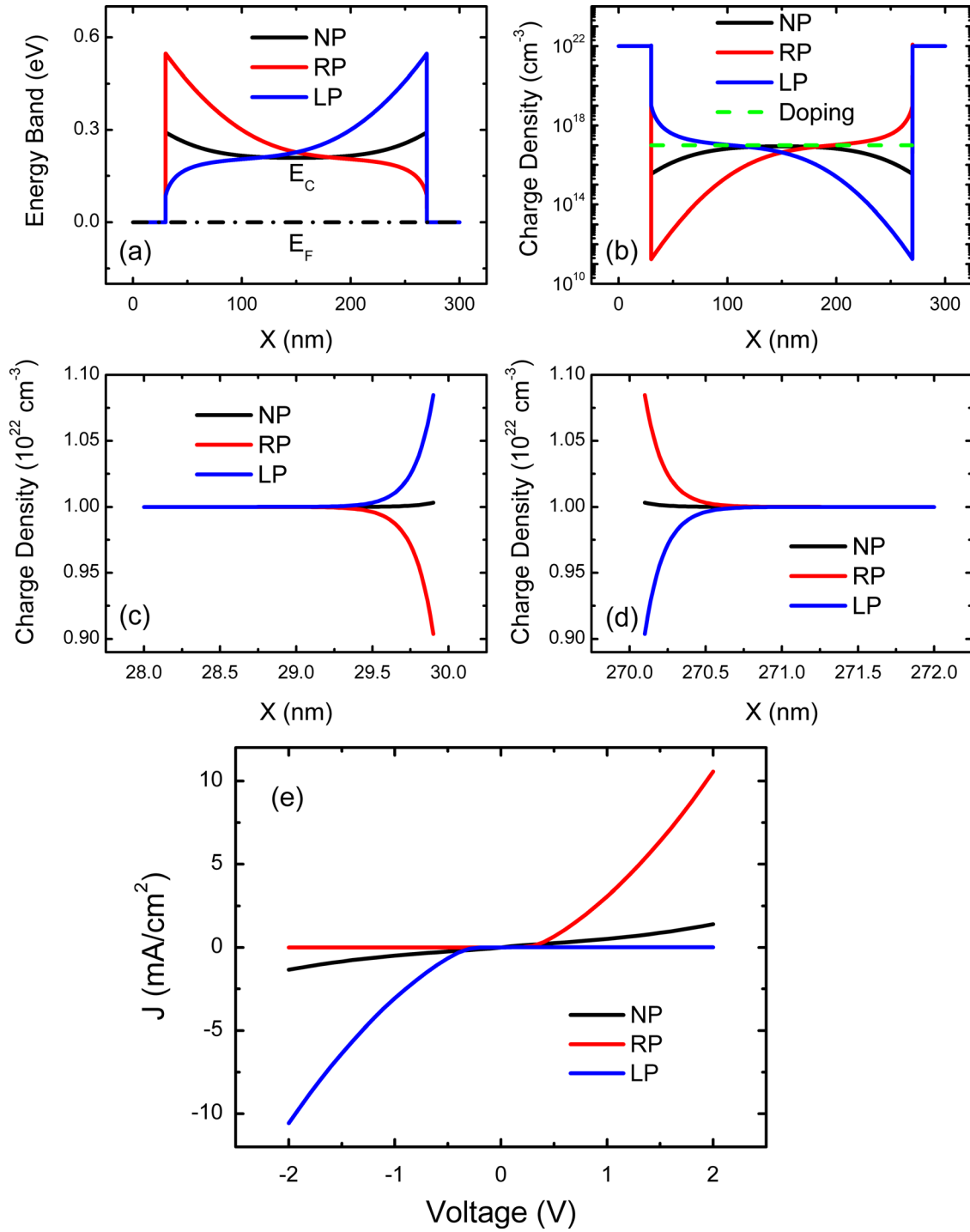


FIG. 2. (Color online) The band diagrams in the case of NP, RP, and LP under short circuit conditions (a). The electron density distributions in the cases of NP, RP, and LP (b). The green dashed line denotes the doping density. The electron density distributions in the case of NP, RP, and LP in the left (c) and right (d) metals. The calculated  $I$ - $V$  curves in the case of NP, RP, and LP (e).

Fig. 3(c). With the increase of the donor doping density, for  $10^{18} \text{ cm}^{-3}$ , the band diagram is rather like that of conventional Schottky junctions as exhibited in Fig. 3(a), the electron depletion region in the ferroelectrics will be much shorter than that of lower doping densities as displayed in Fig. 3(b), and the current becomes larger as shown in Fig. 3(c). There exists a bulk region, that the electron density is equal to the doping density, in the ferroelectrics as displayed in Fig. 3(b). To further verify the effect of the polarization under various doping densities, we calculate the barrier height variations, defined as

$\Delta\phi_B = \phi_B^P - \phi_B^{NP}$ . The calculated values  $\Delta\phi_{B-L}$  are 0.41, 0.40, and 0.35 V for various doping densities  $10^{16}$ ,  $10^{17}$ , and  $10^{18} \text{ cm}^{-3}$ , respectively. Therefore, the polarization could have a limited influence on the energy band when the doping density becomes large enough, giving rise to a small ON/OFF ratio. Here, the ON/OFF ratio is defined as  $I_{\text{ON}}/I_{\text{OFF}}$  (under 1 V voltage). In Fig. 3(d), it can be found that the calculated ON/OFF ratio for the doping density  $10^{16} \text{ cm}^{-3}$  is about one order of magnitude larger than that for the doping density  $10^{18} \text{ cm}^{-3}$ .

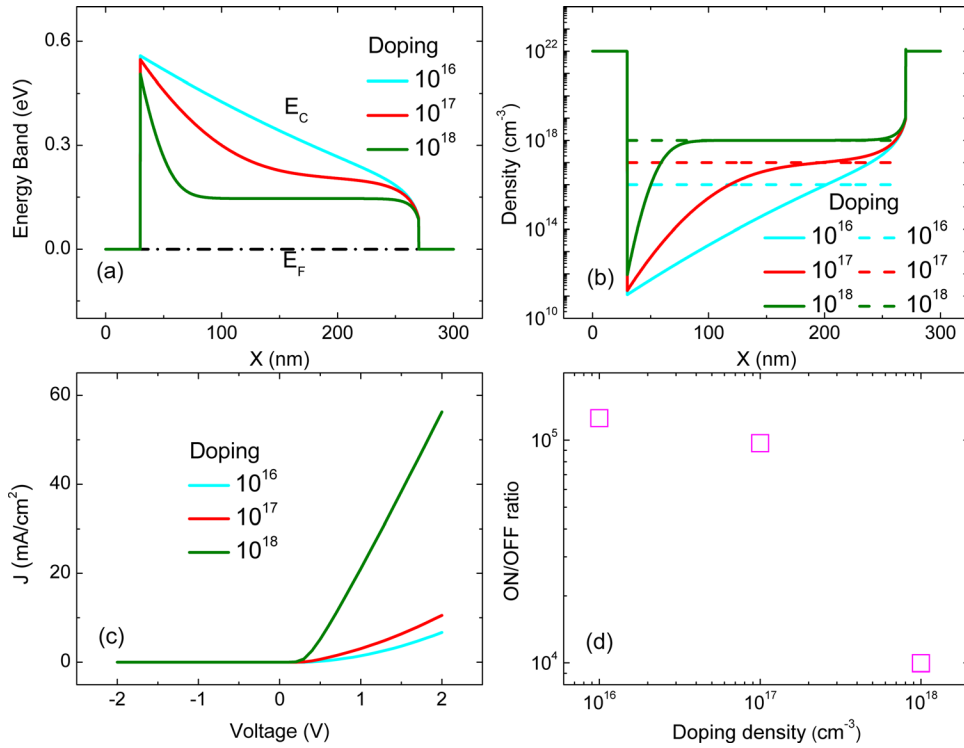


FIG. 3. (Color online) The band diagrams (a), the electron density distributions (b), and the calculated  $I$ - $V$  curves (c) for various doping densities  $10^{16}$ ,  $10^{17}$ , and  $10^{18} \text{ cm}^{-3}$  in the case of RP (a). The dashed lines denote the doping densities. The ON/OFF ratio as a function of the doping density in the ferroelectric film (d).

Further, we investigate the dependence of the band structures, the density distributions, and the  $I$ - $V$  curves on the permittivity in the ferroelectrics. With the increase of the permittivity in the ferroelectrics,  $\phi_{B-L}^{RP}$  becomes smaller and the band diagram becomes similar to that of insulators as shown in Fig. 4(a). More electrons are depleted in ferroelectrics with the increase of the permittivity from Fig. 4(b). The current in this system increases with the increase of the

permittivity in the ferroelectrics as shown in Fig. 4(c). From Fig. 4(d), it can be seen that the calculated ON/OFF ratio decreases with the increase of the permittivity in the ferroelectric, and the calculated ON/OFF ratio for  $\epsilon_f = 50$  is about 2 orders of magnitude larger than that for  $\epsilon_f = 500$ .

In addition, we also calculate the effect of the thickness in the ferroelectrics. With the increase of the thickness in the ferroelectrics, the energy band becomes more like that of

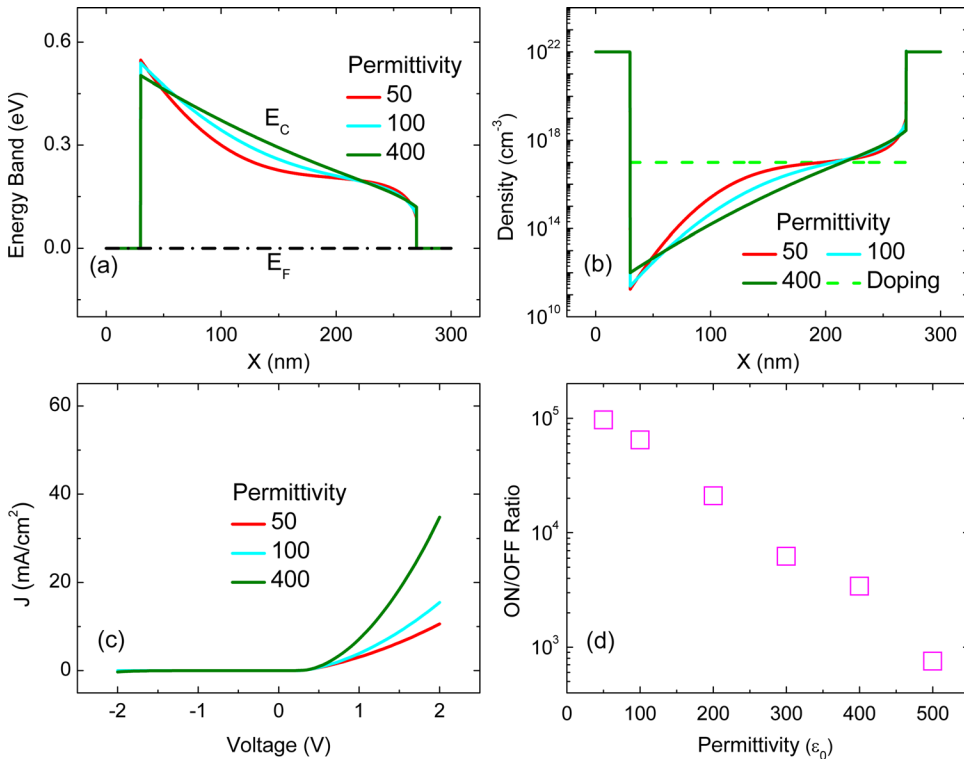


FIG. 4. (Color online) The band diagrams (a), the electron density distributions (b), and the calculated  $I$ - $V$  curves (c) for various permittivity 50, 100, and 400  $\epsilon_0$  in the case of RP. The green dashed lines denote the doping densities. The ON/OFF ratio as a function of the permittivity in the ferroelectric film (d).

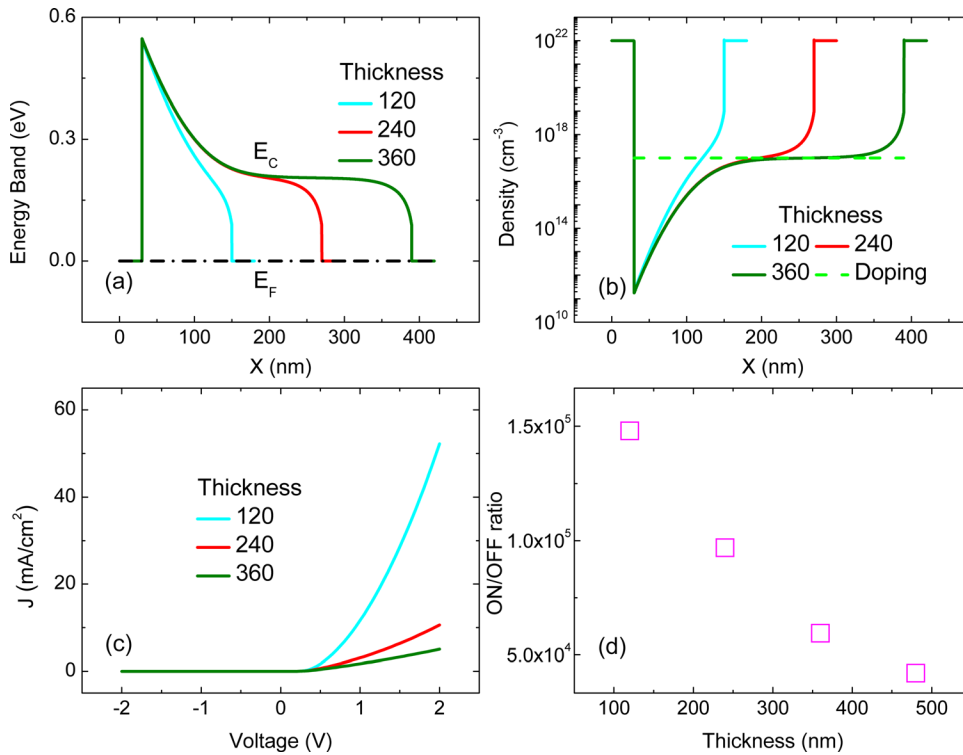


FIG. 5. (Color online) The band diagrams (a), the electron density distributions (b), and the calculated  $I$ - $V$  curves (c) for various thicknesses 120, 240, and 360 nm in the case of RP. The green dashed lines denote the doping densities. The ON/OFF ratio as a function of the thickness in the ferroelectric film (d).

conventional Schottky junctions as shown in Fig. 5(a), there exists a bulk region in the ferroelectrics as shown in Fig. 5(b), and the current becomes smaller as displayed in Fig. 5(c). The calculated ON/OFF ratio decreases with the increase of the thickness in the ferroelectrics, and the ON/OFF ratio with 120 nm ferroelectrics is about three times as large as that with 480 nm ferroelectrics.

#### IV. SUMMARY

In conclusion, we have clarified the operating principle of ferroelectric resistive memories based on the proposed self-consistent numerical model. Our calculation results reveal the effect of the ferroelectric parameters on the band diagrams, the charge density distributions, and the  $I$ - $V$  curves in ferroelectric diodes. The calculated results confirm that the ON/OFF ratio decreases with the increase of the doping density, the permittivity, and the thickness in the ferroelectric films, respectively. We believe that our model will also be helpful in providing theoretical routes into the underlying physical origins in ferroelectric diodes.

#### ACKNOWLEDGMENTS

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