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ABSTRACT

In this work, we theoretically and experimentally investigate the working principle and nonvolatile memory (NVM) functionality of a 2D \(\alpha\text{-In}_2\text{Se}_3\)-based ferroelectric-semiconductor-metal-junction (FeSMJ). First, we analyze the semiconducting and ferroelectric properties of the \(\alpha\text{-In}_2\text{Se}_3\) van der Waals (vdW) stack via experimental characterization and first-principles simulations. Then, we develop a FeSMJ device simulation framework by self-consistently solving the Landau–Ginzburg–Devonshire equation, Poisson’s equation, and charge-transport equations. Based on the extracted Fe-semiconductor (FeS) parameters, our simulation results show good agreement with the experimental characteristics of our fabricated \(\alpha\text{-In}_2\text{Se}_3\)-based FeSMJ. Our analysis suggests that the Fe polarization-dependent modulation of Schottky barrier heights of FeSMJ plays a key role in providing the NVM functionality. Besides, the appearance of mobile carriers in FeS due to its semiconducting properties leads to a non-uniform electric field. This further induces partial polarization switching in the FeS layers, resulting in asymmetry in the FeSMJ characteristics for positive and negative voltages. Moreover, we show that the thickness scaling of FeS leads to a reduction in read/write voltage and an increase in distinguishability. Array-level analysis of FeSMJ NVM suggests a lower read-time and read-write energy with respect to the HfO2-based ferroelectric insulator tunnel junction.

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Ferroelectric (Fe) materials have gained immense research interest for their applications in electronic devices due to their electrically switchable spontaneous polarization and hysteretic characteristics. Fe materials with a high bandgap, called Fe-insulators, have been extensively investigated for versatile nonvolatile memory (NVM) devices, such as Fe-random-access-memory (Fe-RAM), Fe-field-effect-transistors (Fe-FETs), and Fe-tunnel-junctions (FTJs). Unlike Fe-RAM and Fe-FETs, where the Fe layer acts as a capacitive element, the FTJ functionality depends on the tunneling current through the Fe layer. In the FTJ, the Fe layer is sandwiched between two different metal electrodes. Due to the different properties (e.g., the screening length) of the electrodes, the tunneling barrier height at the metal-Fe interface of the FTJ depends on the polarization (P) direction. Thus, the FTJ can exhibit P-dependent tunneling-resistance that facilitates the sensing of its P-state, leading to the design of a two-terminal NVM element. However, as the dominant transport mechanism of the FTJ is direct tunneling, to obtain a desired current density for sufficient operational speed, the Fe-insulator thickness needs to be significantly low (<3 nm for HZO). Unfortunately, with thickness scaling, the Fe-insulator P decreases, which reduces the ratio of the tunneling-resistance and, therefore, the distinguishability of the FTJ memory states decreases. In addition, most of the Fe-insulators (i.e., doped-HfO2) comprise oxygen atoms and the dynamic change in oxygen vacancies can play a major role in their Fe characteristics. Therefore, a decrease in ferroelectricity with scaling and issues related to oxygen vacancies lead to significant challenges in the design and implementation of FTJ-based NVMs.

Similar to the Fe-insulator, Fe material with a low bandgap called the Fe-semiconductor (FeS) also exhibits spontaneous P, which is switchable via the applied electric-field. The van der Waals (vdW) stack of \(\alpha\text{-In}_2\text{Se}_3\) has recently been discovered as a 2D FeS material that can retain the Fe and semiconducting properties, even for a monolayer thickness. This suggests a remarkable possibility for thickness scaling. In addition, as \(\alpha\text{-In}_2\text{Se}_3\) is not an oxide, the issues related to oxygen vacancies are expected to be non-existent in this FeS material. Recently, similar to the FTJ, a metal-FeS-metal junction device (called the FeSMJ) has been demonstrated to exhibit P-dependent resistance states. Unlike the FTJ, the FeSMJ can provide significant current density even with a high FeS thickness and it does not require different metal electrodes for NVM functionalities. To understand such a unique working principle of FeSMJs and to enable
their device-level optimization, a detailed analysis of the material properties of $\alpha$-In$_2$Se$_3$ as well as the device characteristics is needed. To address this need, in this work, we experimentally and theoretically analyze $\alpha$-In$_2$Se$_3$-based FeSMJ devices and examine their thickness scalability. Our analysis is based on experimental characterization, first-principles simulations, and self-consistent device simulation. Moreover, we investigate the FeSMJ thickness scalability and compare it with the FTJ at the device and array levels to analyze its potential for NVM applications.

To begin with, we first discuss the material properties of $\alpha$-In$_2$Se$_3$. Unit cells of the $\alpha$-In$_2$Se$_3$ monolayer are shown in Figs. 1(a)–1(d), indicating a non-centrosymmetric crystal structure, where the central Selenium (Se) atom is displaced from the centrosymmetric position. As a result, where the central Selenium (Se) atom is displaced from the centrosymmetric structure, our device simulation for the calculation of the carrier concentration and density of states (DOS) compared to the valence DOS. Hence, the equilibrium Fermi level ($E_F$) is closer to the conduction band minima ($E_C$) compared to the valence band maxima ($E_V$). We utilize these DOS characteristics in our device simulation for the calculation of the carrier concentration in the FeS layers, as discussed subsequently.

Next, we analyze the Fe properties of the $\alpha$-In$_2$Se$_3$ vdW stack. Figure 2(a) shows the piezorespons force microscopy (PFM) phase vs applied-voltage hysteresis loop of a 120 nm thick $\alpha$-In$_2$Se$_3$ stack that suggests a Fe $P$-switching with a coercive voltage of ~2 V. However, due to the semiconducting properties of $\alpha$-In$_2$Se$_3$, a direct measurement of $P$ through conventional methods is not possible. Therefore, we perform the Berry phase analysis on the DFT wave-functions of $\alpha$-In$_2$Se$_3$. To further understand the Fe properties of $\alpha$-In$_2$Se$_3$, the microscopic potential energy (averaged across the $x$-$y$ plane) along the FeS thickness ($z$-axis) obtained from the DFT simulation is shown in Fig. 2(b). The extracted macroscopic potential [Fig. 2(c)] suggests an
opposite electric-field in FeS layers and vdW gaps. Now, the electrostatic condition at the interface of FeS and vdW gap can be written as

$$\varepsilon_0 E_{\text{vdW}} = \varepsilon_0 E_{\text{FeS}} + P.$$  

(1)

Here, $E_{\text{vdW}}$ and $E_{\text{FeS}}$ are the electric-fields in the vdW gap and FeS layer, respectively, $\varepsilon_0$ is the relative background permittivity of the FeS layer, $\varepsilon_0$ is the vacuum permittivity, and $P$ is the spontaneous polarization. The above equation suggests that $E_{\text{vdW}}$ and $E_{\text{FeS}}$ can be non-zero and hold the opposite sign if and only if the $P$ is non-zero. This further confirms the existence of spontaneous $P$ in the FeS layer. Using the calculated values of $P$, $E_{\text{vdW}}$, and $E_{\text{FeS}}$, we obtain $\varepsilon_r \approx 7$ from Eq. (1). Furthermore, we calculate the total energy ($u$) with respect to the change in $P$ based on the nudge-elastic-band (NEB) method in QE. The change in $P$ is captured by moving the central Se atoms between two stable positions as shown in Fig. 2(d) followed by the Berry phase calculation for $P$. To capture the temperature effect in $u$, we have considered phonon-energy correction for 300 K temperature (discussed in the supplementary material). The resultant $u$-$P$ characteristics are shown in Fig. 2(d), signifying a double-well energy landscape. We fit the simulated $u$-$P$ characteristics with Landau’s free energy polynomial ($u = \frac{1}{2} P^2 + \frac{1}{4} \beta P^4 + \frac{1}{6} \gamma P^6 + \frac{1}{8} \delta P^8$).

The obtained Landau coefficients ($\alpha$, $\beta$, $\gamma$, and $\delta$) are shown in the inset of Fig. 3(a). Based on the extracted parameters of $\alpha$-$In_2Se_3$, we self-consistently solve the Landau–Ginzburg–Devonshire equation, Poisson’s equation, and semiconductor charge equations for the FeSMJ structure. Then, we use the potential profile in a Non-Equilibrium Green’s Function (NEGF) based transport solver to calculate the current in the FeSMJ. The simulation flow and parameters are shown in Fig. 3(a). In our simulation, we consider the vdW gap of 3 Å between the subsequent FeS layers (obtained from DFT simulation with structural relaxation) along with a vdW gap of 1.5 Å between the metal and FeS layer as shown in Fig. 3(b). We utilize this simulation framework along with the experimental results to investigate the FeSMJ device characteristics.

The top view of the fabricated FeSMJ is shown in Fig. 4(a). Here, the FeS thickness ($T_{FeS}$) is 120 nm and the same metal (Ni) is used as the top and bottom contacts. The measured current ($I$) vs voltage ($V$) characteristics [Fig. 4(b)] exhibit a counterclockwise hysteresis due to which the FeSMJ shows two different resistive states. Let us define the current in the low-resistance state (LRS) and high-resistance state (HRS) as $I_{\text{LRS}}$ and $I_{\text{HRS}}$, respectively. Note that the $I_{\text{HRS}}$ to $I_{\text{LRS}}$ switching occurs near $\sim$2 V, which is similar to the coercive voltage of $P$-switching [see the PFM phase in Fig. 2(a)], indicating that the FeS layers are ferroelectric.
change in current is due to the P-switching in the FeS layer. Here, one noticeable thing is that the characteristics are asymmetric with respect to the voltage polarity. For example, the hysteresis window, currents ($I_{\text{LRS}}$ and $I_{\text{HRS}}$), and their ratio ($I_{\text{LRS}}/I_{\text{HRS}}$) are unequal for positive and negative $V$. To understand the possible origin of asymmetry and the FeSMJ operation, we perform device-level simulation. The simulated $I$–$V$ curve considering $T_{\text{FeS}} = 120$ nm and Ni as metal contacts is shown in Fig. 4(b), indicating good agreement with the experimental results. Note that our fabricated device [Fig. 4(a)] has a higher back-metal-FeS interface area compared to the top metal-FeS interface area. Similarly, to compute the current in our simulation, a higher area is considered for the back-metal-FeS interface compared to the top-metal-FeS interface. Due to a Schottky barrier at the metal-FeS interface [Fig. 3(b)], the observed current is due to the electron injection from the metal to FeS via Schottky tunneling along with direct tunneling through the vdW gaps.

Now, to understand the working principle, the equilibrium band diagram of the FeSMJ (along the FeS thickness) is shown in Fig. 4(c-i). Note that the band diagram is for an undoped $\alpha$-In$_2$Se$_3$ in which the $E_F$ is closer to the $E_C$ as discussed before. Without any loss of generality, let us assume that initially, all the FeS layers are in the $-z$ directed polarization state ($-P$). Let us call the left electrode M1 and right electrode M2. Now, the $P$-induced negative (positive) bound charges appear in the FeS near the M1 (M2) interface. The bound charges and the work function difference between the metal and FeS induce an $E$-field within the vdW gap and the FeS layers. As a result, holes (electrons) appear at the FeS-M1 (M2) interface to partially compensate the negative (positive) bound charges. Simultaneously, a built-in potential with opposite polarity appears across the two FeS-M junctions, yielding different Schottky barrier heights ($\phi_B$) for the mobile-carriers. For example, in Fig. 4(c-i), $\phi_B$ at the FeS-M1 interface is higher than at the FeS-M2 interface due to the negative and positive voltage across the respective vdW gaps. Depending on whether the electron-injecting barrier exhibits low or high $\phi_B$, the FeSMJ operates in the LRS or HRS. Moreover, voltage-driven $P$-switching can enable transitioning between the LRS and HRS and vice versa. To understand this, let us consider a positive bias at M2. Hence, the electron injection from the metal to FeS via Schottky tunneling along with direct tunneling through the vdW gaps.

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the M-FeS interface (as the local potential determines the difference between the Fermi level and conduction/valence-band). However, with the decrease in \( T_{\text{FE,S}} \) the built-in potential decreases and that leads to a lower mobile carrier concentration near the M-FeS interface. Now, recall that the mobile-carrier concentration in FeS partially compensates the effect of \( P \)-induced bound charge. As the mobile-carrier concentration decreases with the decrease in \( T_{\text{FE,S}} \), the effect of \( P \)-induced bound charge becomes more prominent. Hence, the \( P \)-dependent modulation in \( \phi_D \) increases with the decrease in \( T_{\text{FE,S}} \) which leads to an increase in \( I_{\text{HS/ILRS}} \) [Fig. 5(b)]. Consequently, improved distinguishability \( (I_{\text{HS/ILRS}}) \) along with low voltage NVM operation can be achieved by scaling down the \( T_{\text{FE,S}} \).

Next, we evaluate the FeSMJ NVM performance in comparison with the FTJ. In an array, each NVM cell \(^2\) [Fig. 5(c)] is composed of a FeSMJ/FTJ connected in series with an access-transistor (T1) and their internal node (n) is connected to the gate of another transistor (T2) that senses the FeSMJ/FTJ resistive state-dependent discharging of the internal node potential. The read and write methodologies of this 2 T-1 R memory cell are described in the supplementary material. In this analysis, we compare the different flavors of HfO\(_2\)-based FTJs\(^{25-28}\) with our FeSMJ devices for an array size of 1 Mb by considering iso-cell-area and iso-sense-margin (discussed in the supplementary material). The device-level comparison [Fig. 5(d)] suggests that the FeSMJ has a key advantage of higher current density than the HfO\(_2\)-based FTJ (due to Schottky transport in the former as opposed to direct tunneling in the latter). Therefore, for the same area, the FeSMJ provides lower resistance (~10\(^{-3}\) times) compared to the FTJs. As the discharging of the internal node (n) depends on the FeSMJ/FTJ resistance, the FeSMJ provides faster discharge and, hence, smaller read-time compared to FTJs [Fig. 5(e)]. Furthermore, due to the slow discharging of the internal node, the T2 transistor remains turned off for a longer period of time for the FTJ. As a result, we observe significantly higher read energy for the FTJ compared to the FeSMJ. Moreover, we observe a little higher write energy for the FTJ\(^{25,26,28}\) due to its higher write voltage (>3 V) compared to the FeSMJ (2.5 V). Due to such a notable benefit of the FeSMJ over HfO\(_2\)-based FTJs for NVM applications, further exploration of the FeSMJ is required to investigate its retention characteristics in addition to its correlation with scaling. Note that, in this comparison, we only consider HfO\(_2\)-based FTJs because of their aggressive scalability.\(^2\) However, there are different perovskite-based FTJs (with significantly high current and high \( I_{\text{HS/ILRS}} \)) where the memory operation not only depends on the \( P \)-switching but also depends on the migration of oxygen vacancies, ions, and formation of the conductive paths.\(^3\) The scalability and variability of such devices are yet to be investigated and, therefore, not included in this comparison.

In summary, the FeS polarization induces a built-in potential across the vdW gap between FeS and metal contact, leading to a \( P \)-dependent Schottky barrier for electron injection. By invoking voltage-driven \( P \)-switching, the barrier height can be modulated, which leads to transitions between the HS and LS in the FeSMJ. Furthermore, we show that the appearance of mobile-carriers in FeS can lead to a partial \( P \)-switching, yielding asymmetric \( I-V \) characteristics of FeSMJ. Also, with \( T_{\text{FE,S}} \) scaling, \( I_{\text{HS/ILRS}} \) increases and read/write voltages decrease. Most importantly, the exhibits a significantly high current density due to Schottky tunneling. Due to such appealing characteristics and fundamental differences in the transport mechanisms, FeSMJ-NVM exhibits significantly improved performances compared to FTJ-NVM.

See the supplementary material for the phonon energy correction, NVM array design, layout design, and read-write schemes.

**DATA AVAILABILITY**

The data that support the findings of this study are available within this article and its supplementary material.

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