

Original Article

# Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>: A Potential Dielectric Layer for GaP Based Metal-Insulator-Semiconductor Structures

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**Abstract** - Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> is a mixed alloy that has the potential to function as an insulating layer in metal insulator semiconductor (MIS) systems. A theoretical investigation of the structural and dielectric properties of Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> and its binary fluorides (CdF<sub>2</sub> and SrF<sub>2</sub>) is reported utilizing the Pseudopotential Plane-Wave (PP-PW) approach in Density Functional Theory (DFT) and Density Functional Perturbation Theory (DFPT). For the exchange-correlation (XC) potentials, this method employs the generalized gradient approximation (GGA). The binary compounds' and alloy's lattice constant, bulk modulus, refractive index, static dielectric constant, band gap, intrinsic breakdown field, energy density, storage density, and lattice misfit are all reported. The estimated lattice constants agreed with the experimental data. The bulk modulus for SrF<sub>2</sub> is consistent with experimental results. The computed bulk modulus of Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> (87.6GPa) shows it is moderately hard. The intrinsic breakdown field depends on the band gap, while the energy storage density depends on the band gap and dielectric constant. A linear relationship is obtained between the intrinsic breakdown field and band gap of considered fluorides and oxides. The intrinsic breakdown field increases in the order HfO<sub>2</sub>—CdF<sub>2</sub>— Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>—SiO<sub>2</sub>—SrF<sub>2</sub> while the energy density increases in the order HfO<sub>2</sub>—SiO<sub>2</sub>—CdF<sub>2</sub>—SrF<sub>2</sub>— Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>. The predicted band gap and dielectric constant of Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> are 8.19eV and 8.714, respectively. The intrinsic breakdown field of Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> is 2.78V/nm. Its energy storage density is 299.13J/cm<sup>3</sup>. There is an improvement in the values of dielectric constant and energy storage density for Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> when compared with SiO<sub>2</sub>. These properties of Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> make it a potential insulating layer for MIS devices. From the calculation of lattice mismatch, Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> and CdF<sub>2</sub> have a mismatch of <1%, which makes them suitable dielectric layers on the Gallium Phosphide (GaP) substrate.

**Keywords** - DFT, DFPT, Dielectric constant, Insulating layer, Intrinsic breakdown field, Energy storage density.

## 1. Introduction

The discovery of novel materials or the progressive application of existing ones is critical for technological progression in domains such as electronics, optics, engineering, and so on. To prevent extinction due to the overuse of existing materials and to supplement the latter, more materials must be studied to determine their prospective applications. Dielectrics play a crucial role in the operation of Metal-Insulator-Semiconductor (MIS) systems because they serve as insulators and store electric charges. In electronic devices, dielectric materials act as insulation between conductors. An excellent dielectric material has a high breakdown field, as well as resilience to stress, heat, and chemical reactions. The dielectric constant (k) is a measure of a dielectric's ability to store electrical charges. The properties and behavior of dielectric materials must be understood for designing high-quality MIS structures for various electronic applications. MIS devices include MIS capacitors, transistors, memories, charge-coupled devices, deep ultraviolet light emitting diodes, MIS solar cells, field effect diodes, etc.

SiO<sub>2</sub> is a widely used insulating layer due to its insulating properties. It has a band gap of 8.90 and a dielectric constant of 3.9. Its breakdown field is recorded as 2.7V/nm. Due to the scaling down of the thickness of SiO<sub>2</sub> to a few nanometers, the performance of MIS devices has been improved because smaller MIS structures operate faster than larger MIS structures due to high current drive. However, the reduction leads to the problem of leakage current, which results in heating, high power usage, and short-term performance of MIS devices. Since the dielectric constant is inversely proportional to the leakage current, many high k oxides have been proposed to replace SiO<sub>2</sub> to overcome the leakage effects. However, band gap reduces with increasing k, indicating low dielectric strength or breakdown field. The band gaps of most of the proposed materials are relatively low (between 4eV and 6eV) [1] compared with that of SiO<sub>2</sub>. Hence, designing MIS structures requires a balance for dielectric constant k, band gap E<sub>g</sub>, and intrinsic breakdown field E<sub>BD</sub> [1]. The insulating dielectric is deposited on a



substrate which is a semiconductor. To maintain interfacial stability between the dielectric layer and the substrate, the difference between the lattice parameters of the dielectric and substrate must be less than 1% for a stable structure.

The alkaline earth fluorides are good materials for insulating layers on semiconductors because they have wide band gaps. They have a fluorite structure, which is similar to the zinc blend or diamond structure of frequently used substrates with good lattice matching.

There are records in the literatures of epitaxial growth of  $\text{CaF}_2$  and  $\text{CdF}_2$  on Si substrate [2, 3], growth and characterization of  $\text{SrF}_2$  on InP substrate [4], the structure of  $\text{Ca}_x\text{Sr}_{1-x}\text{F}_2$  epilayer on GaAs and Ge substrates [5] and growth characteristics of ultra-thin  $\text{Ca}_x\text{Mg}_{1-x}\text{F}_2$  alloys on Si substrate [6].

In 2004, Buchinskaya and Fedorov [7] discovered a  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  solid solution to have the fluorite structure after it was formed by the Bridgman Stockbarger method [8]. They found the melting point of the crystal to be 1298K.

The lattice parameter variation with temperature of  $\text{CdF}_2$ ,  $\text{SrF}_2$  and  $\text{Cd}_{1-x}\text{Sr}_x\text{F}_2$  ( $x = 0.23, 0.50$ ) solid solutions was investigated through experiments at 5-300 K [9]. The heat capacity of  $\text{Cd}_{0.50}\text{Sr}_{0.50}\text{F}_2$  was investigated at various temperatures, and structural disorder of the crystal occurred at low temperatures causing the crystal to behave as a glass [10].

The ionic, electrical and thermal conductivities of  $\text{Cd}_{0.77}\text{Sr}_{0.23}\text{F}_2$  solid solution have been studied [11]. The crystal has a low thermal conductivity of 1.1W/mK at 300K. As temperature increases, the thermal conductivity of the crystal reduces only slightly [12]. The thermal conductivities of all the compositions of  $\text{Ca}_{1-x}\text{Sr}_x\text{F}_2$  ( $0 \leq x \leq 1$ ) crystal are high (i.e.  $\lambda > 3\text{W/mK}$  at 300K) [13].

In this work, we would like to study the structural and dielectric properties of  $\text{CdF}_2$ ,  $\text{SrF}_2$ , and  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$ . The structural properties include the lattice parameter, bulk modulus and lattice mismatch. In contrast, the dielectric properties include the static dielectric constant, the band gap, the intrinsic breakdown field and electrical energy density. The discovery of new insulating layers for MIS structures requires a balance for the dielectric constant, band gap and intrinsic breakdown field [14].

## 2. Computational Details

The structural characteristics of  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  and its binary fluorides are studied using density functional theory (DFT) with the ultrasoft pseudo-potential, plane wave approach, which is implemented in Quantum Espresso code [15]. The orbitals of Cd ( $4d^{10}, 5s^2$ ), Sr ( $4s^2 4p^6 4d^{10}, 5s^1$ ), and F ( $2s^2 2p^5$ ) are treated as valence electrons. Perdew, Burke, and Ernzerhof's exchange-correlation (PBE) [16] is

employed. Brillouin zone integration is accomplished using the Monkhorst and Pack meshes [17]. We sampled  $6 \times 6 \times 6$  k locations to calculate the alloy's total energy accurately. The kinetic energy cutoff is 60Ryd.

DFT is a well-accepted theory for calculating the physical characteristics of materials. When a system is agitated, specific physical properties are obtained. Examples include an electronic contribution to the dielectric constant, phonon frequencies, Born effective charges, *etc.* These properties are calculated by powerful techniques known as Density Functional Perturbation Theory (DFPT). Most physical properties of solid materials depend on the valence electrons. The valence electron is modeled by the pseudopotential approximation.

The structural properties of the binary compounds  $\text{CdF}_2$  and  $\text{SrF}_2$  in the fluorite phase are first calculated, followed by  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  using the GGA scheme. For the considered materials, we performed structural optimization by minimizing the total energy with respect to the cell parameters and also the atomic positions. The alloy was studied by using a primitive mesh of 12 atoms. The total energies calculated as a function of cell parameters were fitted to Murnaghan's equation of state [18] to obtain the equilibrium structural properties both for the binary compounds and ternary alloy. The equation of state for energy is given as;

$$E(V) = E_0 + \frac{B_0 V}{B_0'} \left[ \frac{(V_0/V)^{B_0'}}{B_0' - 1} + 1 \right] - \frac{B_0 V_0}{B_0' - 1} \quad (1)$$

The equation of state for pressure is given as;

$$P(V) = \frac{B_0}{B_0'} \left[ \left( \frac{V_0}{V} \right)^{B_0'} - 1 \right] \quad (2)$$

Quantities such as electronic contribution to dielectric constant, Phonon frequencies and Born effective charges that can be obtained by perturbing the total energy are calculated by using DFPT. Here, the total energy is differentiated with respect to the perturbation.

$$E_n = \frac{1}{k!} \frac{d^k E_n}{d\lambda^k} \quad (3)$$

Where E=total energy, n=number of atoms, k=order of perturbation,  $\lambda$ =perturbations, which could be atomic displacement, electric field, *etc.*

The total or static dielectric constant is divided into electronic contribution and ionic contribution. That is,

$$k = k_e + k_i \quad (4)$$

Where  $k$  is the total dielectric constant,  $k_e$  is the electronic dielectric constant and  $k_i$  is the ionic dielectric constant.

The electronic contribution to the dielectric constant is given as a tensor.

$$k_e = \delta_{\alpha\beta} + 4\pi \frac{\partial P_\alpha}{\partial \varepsilon_\beta} \quad (5)$$

Where  $\alpha$  and  $\beta$  are the directions of the electric field ( $\varepsilon$ ) and electronic polarization (P).

When  $\alpha=\beta$ ,  $\delta_{\alpha\beta} = 1$  and when  $\alpha \neq \beta$ ,  $\delta_{\alpha\beta} = 0$ .

The refractive index, n, is related to the average  $k_e$  by the relation [19]

$$k_e = n^2$$

So that,

$$n = \sqrt{k_e} \quad (6)$$

The band gap energy is related to the refractive index by the Herve-Vandamme relation [20]

$$n^2 = 1 + \left( \frac{A}{E_g + B} \right)^2 \quad (7)$$

Where  $A=13.6\text{eV}$ ,  $B=3.46\text{eV}$  and  $E_g$  is the band gap energy.

The relationship between intrinsic breakdown field ( $E_{BD}$ ) and band gap ( $E_g$ ) [21] is given as

$$E_{BD} = 1.36 \times \left( \frac{E_g}{E_{gc}} \right)^\alpha \quad (8)$$

Where  $\alpha=1$  for insulator,  $E_{gc}$ =critical band gap= $4\text{eV}$

Equation (8) can be modified as

$$E_{BD} = \frac{1.36}{4} \times E_g = 0.34 \times E_g \quad (9)$$

Born effective charge,  $Z^*$  is also known as a transverse or dynamic effective charge. It is a basic parameter. Born effective charge is the change in polarization when an atom is displaced or the change in force induced on a given atom when an electric field is applied.

$$Z^* = \Omega_o \frac{\partial P_\beta}{\partial \tau_{k\alpha}(q=0)} = \frac{\partial F_\alpha}{\partial \varepsilon_\beta} \quad (10)$$

$\Omega_o$ =unit cell volume,  $F_\alpha$  = force on an atom in  $\alpha$  direction,  $P_\beta$  = polarization in  $\beta$  direction,  $\varepsilon_\beta$ =electric field in  $\beta$  direction and  $\tau_{k\alpha}$  = atomic displacement of atom k in  $\alpha$  direction. It is a tensor.

The second derivative of the energy with respect to atomic displacement is a  $3N \times 3N$  matrix where N is the number of atoms per unit cell. The matrix contains the inter-atomic force constants whose diagonalization produces phonon frequencies and eigenvectors (displacement).

The ionic contribution to the dielectric constant is given by [22]

$$k_i = \sum \frac{Ne^2 Z^{*2}}{m\omega_{TO}^2} \quad (11)$$

N= number of ions per unit volume

e= electronic charge

$Z^*$ = transverse effective charge

m= reduced mass

$\omega_{TO}$ = transverse optical phonon frequency

Another important parameter is the electrical energy storage density [1], which can be used for the appropriate selection of dielectric materials for MIS structures.

$$F_{ED} = 8.1882 \times k \left( \frac{E_g}{E_{gc}} \right)^{2\alpha} \quad (12)$$

Equation (12) can be modified as

$$F_{ED} = \frac{8.1882}{16} \times k E_g^2 = 0.5118 \times k E_g^2 \quad (13)$$

### 3. Results and Discussion

#### 3.1. Structural Properties

Table 1 displays the crystals' lattice properties. The lattice parameters for  $\text{CdF}_2$ ,  $\text{SrF}_2$ , and  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  are  $5.448\text{\AA}$ ,  $5.816\text{\AA}$ , and  $5.562\text{\AA}$ , respectively. They concur with the experiment's findings. The experimental lattice parameters for binary compounds are derived from [23], whereas those for alloys are taken from [7].

Table 1 also includes information on the bulk modulus. Only the experimental bulk modulus of  $\text{SrF}_2$  [24] is known, and it is consistent with our results. The bulk moduli of the fluorides are  $96.5\text{GPa}$ ,  $69.1\text{GPa}$ , and  $87.6\text{GPa}$  for  $\text{CdF}_2$ ,  $\text{SrF}_2$ , and  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$ , respectively, indicating that they can sustain stress. The bulk modulus of the alloy demonstrates that it is relatively hard, making it suitable as an insulating layer.

**Table 1. Lattice constants a( $\text{\AA}$ ) and Bulk modulus B(GPa) of  $\text{CdF}_2$ ,  $\text{SrF}_2$  and  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$**

Materials	a( $\text{\AA}$ )	a <sub>exp</sub> ( $\text{\AA}$ )	B(GPa)	B <sub>exp</sub> (GPa)
$\text{CdF}_2$	5.448	5.388	96.5	—
$\text{SrF}_2$	5.816	5.799	69.1	69.0
$\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$	5.562	5.478	87.6	—

3.2. Dielectric Properties

The electronic contribution to the dielectric constant and refractive indices of CdF<sub>2</sub>, SrF<sub>2</sub> and Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> are presented in Table 2. The dielectric constants are 2.778, 2.201 and 2.600, respectively. The value of k<sub>e</sub> for SrF<sub>2</sub> compared well with the experiment [25]. The refractive indices of the systems are obtained from (6). The values of n for the binary compounds also compared well with experimental values [25, 26].

Table 2. Electronic contribution to dielectric constant k and refractive indices n of CdF<sub>2</sub>, SrF<sub>2</sub> and Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>

Materials	k <sub>e</sub>	k <sub>e</sub> (exp)	n	n(exp)
CdF <sub>2</sub>	2.778	—	1.667	1.66
SrF <sub>2</sub>	2.201	2.2106	1.484	1.4868
Cd <sub>0.75</sub> Sr <sub>0.25</sub> F <sub>2</sub>	2.600	—	1.612	—

Table 3 shows the band gap and static dielectric constants of considered materials. For the band gap of Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>, we used the Herve-Vandamme relation (7), and the predicted band gap of Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> is 8.19eV. The band gaps of CdF<sub>2</sub> and SrF<sub>2</sub> are experimental values [27, 28]. The static dielectric constants of the materials are also presented in Table 3. For CdF<sub>2</sub>, k=8.827, for SrF<sub>2</sub>, k =6.151 and for Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>, k =8.714. The dielectric constants of CdF<sub>2</sub> and SrF<sub>2</sub> compared well with reported values [29, 30]. Since the dielectric constant of Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> is higher than the dielectric constant of SiO<sub>2</sub>, Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>, the dielectric layer can be thicker for the same stored charges as shown in Fig.1(a) and Fig. 1(b). The thickness reduces the problem of leakage current which leads to heating, high power consumption and device breakdown.

Table 3. Band gap energies E<sub>g</sub>(eV) and static dielectric constants k of CdF<sub>2</sub>, SrF<sub>2</sub> and Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>

Materials	E <sub>g</sub> (eV)	k	k(rep)
CdF <sub>2</sub>	7.80	8.827	8.33
SrF <sub>2</sub>	10.00	6.151	6.465
Cd <sub>0.75</sub> Sr <sub>0.25</sub> F <sub>2</sub>	8.19	8.714	—

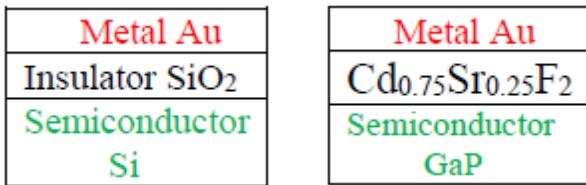


Fig.1(a) MIS Structure With SiO<sub>2</sub> dielectric layer (b) MIS Structure with Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> layer thicker than SiO<sub>2</sub> for the same application

The intrinsic breakdown field of the materials is presented in Table 4 and calculated from (8). The E<sub>BD</sub> are 2.65V/nm, 3.31V/nm and 2.78V/nm for CdF<sub>2</sub>, SrF<sub>2</sub> and Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>, respectively, as presented in Table 4. The calculated E<sub>BD</sub> for

SiO<sub>2</sub> is 3.03V/nm, comparable to the experimental value. The E<sub>BD</sub> for the considered materials is closely the same as SiO<sub>2</sub> (≈3V/nm). Most of the proposed oxides for the dielectric layer have E<sub>BD</sub> < 2V/nm because of their relatively smaller band gaps. There is an improvement in the values of E<sub>BD</sub> for the fluorides. Fig. 2 shows the relationship between the intrinsic breakdown field (E<sub>BD</sub>) and band gap (E<sub>g</sub>) of fluorides and oxides. The fluorides are CdF<sub>2</sub>, SrF<sub>2</sub> and Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>. The oxides are SiO<sub>2</sub> (commonly used dielectric layer) and HfO<sub>2</sub> which is the most attractive oxide among the proposed oxides because of its high value of k (16) [31]. The band gap of HfO<sub>2</sub> is 3.95eV [32]. The graph is linear with E<sub>BD</sub> directly proportional to E<sub>g</sub>. The intrinsic breakdown field increases in the order HfO<sub>2</sub>—CdF<sub>2</sub>— Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>—SiO<sub>2</sub>—SrF<sub>2</sub>. SrF<sub>2</sub> has the highest intrinsic breakdown field because of its highest band gap (9.73eV).

Table 4. Intrinsic breakdown field E<sub>BD</sub> (V/nm) and energy storage densities F<sub>ED</sub> (J/cm<sup>3</sup>) of CdF<sub>2</sub>, SrF<sub>2</sub> and Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>

Materials	E <sub>BD</sub> (V/nm)	F <sub>ED</sub> (J/cm <sup>3</sup> )
CdF <sub>2</sub>	2.65	274.83
SrF <sub>2</sub>	3.31	298.02
Cd <sub>0.75</sub> Sr <sub>0.25</sub> F <sub>2</sub>	2.78	299.13

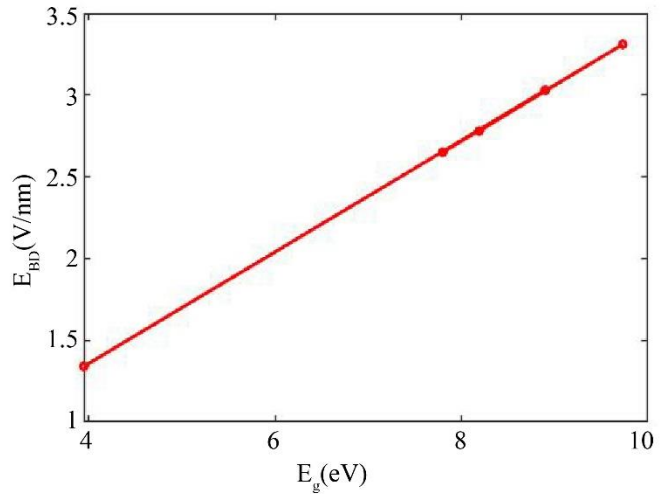


Fig. 2 Intrinsic Breakdown Field versus Band gap of Fluorides and Oxides

Fig. 3 presents the graph of energy density F<sub>ED</sub> of the materials against kE<sub>g</sub><sup>2</sup>. F<sub>ED</sub> is the electrical energy stored by the insulating layer per unit cm<sup>3</sup>. Energy density increases in the order HfO<sub>2</sub>—SiO<sub>2</sub>—CdF<sub>2</sub>—SrF<sub>2</sub>— Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>. The material with the highest value of F<sub>ED</sub> is Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub>. This is because Cd<sub>0.75</sub>Sr<sub>0.25</sub>F<sub>2</sub> has the highest value of kE<sub>g</sub><sup>2</sup> — 584.50(eV)<sup>2</sup>. F<sub>ED</sub> increases as kE<sub>g</sub><sup>2</sup> increases. In spite of its high k, F<sub>ED</sub> is low for HfO<sub>2</sub> because of its low band gap (E<sub>g</sub>). The combination of k and E<sub>g</sub> are important in determining the quality and reliability of an insulating layer, and the combination will help in the discovery of more usable materials. The electrical energy storage densities are 274.83J/cm<sup>3</sup>, 298.02J/cm<sup>3</sup> and 299.13J/cm<sup>3</sup> for CdF<sub>2</sub>, SrF<sub>2</sub> and

$\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  respectively. They are calculated from (12) and presented in Table 4. The  $F_{\text{ED}}$  for the three materials is relatively high, about twice the value for  $\text{SiO}_2$  ( $158.09\text{J}/\text{cm}^3$ ). Although the proposed oxides have relatively high dielectric constants, their energy storage densities and intrinsic breakdown fields are low because of their lower band gaps when compared with those of the fluorides. Based on the investigated intrinsic breakdown field and energy storage density,  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$ ,  $\text{CdF}_2$  and  $\text{SrF}_2$  are high  $k$  dielectrics with improved electrical characteristics.

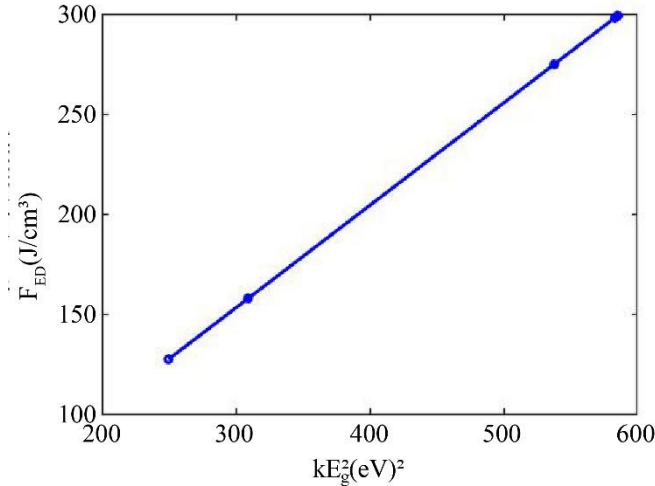


Fig. 3 Dependence of Energy storage density on  $kE_g^2$  of Fluorides and Oxides

Lattice mismatch of the insulator on the semiconductor is given as  $\Delta a/a$ .  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  and  $\text{CdF}_2$  can be grown on a Gallium Phosphide (GaP) semiconductor. The experimental lattice parameters of  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  and  $\text{CdF}_2$  are  $5.4778\text{\AA}$  and  $5.448\text{\AA}$ , respectively. For GaP,  $a=5.45\text{\AA}$  [33]. There is a lattice mismatch of 0.88% and 0.50%, respectively, for  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  and  $\text{CdF}_2$ , respectively. Since the lattice mismatch is less than 1%,  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  and  $\text{CdF}_2$  can be used as insulating layers in GaP-based MIS devices with stable structures. Although  $\text{CdF}_2$  has been grown on Si but, there is a problem of a chemical reaction between  $\text{CdF}_2$  and Si. There is no record of a chemical reaction between  $\text{CdF}_2$  and GaP in the literatures as far as we know. For  $\text{SrF}_2$ , the lattice mismatch is 7%, making the GaP

substrate not ideal for the  $\text{SrF}_2$  layer. However, the growth of  $\text{SrF}_2$  on InP substrate has already been reported [34].

#### 4. Conclusion

In this paper, we used GGA inside the PP-PBE method to investigate the structural and dielectric properties of the cubic alkaline earth fluorides  $\text{CdF}_2$ ,  $\text{SrF}_2$ , and  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$ . The lattice parameter and bulk modulus are determined. To facilitate comparison, the structural characteristics of the alloy's constituent binary compounds were computed. Our calculations and experiments show good agreement. The electronic contribution to the dielectric constant and ionic contribution parameters are calculated using density functional perturbation theory. We computed the intrinsic breakdown field and energy storage density for  $\text{CdF}_2$ ,  $\text{SrF}_2$ , and  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$ . The calculations allowed us to identify  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  as a better material for insulating layers in GaP-based MIS systems.  $\text{CdF}_2$  is likewise applicable, although  $\text{SrF}_2$  cannot be grown on GaP substrate due to a large lattice mismatch. It is worth noting that  $\kappa$  is important in the choice of dielectric material.

However, band gap energy is also crucial because barrier height increases with increasing band gap, and as  $k$  increases, band gap decreases. To minimize leakage current, a large barrier height is essential. Thus, a balance must be ensured between  $k$ , and  $E_g$ . Energy storage density of  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  is closely two times greater than  $\text{SiO}_2$ . Their  $E_{\text{BD}}$  are closely equal. The intrinsic breakdown field increases in the order  $\text{HfO}_2$ — $\text{CdF}_2$ — $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$ — $\text{SiO}_2$ — $\text{SrF}_2$  while the Energy density increases in the order  $\text{HfO}_2$ — $\text{SiO}_2$ — $\text{CdF}_2$ — $\text{SrF}_2$ — $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$ . Since a high  $\kappa$  material does not necessarily result in high energy density and high intrinsic breakdown field, more materials can be discovered for application as dielectrics in MIS devices by carefully looking at their dielectric constants as well as their band gaps. This study stimulates the design and construction of GaP-based MIS devices with a  $\text{Cd}_{0.75}\text{Sr}_{0.25}\text{F}_2$  insulating layer.

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