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**Research Article** 

# The investigation of the complex dielectric and electric modulus of $Al/Mg_2Si/p-Si$ Schottky diode and its AC electrical conductivity in a wide frequency range

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Abstract: The Al/Mg<sub>2</sub>Si/p-Si Schottky diode was fabricated using spin coating. The real ( $\varepsilon$ ) and imaginary ( $\varepsilon$ ) components of complex dielectric ( $\varepsilon^*$ ), the real (M) and imaginary (M) components of complex electric modulus (M\*) and AC electrical conductivity ( $\sigma_{AC}$ ) of the fabricated Al/Mg<sub>2</sub>Si/p-Si Schottky diode (SD) were examined by using the impedance spectroscopy (IS) measurements in a wide frequency range of 1 kHz-1 MHz. The  $\varepsilon$  and  $\varepsilon$ ?? were obtained using the value of measured capacitance and conductance while the values of dielectric loss tangent ( $\tan \delta$ , M', M'' and  $\sigma_{AC}$  were obtained using the value of  $\varepsilon$ ? and  $\varepsilon$ ??. While the values of  $\varepsilon$ ?,  $\varepsilon$ ?? and  $\tan \delta$  are almost independent of the frequency in the inversion and accumulation region, their value changes with the frequency, especially in the depletion region. The  $\sigma_{AC}$  was examined depending on the frequency and it was seen that its value increased with increasing frequency especially in depletion and accumulation region. The experimental results showed that the Mg<sub>2</sub>Si can be used instead of conventionally used dielectric materials (SnO<sub>2</sub>, SiO<sub>2</sub>).

## 1. Introduction

The dielectric material is electrically insulating. Metal-oxide-semiconductor (MOS), metal-polymer-semiconductor (MPS) or metal-ferroelectric-semiconductor (MFS) structures can store charge thanks to the properties of the dielectric material used at the interface between metal and semiconductor. In these structures, charge storage depends on the thickness of the dielectric material and especially on the dielectric constant ( $\varepsilon$ ) of the dielectric material. Such an interface layer separates the metal from the semiconductor and regulates the charge transitions. Additionally, the interfacial layer provides to realize the decrease in the magnitude of the leakage current, series resistance ( $\mathbf{R}_s$ ) values and interface states ( $\mathbf{N}_{ss}$ ) in the devices, it also increases the short circuit resistance ( $\mathbf{R}_{sh}$ ), barrier height and rectification ratio. In other words, such a layer affects the performance and reliability of the structure. Dielectrics materials are affected by an applied alternating electric field. By the formation of polarization in the material, it gains a dipole moment. By providing electrical charge accumulation on the dielectric surface, it exhibits capacitor behavior and can store charge [1–3]. The performance of semi-conductor devices affects some factors such as the  $\mathbf{N}_{ss}$ ,  $\mathbf{R}_s$ , the density of the interface states, temperature, frequency, voltage, and the form of the barrier between metal and semiconductor.

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Magnesium silicide (Mg<sub>2</sub>Si) is an intermetallic compound with relatively high melting temperature (=1085 °C), low density (=1.99 g/cm<sup>3</sup>), a narrow-gap semiconductor (=0.6–0.7 eV), and a low thermal expansion coefficient (= $7.5 \times 10^{-6}$  K) [4–6]. Its conduction types are p-type and it has been widely used as a semiconductor and thermoelectric material [6–10]. Mg<sub>2</sub>Si is one of the attractive materials for optoelectronic application [11–13]. Additionally, researchers mostly focused on ceramic materials such as MgSiN<sub>2</sub> and Mg<sub>2</sub>Si<sub>(1-x)</sub>V<sub>x</sub>O<sub>4</sub>[14, 15].For instance; according to Lenčéš et al. [14], the relative dielectric constant for MgSiN<sub>2</sub> powder obtained from a mixture of Mg<sub>2</sub>Si is 9.0 at 100 kHz.

The research on the dielectric properties of Mg<sub>2</sub>Si has been limited in the literature. Additionally, the change in frequency has a significant effect on the dielectric properties of structures that can store charge. Thus, in this study, the frequency-dependent properties of  $\varepsilon'$ ,  $\varepsilon''$ ,  $\tan \delta M'$ , M'' and  $\sigma_{AC}$  for Al/Mg<sub>2</sub>Si/p-Si SD were examined by using the admittance measurements including measured capacitance and conductance data in a wide frequency range from 1 kHz to 1 MHz, and detailed.

#### 2. Materials and methods

The wafer (p-Si) with boron-doped p-Si with 1–10  $\Omega$  cm resistivity, approximately 525  $\mu$ m thickness and (??) orientation was chemically cleaned using acetone (C<sub>3</sub>H<sub>6</sub>O), isopropanol (C<sub>3</sub>H<sub>8</sub>O), and deionized (DI) water for 5 min, respectively. To remove the native oxide layer on the surface of the wafer was washed with HF. The wafer was washed again with DI for 5 min and dried with nitrogen. For omic contact, Al was coated on the back of the wafer in thermal evaporation. For a low resistance, the Al metal was precipitated into the semiconductor by annealing at 450 °C in N<sub>2</sub> environment for 5 min. A mixture of 1 mL of chloroform and 50 mg of Mg<sub>2</sub>Si in powder form was thoroughly mixed with the aid of a centrifuge and synthesis of the interface layer was completed. Then, the interface layer was covered by spin-coating on the front of the wafer. To form rectifier (Schottky) contacts with 0.5 mm radius, Al was evaporated on the interface-covered surface and Al/Mg<sub>2</sub>Si/p-Si SD was fabricated. Frequency-dependent capacitance (C) and conductance (G/ $\omega$ ) measurements of Al/Mg<sub>2</sub>Si/p-Si SD were performed by using HP4192A impedance analyzer. Figure 1 shows the capacitance and conductance measuring system and the cross section of Al/Mg<sub>2</sub>Si/p-Si SD.

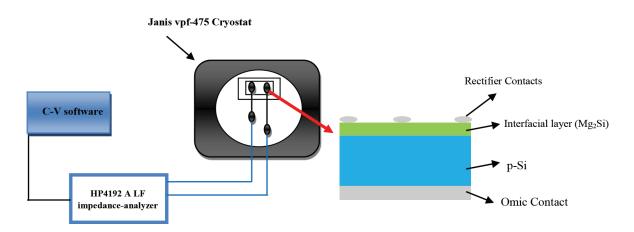


Figure 1. The capacitance and conductance measuring system and the cross section of Al/Mg<sub>2</sub>Si/p-Si SD.

#### 3. Results

The equivalent circuit for Al/Mg<sub>2</sub>Si/p-Si SD is shown in Figure 2. As can be seen from Figure 2, the equivalent circuit consists of the total series resistance ( $R_s$ ), a parallel junction capacitance (C) and the shunt resistance ( $R_{sh}$ ), where C and  $R_{sh}$  are connected in parallel while  $R_s$  is connected in series to both C and  $R_{sh}$  [16,17].

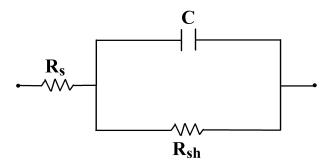


Figure 2. The equivalent electrical circuit for Al/Mg<sub>2</sub>Si/p-Si SD.

Metal/semiconductor contacts behave like a parallel plate capacitor. In the presence of an insulating or organic interface layer, a capacitance (C) is formed between the metal and the semiconductor. The relationship of this capacitance and the capacitance of the interface layer ( $C_{ox}$ ) and the capacitance of the semiconductor ( $C_{sc}$ ) is given as follows [17,18]:

$$\frac{1}{C} = \frac{1}{C_{oc}} + \frac{1}{C_{sc}}.$$
(1)

The capacitance (C) and conductance (G) measurements for Al/Mg<sub>2</sub>Si/p-Si SD are carried out in a wide range of frequencies (1 kHz–1 MHz). The dielectric properties of the structures are examined using these measurements. The  $\varepsilon^*$  of a structure provides information on its  $\varepsilon'$  and  $\varepsilon''$ . Thus,  $\varepsilon^*$  is given as follows [19,20]:

$$\varepsilon^* = \varepsilon' - j\varepsilon'' = \left(\frac{C_m d_i}{\varepsilon_0 A}\right) - j\left(\frac{G_m d_i}{\varepsilon_0 A}\right),\tag{2}$$

where  $\varepsilon_{I}, \varepsilon_{I'}$ ,  $C_m$ ,  $G_m$ ,  $d_i$ , A and  $\varepsilon_0$  are the real part and the imaginary part of complex dielectric permittivity, measured capacitance, measured conductance, the interfacial layer thickness, the area of the diode and the permittivity of vacuum, respectively [21–24].  $\varepsilon_{I}$  is the maximum value of the energy stored in the dielectric material under the external electric field and it depends on some physical and chemical factors such as frequency, defects of dielectric materials and the chemical structure [2,25,26].  $\varepsilon_{II}$  is the energy loss caused by the slow polarization currents and the orientation of molecular dipoles in the dielectric material under the external electric field [26]. Briefly,  $\varepsilon_{I}$  represents the charging while  $\varepsilon_{II}$  represents the loss current. The  $\varepsilon_{I}$ -V and  $\varepsilon_{II}$ -V plots for the Al/Mg<sub>2</sub>Si/p-Si SD were given in Figures 3 and 4, respectively. The  $\varepsilon_{I}$ -V and  $\varepsilon_{II}$ -V plots have regions of inversion, depletion, and accumulation for each frequency. As shown in Figure 3,  $\varepsilon_{I}$ was taken an almost constant value in the inversion and accumulation region and it increases with decreasing frequency in the depletion region. The space charges have not enough time to orient themselves in the direction of the alternating field at high frequencies. However, they have enough time for orientation at low frequencies. Hence, dielectric constant increases due to such behavior of space charges at low frequencies [27–32].

The  $\varepsilon \prime \prime$  value of Al/Mg<sub>2</sub>Si/p-Si SD behaves just like  $\varepsilon \prime$  in the inversion and accumulation region. Especially at low frequencies, the high values of  $\varepsilon \prime$  and  $\varepsilon \prime$  are higher than their high-frequency values due to

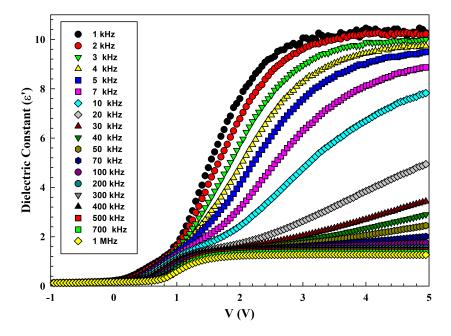


Figure 3.  $\varepsilon$  '-V plot for Al/Mg<sub>2</sub>Si/p-Si SD in a wide frequency range.

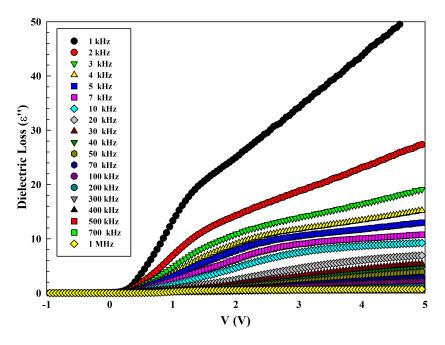


Figure 4.  $\varepsilon$  //-V plot for Al/Mg<sub>2</sub>Si/p-Si SD in a wide frequency range.

interfacial polarization. The distributions in  $\varepsilon'$  and  $\varepsilon''$  with frequency may be caused by electronic and ionic polarization effective at high frequencies (f  $\geq 10^9$  Hz) and bipolar and surface polarizations that are effective at low frequencies (f  $\leq 10^3$  Hz). Also, the correlation of  $\varepsilon'$  and  $\varepsilon''$  with frequency is related to the capacitance and conductance values. Additionally, while the existence of N<sub>ss</sub>, which can follow the alternating signal at low or intermediate frequencies, contributes to the capacitance and conductivity values in depletion and inversion regions,  $\mathbf{R}_s$  is effective in the accumulation region.

The tan  $\delta$ , indicating the energy loss of the structure during AC current conduction, is a measure of the ratio of electrical energy loss to stored energy at applied bias voltage and is given as follows [33]:

$$\tan \delta = \frac{\varepsilon''}{\varepsilon'}.\tag{3}$$

tan $\delta$  depends on interface polarization and dipole orientations [34]. The tan $\delta$ -V plot for Al/Mg<sub>2</sub>Si/p-Si SD was given in Figure 5. As shown in Figure 5, it was taken an almost constant value in the inversion and accumulation region. However, it has appronunced and sharp peak that arises from the N<sub>ss</sub> at low frequencies. The peak behavior of the tan $\delta$ -V has occurred especially in the depletion region between ~0 V and ~2 V. Such phenomena of tan $\delta$  are due to a particular distribution of charges and interfacial polarization mechanism, the density of the N<sub>ss</sub> and the thickness of the interface layer (Mg<sub>2</sub>Si) [3, 25]. Additionally, the peak value loses its effect with increasing frequency since charge carrier hopping cannot follow the external signal in high frequency. This indicates a relationship between dielectric behavior and conduction mechanisms of the diode.

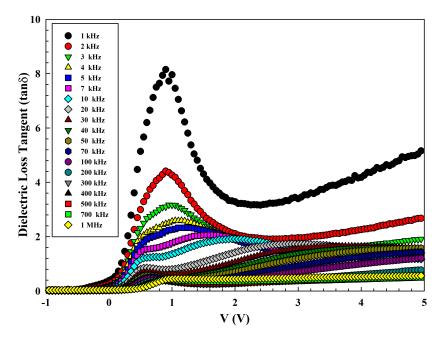


Figure 5.  $\tan \delta$ -V plot for Al/Mg<sub>2</sub>Si/p-Si SD in a wide frequency range.

Physically, the complex electric modulus (M\*) is used to understanding the dielectric relaxation process of the material. M\* provides information about polarization mechanisms in the material and electrical transport process parameters such as carrier hopping rate and conductivity relaxation time. M\* is calculated using  $\varepsilon$ ' and  $\varepsilon$ " and is given as follows [35, 36]:

$$M^* = \frac{1}{\varepsilon^*} = M' + jM'' = \left(\frac{\varepsilon'}{(\varepsilon')^2 + (\varepsilon'')^2}\right) + j\left(\frac{\varepsilon''}{(\varepsilon')^2 + (\varepsilon'')^2}\right),\tag{4}$$

where M' and M'' the real and the imaginary part of M<sup>\*</sup>, respectively. Thus, M'-V and M''-V plots for the  $Al/Mg_2Si/p$ -Si SD were given in Figures 6 and 7, respectively. As shown in Figure 5, the M' is independent of

frequency in the accumulation region. The M<sup> $\prime$ </sup> value reaches its maximum value at high frequencies since the dielectric relaxation mechanisms depend on frequency [37]. As seen in Figure 7, while M<sup> $\prime\prime$ </sup> is independent of frequency in the inversion and accumulation region, it has a peak of different magnitude for all frequencies in the depletion region. M<sup> $\prime\prime$ </sup> reaches the maximum value in high frequency. The peak is shifting to the accumulation region with increasing frequency and its magnitude decreases. This situation is due to the Maxwell–Wagner type (MWt) interface polarization and the distribution of N<sub>ss</sub> ingrained at the junction of the interfacial layer (the Mg<sub>2</sub>Si) and the semiconductor (p-Si) [38,39]. The charges placed in N<sub>ss</sub> affect both the electrical and dielectric properties. Because these traps or permitted energy levels can both hold and release some loads under an electric field or applied bias voltage. Most types of N<sub>ss</sub> that have different lifetimes can be used at low frequencies because they can catch up with the ac signal.

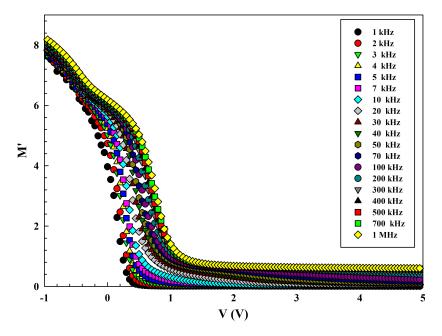


Figure 6. M/-V plot for Al/Mg<sub>2</sub>Si/p-Si SD in a wide frequency range.

The conductivity properties and load storage capability of the structure can be examined using the AC electrical conductivity ( $\sigma_{AC}$ ) given in Eq. 5 [40,41].

$$\sigma_{AC} = \omega C \left( \tan \delta \right) \left( \frac{d_i}{A} \right) = \omega \varepsilon_0 \varepsilon''.$$
(5)

According to Eq. (5),  $\sigma_{AC}$  only depends on  $\varepsilon$ ". Figure 8 shows the  $\sigma_{AC}$ -V plot of Al/Mg<sub>2</sub>Si/p-Si SD in a wide frequency range. As shown in Figure 8,  $\sigma_{AC}$  is independent of frequency in the inversion and accumulation region and it takes a constant value in these regions. As the frequency increases, the value of  $\sigma_{AC}$  increases due to the decrease of the interface polarization, especially in depletion and accumulation regions. This increase causes an increase in eddy current. Such phenomena can be explained by a gradual decrease in series resistance (R<sub>s</sub>) of the structure with increasing frequency [42–44]. In other words, the energy loss increases due to the increasing eddy currents. As the electrical conductivity increases, the value of tan $\delta$  also increases. The increasing  $\sigma_{AC}$  values are the result of  $\varepsilon$ ", especially at high frequencies. In recently, similar results have been reported in the literature by various workers [37, 45–48].

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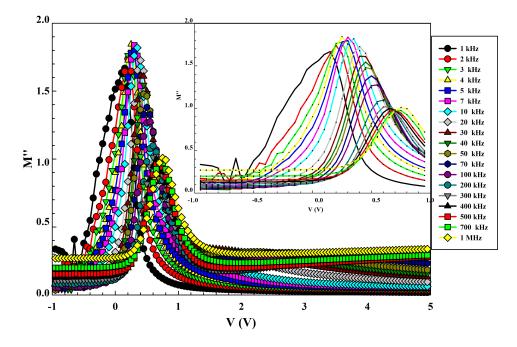


Figure 7. M//-V plot for  $Al/Mg_2Si/p-Si$  SD in a wide frequency range.

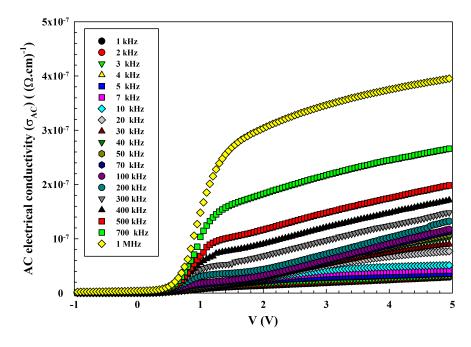


Figure 8.  $\sigma_{AC}$ -V plot for Al/Mg<sub>2</sub>Si/p-Si SD in a wide frequency range.

#### 4. Discussion

The complex dielectric permittivity ( $\varepsilon^* = \varepsilon' - j\varepsilon''$ ), dielectric loss tangent (tan  $\delta$ ), the complex electric modulus (M<sup>\*</sup>=M'+jM'') of the Al/Mg<sub>2</sub>Si/p-SiSD and its AC electrical conductivity ( $\sigma_{AC}$ ) were calculated using the admittance measurements including measured capacitance and conductance data in a wide range from 1 kHz

to 1 MHz. The variation of the frequency-dependent dielectric properties mainly depends on the electric dipole polarization, the interface polarization and the density distribution of the  $N_{ss}$ . Additionally, the values of  $\varepsilon \prime$ ,  $\varepsilon''$ , tan $\delta$ , M/ and M// for the Al/Mg<sub>2</sub>Si/p-Si SD were found as 0.756, 0.425, 0.562, 1.005 and 0.565 for 1 MHz at +5 V bias, respectively. The  $\varepsilon$ ' is associated with interfacial and directional polarization while  $\varepsilon$ ''is associated with transmission loss. The variation in values of  $\varepsilon$ ',  $\varepsilon$ " and tan  $\delta$  was attributed to the surface states, interfacial polarization and the decrease of C and G with increasing frequencies.  $N_{ss}$  follows the alternating signal especially at low or intermediate frequencies and affects the capacitance and conductivity values. The  $\tan \delta$  has a peak at low frequencies and this peak decreases with increasing frequency. This decrease was attributed to the inability of the hopping electrons to follow the external ac signal, with the dipole and surface polarizations reaching a constant value at high frequencies. The maximum value of the M<sup>1</sup> at high frequencies is due to the frequency sensitivity of the dielectric relaxation mechanisms. The peak behavior of M'' in the depletion region has been attributed to the distribution of  $N_{ss}$  ingrained at the junction of the Mg<sub>2</sub>Si and the p-Si and the MWt interface polarization. The increase in  $\sigma_{AC}$  with increasing frequency only contributes to the dielectric loss. Besides, the lost current caused by this increase increases the tan $\delta$ . This situation has been explained as the  $R_s$  decreases gradually with the increase in frequency. The obtained results showed that all-dielectric parameters ( $\varepsilon'$ ,  $\varepsilon''$ , tan $\delta$ , M<sup>I</sup>, M<sup>II</sup> and  $\sigma_{AC}$ ) of the fabricated Al/Mg<sub>2</sub>Si/p-Si SD depend on extreme frequency. Additionally, experimental results showed that the  $Mg_2Si$ , which is coated between the metal and semiconductor interface via spin coating method, can be used for more electronic charge storage instead of conventionally used dielectric materials  $(SnO_2, SiO_2)$ .

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