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Dielectric properties and ac electrical conductivity of MIS structures in the wide frequency and temperature range

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Dielectric properties and electrical conductivity of the Al/SiO$_2$/p-Si (MIS) structures have been investigated in the temperature and frequency range of 80-400 K and 1 kHz-100 kHz, respectively. Experimental results show that the dielectric constant (ε'), dielectric loss (ε''), loss tangent (tanδ) and ac electrical conductivity (σ_{ac}) were found expect 100 kHz a strong function of frequency and temperature. The dielectric constant ε' especially shows a maximum about at 300 K, which shifts to high temperature with increasing frequency. On the other hand dielectric loss ε'' decreases with increasing both frequency and temperature, and at high temperature becomes frequency- independent. The decrease in the ε" with increasing frequency can be understood in terms of a decrease in electrical conductivity. In addition, the experimental dielectric data have been analyzed in the light of electric modulus formalism. The values of σ_{ac} conductivity show strong frequency dependence at high temperatures while at low temperatures becomes almost constant. The Lnσ_{ac} vs q/kT plots show that the activation energy (E_a) decreases with increasing frequency and they are found as 65.8 meV and 56.5 meV for 1 kHz and 100 kHz, respectively. It was observed that at low temperature, the dipolar and space charge polarization process may be dominating the dielectric relaxation, while at high temperature; the thermally activated mechanism is more significant.

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1. Introduction

In general, there are several possible sources of error, which cause deviations of the ideal behavior such as dielectric and electrical conductivity properties, must be taken into account. These include the preparation condition, effects of interfacial insulator layer, localized electric charge carriers, series resistance and formation of barrier height. The study of dielectric properties produces valuable information on the behavior of localized electric charge carriers leading to greater understanding of the mechanism of dielectric polarization in the studied such as metal-insulator-semiconductor (MIS) and metal-oxide-semiconductor (MOS) structures. Nevertheless satisfactory understanding in all details has still not been achieved. If measurements are carried out at efficiently high frequencies (f≥1MHz), such the carrier life time τ is much larger than period (T), the charges at the interface cannot follow an ac signal. In contrary, at low frequencies the charges can easily follow an ac signal and they are capable of these charges increase with decreasing frequency [1-8]. Therefore, the frequency and temperature dependent dielectric and electrical conductivity characteristics are very important according to accuracy and reliability result [9-21].

In generally, there are four mechanisms which contribute to the dielectric polarization of a material: (a) electronic, (b) ionic, (c) space charge or interfacial and (d) dipolar polarization. The first two contribute to the dielectric constant at higher frequencies and later two to that at the lower frequencies. Both the ionic and electronic polarization decreases marginally with an increase in temperature. With the increase in temperature, ionic distances increase which affects both the ionic as well as the electronic contributions to polarization, both is getting weaker as the temperature rises [17, 22, 23]. The dipolar polarization being inversely proportional to temperature decreases with increasing temperature [22, 23]. It is well-known that the contribution of dipolar and space charge polarization is most significant at low frequency [24].

In this study, dielectric and electrical conductivity properties of MIS structure are measured with the help HP 4192A LF impedance analyzer. The dependence of temperature and frequency on the dielectric constant (ε'), dielectric loss (ε''), loss tangent (tanδ) and the ac electrical conductivity (σ_{ac}) of MIS structures have been studied by using C-V and G/ω-V measurements technique in the frequency and temperature range of 1 kHz-100 kHz and 80-400 K, respectively. Experimental results show that the values of ε', ε'' and tanδ changes with both frequency and temperature.

2. Experimental procedure

Al/SiO$_2$/p-Si (MIS) structures were fabricated on float zone <100> boron-doped (p-type) single crystal Si wafer, having a thickness of 280 μm with 8 Ω-cm resistivity. For the fabrication process, Si wafer was degreased in organic solvent of CHClCCl2, CH3COCH3 and CH3OH, etched in a sequence of H2SO4 and H2O2, 20% HF, a solution of 6HNO3:1HF:35H2O, 20% HF and finally quenched in de-ionised water of resistivity of 18 MΩ.cm for a prolonged time. High purity (99.999 %) aluminium with a thickness of ~2000 Å was thermally evaporated from the tungsten filament onto the whole backside of half wafer at a pressure of ~2x10^{-6} Torr. The ohmic contacts were prepared by sintering the evaporated Al back contact at 650 °C for 75 minutes under dry nitrogen flow at rate of 2 lit./min. This process served to sinter the aluminium on the upper surface of the Si wafer. After deposition of ohmic contact, the front surface of the Si wafer was exposed to air in sterile glass box for two years at room temperature. The front rectifier contacts were produced by the evaporation of 2500 Å thick aluminium dots of ~1 mm in diameter onto the Si wafer. The thickness of metalic layer and the deposition rate were monitored with the help of Inficon XTM/2 thickness monitor. By this way, metal-semiconductor (MS) diode with a thin interfacial insulator layer (SiO_2) was fabricated on p-type Si. The interfacial layer thickness was estimated to be about 55 Å from the oxide capacitance measurement in the strong accumulation region at high frequency. Temperature dependence of admittance measurements (C-V and G/w-V) characteristics of Al/SiO_2/p-Si (MIS) structures were measured in the frequency and temperature range of 1 kHz-100 kHz and 80-400 K, respectively. The C-V and G/w-V measurements carried out by using an HP4192 A LF impedance analyzer and the test signal of 40 mV_{rms}. All measurements were carried out in a Janes VPF-475 cryostat with the help of a microcomputer through an IEEE-488 ac/dc converter card. The sample temperature was always monitored by means of a copper-constantan thermocouple and a Lakeshore 321 auto-tuning temperature controller with sensitivity better than ± 0.1 K.

3. Results and discussion

The frequency and temperature dependence of admittance measurements (C-V and G/w-V) are widely used to obtain accurate information concerning both electrical and dielectric properties in MIS or MOS structures. The applied ac signal causes the Fermi level to oscillate about the mean positions governed by the dc bias, when the MIS structure is in the depletion region. The variation of capacitance and conductance with temperature at different frequencies of the MIS structure are shown in Fig. 1(a) and (b), respectively. As can be seen in Fig. 1, both C-V and G/w-V characteristics especially at low frequencies and temperatures are very sensitive both to frequency and temperature. As can be seen in Fig.1(a), the values of C gives a peak in almost each frequency and this anomalous peak has a tendency to disappear at high frequencies.

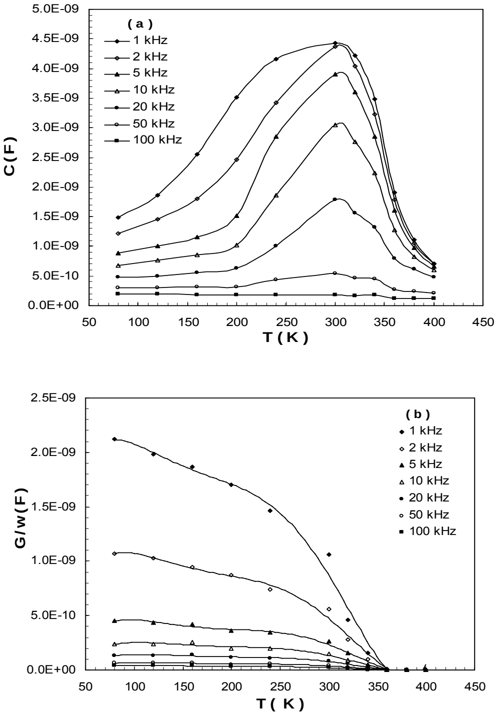

Fig. 1. Variation of the (a) capacitance (C) and (b) conductance (G/ω) with temperature at different frequencies for Al/SiO$_2$/p-Si (MIS) structure at various frequencies.

Such behaviour shows that there are various kinds of interface states with different lifetimes and they can follow an ac signal at low frequencies, but cannot follow at high frequencies [1,6,11]. Similarly, Fig. 1(b) shows the variation of conductance in depletion region for the same frequency interval, indicating the existence of different time-dependent responses of interface states. In addition, such behaviour is mainly attributed to the molecular restructuring and reordering of the interface states and series resistance depend on temperature. The presence of the capacitance peak in the forward C-V plots are investigated by a number of experimental results on MIS or MOS structures [11,25,26].

The temperature dependence of the real part of complex permittivity ε' (dielectric permittivity), and the imaginary part of complex permittivity ε'' (dielectric loss factor), loss tangent (tanδ), ac electrical conductivity (σ_{ac}) and the complex electric modulus (M' and M'') were studied for Al/SiO_2/p-Si (MIS) structures as a function of frequency. The values of the dielectric properties measured in the frequency range of 1 kHz-100 kHz and at the temperature range of 80 - 400 K, respectively. The complex permittivity can be defined in the following complex form [27,28]:

$$\varepsilon^* = \varepsilon' - j\varepsilon'' \tag{1}$$

where j is the imaginary root of -1. The complex permittivity formula has been used to describe the electrical and dielectric properties. In the ε^* formulation, in case of admittance measurements (C-V and G/w-V), the following relation equations:

$$\varepsilon^* = \frac{Y^*}{j\omega C_o} = \frac{C}{C_o} - j\frac{G}{\omega C_o} \tag{2}$$

where; Y^*, C and G are the measured admittance, capacitance and conductance of the dielectric respectively and ω is angular frequency ($\omega=2\pi f$) of the applied electric field [29]. The dielectric constant (ε'), at various frequencies was calculated by using the measured capacitance values at the strong accumulation region via the formula [30,31]:

$$\varepsilon' = \frac{C}{C_o} \tag{3}$$

where C_o is capacitance of an empty capacitor. $C_o = \varepsilon_o(A/d)$; where A is the rectifier contact area in cm^{-2}, d is the interfacial insulator layer thickness and ε_0 is the permittivity of free space charge ($\varepsilon_o = 8.85\times10^{-14}$ F/cm). In strong accumulation region, the maximal capacitance of devices corresponds to the insulator layer capacitance ($C_{ac} = C_{ox} = \varepsilon'\varepsilon_o A/d$). The dielectric loss (ε''), at various frequencies was calculated by using the measured conductance values from the below equation;

$$\varepsilon'' = \frac{G}{\omega C_o} \tag{4}$$

The loss tangent (tanδ) can be expressed as follows [27,28,30-32],

$$\tan\delta = \frac{\varepsilon''}{\varepsilon'} \tag{5}$$

The effect of conductivity can be highly suppressed when the data are presented in the modulus representation.

The ac electrical conductivity (σ_{ac}) of the dielectric materials is proportional to tanδ, in other words ε'' and can be given by the following equation [27,33,34],

$$\sigma_{ac} = \omega C \tan\delta(d/A) = \varepsilon''\omega\varepsilon_o \tag{6}$$

The dielectric properties of Al/SiO$_2$/p-Si (MIS) structures are measured with the help HP 4192A LF impedance analyzer. The instrument directly provides the values of capacitance and conductance (Fig. 1(a) and (b). The variation of the dielectric constant (ε'), dielectric loss (ε''), loss and tangent (tanδ) as a function temperature at few selected frequencies for the MIS structure are shown in Fig. 2(a)-(c), respectively. Experimental results show that the values of ε', ε'' and tanδ were found strongly frequency and temperature dependent. As can be seen from Fig. 2(a), the variation of dielectric constant (ε') provides a peak at particular temperature for each frequency except for 100 kHz. The peaks are shifted towards higher temperature side on increasing frequency. The temperature at which dielectric constant (ε') become maximum (i.e., ε'_{max}) is denoted by T_{max} for a particular frequency. The values of ε'_{max} and T_{max} at different frequencies are listed in Table 1. It is clear from the table that ε'_{max} varies from 3.68 at (1 kHz, 280 K) to 0.40 at (50 kHz, 315 K).

Such behaviour shows that there are various kinds of interface states with different lifetimes and they can follow an ac signal at low frequencies. On the other hand, the values of ε'' and tanδ decreases with increasing temperature for each frequency and becomes almost constant in the high temperature region.

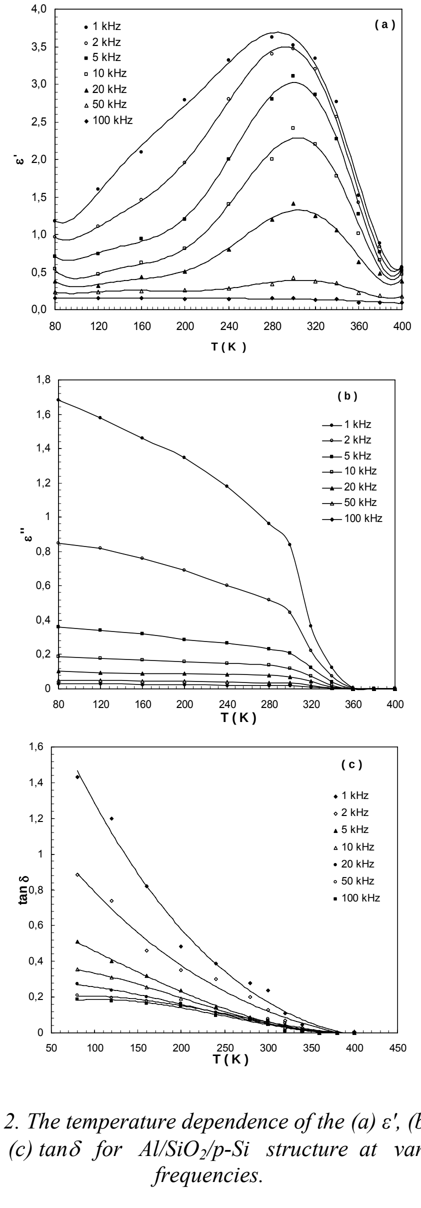

Fig. 2. The temperature dependence of the (a) ε', (b) ε'' and (c) tanδ for Al/SiO$_2$/p-Si structure at various frequencies.

Table 1. Comparison of T_{max} and ε'_{max} of $Al/SiO_2/p$-Si (MIS) structure at various frequencies.

f (kHz)	T_{max} (K)	ε'_{max}
1	280	3.68
2	295	3.50
5	300	3.00
10	305	2.30
20	310	1.30
50	315	0.40

These variation of ε', ε'' and tanδ may be attributed to especially, dipolar and space charge polarization which may come into play at different stages of its responses to varying temperature and frequency of the applied alternating field.

The temperature dependence of ac conductivity (σ_{ac}) for different frequencies is shown in Fig. 3(a). As shown in Fig. 3 (a), the values of ac conductivity increase with increasing temperature for all frequencies. The variation of σ_{ac} was remarkably high at high temperatures, but it was very small at low temperatures. This behavior of conductivity with increase temperature is typical of semiconductor behavior. As ac conductivity (σ_{ac}) is thermally activated processes, we calculated the activation energy (E_a) using a well-established empirical relation;

$$\sigma_{ac} = \sigma_o \exp(-qE_a / kT) \tag{7}$$

where σ_o pre-exponential factor, k the Boltzmann constant. The temperature dependent ac conductivity data obtained in the range of 80 - 400 K can be fitted to Arrhenius plot Eq.7 as shown in Fig. 3(b). As shown in Fig. 3(b), there are a linear relationship between the total conductivity and the inverse absolute temperature.

The values activation energy (E_a) obtained from the slope of Ln (σ_{ac}) vs q/kT plot for each frequency and are given in Table 2. It is clear that from Table 2, the value of E_a decreases with increasing frequency and varies from 65.8 meV at 1 kHz to 56.5 meV at 100 kHz. These values are far away from the mid-gap energy, which is around 1.12 eV for Si. Thus, it can be assumed that the observed exponential behaviour is not due to intrinsic conduction. This small activation energy corresponds to the first ionized oxygen vacancy, which indicates that in this temperature range, the free conduction electrons results from the first ionization of oxygen vacancies. In addition, from the same Arrhenius plot, the parameter σ_o can be calculated as $8.37\text{x}10^{-8}$ S.cm^{-1} and $18.11\text{x}10^{-8}$ S.cm^{-1} for 1 kHz and 100 kHz, respectively. It can be concluded that electrical conductivity (σ_{ac}) depends on frequency and temperature and it is reasonable to assume that a range of E_a is involved. Similar behaviour of the ε', ε'', tanδ and σ_{ac} has recently been reported in literature [35,36].

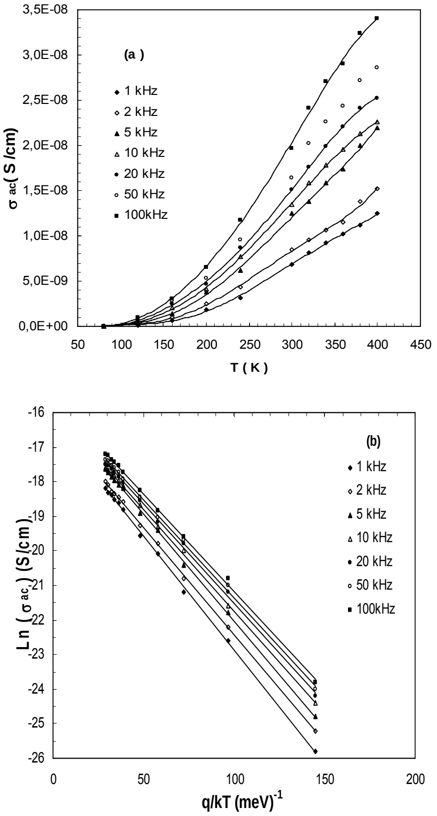

Fig. 3. Temperature dependence of ac electrical conductivity (σ_{ac}) and Arhenius plots, respectively, for $Al/SiO_2/p$-Si (MIS) structure at various frequencies.

Fig. 4 shows the Lnσ_{ac} vs frequency curves at different temperatures. As shown in Fig. 4, the dependence of ac electrical conductivity (σ_{ac}) decreases with increase of temperature at higher frequencies. Such behavior of temperature dependence of σ_{ac} can be attributed to the ionic hopping conduction could be dominant at lower temperatures in the high frequency range. It is clear that the values of σ_{ac} are weakly dependent on frequency especially at high temperatures. Similar results have recently been reported in literature [14,17,37].

Table 2. The values of E_a and σ_o of $Al/SiO_2/p$-Si(MIS) structure at various frequencies.

f (kHz)	E_a (meV)	σ_0 (Ωcm^{-1})
1	65.8	$8.370\text{x}10^{-8}$
2	62.0	$8.914\text{x}10^{-8}$
5	61.7	$1.297\text{x}10^{-7}$
10	59.0	$1.312\text{x}10^{-7}$
20	57.4	$1.406\text{x}10^{-7}$
50	56.6	$1.529\text{x}10^{-7}$
100	56.5	$1.811\text{x}10^{-7}$

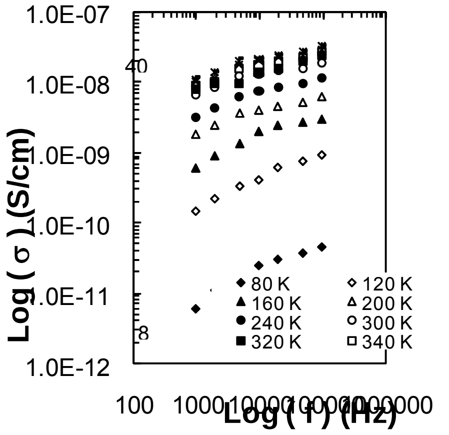

Fig. 4. The variation of Lnσ_{ac} vs logf of Al/SiO$_2$/p-Si(MIS) structure at various temperatures.

4. Conclusions

Frequency and temperature dependence of dielectric properties and ac electrical conductivity of Al/SiO$_2$/p-Si (MIS) structure have been studied in detail at low frequencies ($f \leq 100$ kHz) and a wide range of temperature (80-400 K). Experimental data show that the dielectric constant (ε'), dielectric loss (ε''), loss tangent ($\tan\delta$), ac electrical conductivity (σ_{ac}) were found a strong function of frequency and temperature. While the values of ε'' and $\tan\delta$ decreases with increasing temperature the ε' provides a peak at particular temperature for each frequency except for 100 kHz. The peaks are shifted towards higher temperature side on increasing frequency. The Ln(σ_{ac}) vs q/kT plots show that the activation energy (E_a) decreases with increasing frequency and varies from 65.8 meV at 1 kHz to 56.5 meV at 100 kHz. In addition, from the same Arrhenius plot, the parameter σ_o can be calculated as 8.37×10^{-8} S.cm^{-1} and 18.11×10^{-8} S.cm^{-1} for 1 kHz and 100 kHz, respectively. From the E_a at different frequencies, it is clear that space charge and oxygen vacancies play an important role in the conduction processes. In summary, at low frequencies and temperature, especially the dipolar and space charge the polarization process may be dominating the dielectric relaxation, while at high temperature; the thermally activated mechanism is more significant.

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