CHAPTER 2

THEORY AND EXPERIMENTAL TECHNIQUES.

Various experimental techniques have been used to study the thickness, electrical and optical behaviour of the deposited tantalum oxide films. A brief detail of these techniques and the theory are presented in this chapter.

2.1. THICKNESS MEASUREMENT.

The measurement of the thickness of the film is an essential parameter. It largely determines the optical and electrical properties of the film. As a matter of fact almost all the properties of a thin film are found to be functions of thickness. The thickness of a thin film is generally is of the order of a few angstroms to nearly a 100nm. Special techniques have been employed, as common thickness measurements do not suit the measurements of thickness of a thin film. The most commonly used methods are

1. Ellipsometry

2. Stylus method

3. Multiple beam interferometry.

Ellipsometry [1] is a non-destructive method for measuring both thickness and refractive index of transparent thin films. It is based on measurement of angles, phase angles, phase difference and amplitude ratios. The measurements in this investigation have been made using Rudolph-auto ellipsometer.

36
When a plane-polarized light is reflected from a thin film the state of polarization of the reflected light is altered usually becoming elliptically polarized. The magnitude of these changes depends on the thickness and refractive index of the film. Hence the change in the magnitudes of polarization can reveal both thickness and refractive index of the film. The ratios of the reflected amplitude for light polarized parallel to and perpendicular to the plane of incidence gives $\tan \psi$ and the relative phase difference between them is given by $\Delta$. These two parameters can be measured directly by the ellipsometer. These experimental results are converted into thickness by substituting the known value of the refractive index of the film.

The Stylus (Talysurf) method [1] is a surface profile measurement technique. The thickness of a film of any material is measured by moving a small diamond stylus across a test groove formed in the material or over the edge of a step from the deposit of a substrate.

The vertical shift movement at this step of the stylus on the film is converted onto electrical output by a transducer system. The amplitude of the electrical signal will be proportional to the thickness of the film. The steps on the film for stylus measurement are produced by masking a little portion of this substrate during a deposition process.

Talysurf comprises of a fine diamonds tip with a radius of 0.7–1μm, which is gently pressed on to the surface (with a pressure of nearly 100kp/cm²). The diamond tip moves uniformly on the test surface and a strip chart recorder records the output. As and
when it crosses the step the amplitude of the output increases proportionately and the recorder records the step height.

The results obtained by ellipsometer measurement are in good agreement with the results of the Talysurf method. The stylus method is not only used for thickness measurements but also for surface topography. The disadvantage of this method is it is a destructive method, if the films are soft.

2.2. STRUCTURE OF THE FILM.

X-ray diffractometry is a technique for the characterization of thin films [1.2,3] since it provides a very broad range of information about the material in its thin film form. The data that can be interpreted from an XRD includes nature of capability, existence of preferred orientation stress and strains in the films and its composition in the near surface regime. XRD can reveal more information about the film than any other single type of characterization. It is purely non-destructive and film does not get damaged due to prolonged exposure to X-rays.

The incident X rays undergo diffraction according to Bragg’s relation \( \lambda = 2d \sin \theta \). Since the wavelength \( \lambda \) and diffraction angle \( \theta \) are known from the experiment, the lattice spacing \( d \) can be evaluated.[2,3]. [The value of \( \lambda = 1.5418 \text{\AA} \) for \( Cu \) K\( \alpha \) radiation, \( \lambda = 1.7902 \text{\AA} \) for \( Co \) K\( \alpha \) radiation]. The obtained values (SCINTAG X RAY DIFFRACHTOMETER) are compared with available standard patterns ASTM Charts [4,5] to index each of the peaks. Thus the existence of diffracting planes of the film can be
established [6,7]. The width of the peak also gives some useful information. The full width at half maximum (FWHM) can be used to determine grain size using the formula.

\[ D = 0.9 \lambda \cos \theta. \]

\[ \lambda = \text{The wavelength of X-ray}. \quad B = (B_m^2 - B_s^2)^{1/2} \quad \text{where } B_m \text{ is the full width at half maximum of the peak of the sample and } B_s \text{ is the full width at half maximum of the peak of the powder sample (standard) in radian. } \theta = \text{angle at which the peak occurs}. \]

However, grain size by this calculation is approximate and it is the average value for the film. The shift in the reflection from the standard value can be used estimate the total residual stress in the film assuming that the shift is not due to any instrumental errors.

The expression that relates the stress \( \alpha \) to the observed inter planar spacing \( d \), the standard \( d_0 \) and the elastic constant \( E \) (Young’s modulus) and \( \gamma \) the Poisson’s ratio of the material (bulk) is

\[ \alpha = \frac{E}{1-\gamma} (d - d_0/ d_0 ). \]

When \( \alpha \) is positive the stress is tensile. When \( \alpha \) is negative the stress is compressive. The expression assumes bulk values of elastic constants of the material. Therefore the magnitude of the stress calculated may not be accurate, however the direction of the stress is correct.

2.3. OPTICAL PROPERTIES

The deposited films were characterized for their following optical properties:

1. Spectral transmittance in the wavelength region 200nm to 900nm
2. Refractive index

3. Extinction co-efficient

4. Optical band gap

The spectral transmittance of the films was measured in the wavelength region of 200 - 900 nm using HITACHI 330 model spectrophotometer. Using the transmittance data, refractive index and extinction co-efficient of the film were calculated using the envelope technique developed by Swanepoel [8]. The refractive index of the film $n(\lambda)$ is given by

$$n(\lambda) = \sqrt[4]{N + (N^2 - S^2)^{1/2}}$$

Where

$$N = \{2S[(T_M(\lambda) - T_m(\lambda)) / T_M(\lambda)] T_m(\lambda) / (S^2 + 1) / 2\}$$

$S$ is the refractive index of the substrate

$T_M$ is the transmittance maximum

$T_m$ is the transmittance minimum in the envelope of the transmittance spectrum.

The refractive index of the film is calculated at two wavelengths $\lambda_1$ and $\lambda_2$ in the envelope. The thickness of the film is calculated using the formula,

$$t = \lambda_1 \lambda_2 / 2 (n_1 \lambda_2 - n_2 \lambda_1).$$

The extinction co-efficient is determined using the equation

$$K = \alpha \lambda / 4\pi$$

Where $\alpha = -\log x / t$ and

$$x = E - [E_m - (n^2 - 1)^3 (n^2 - s^2) / (n - 1)^3 (n - s^2)]^{1/2} / (n - 1)^3 (n - s^2)$$

$$E_m = \{8n^2s / T_M\} + (n^2 - 1) (n^2 - s^2).$$

A computer program to calculate constants $n$ and $k$ was developed.
2.4 OPTICAL BAND GAP:

The optical band gap of dielectric material provides information about its stoichiometry. It is therefore a very useful parameter in indirect estimation of stoichiometry. Taking the bulk band gap values as reference a qualitative approximation of the oxygen content in the film can be made. To calculate the band gap of films in the present study the following method was adopted.

The dispersive curve for refractive index was extrapolated linearly to obtain \( n_f \) values at the wavelengths below, which the \( T_{max} \) and \( T_{min} \) envelopes intersect. These wavelengths in the case of tantalum oxide films between 240nm and 280nm. From the expressions given by Swanepol [8] for the extinction co-efficient in the regions of strong absorptions the values of \( k \) is given by

\[
 k = \left\{ \left( n_f + 1 \right)^3 \left( n_f + S^2 \right) \right\} / 16 n_f^2 S = e^{-\alpha l}
\]

\( \alpha = 4\pi k/\lambda \) is the absorption in cm\(^{-1} \) at wavelength \( \lambda \).

\( k \) is the extinction co-efficient and

\( t \) is thickness of the film.

The fundamental absorption probability [9] or the direct transition probability due to the absorption of photon energy is given by

\[
\alpha h\nu = A (h\nu - E_g)^{1/2}
\]

Where \( A \) is a constant and \( E_g \) is the optical band gap (in eV) and \( h\nu \) is the energy of photon. Hence a graph can be obtained by plotting \( \alpha \) against \( h\nu \). The extrapolation of the linear region of the curve meets the X-axis giving an intercept. The value of the intercept on X-axis represents the value of the optical band gap \( E_g \) for fundamental absorption.
2.4.1. INTER-BAND TRANSITIONS:

The energy band gap is found to be composition dependent in dielectric films [9,10]. The reflectance spectrum obtained shows absorption of optical energy at different regions. The photon electron interaction leads to indirect transition probability. Electron interacting with a photon absorbs the radiation without being excited into the other band, but the probability is to make a transition to another state in the same band, which is referred to as interband transition. It takes place even when \( h\nu \) is less than \( E_g \) and they dominate below the absorption edge. For \( h\nu \) greater than \( E_g \) both fundamental absorption and indirect absorption occur simultaneously. The indirect absorption probability is given by the equation:

\[
(\alpha h\nu)^{1/2} = A(h\nu - E_g)
\]

\( E_g \) gives the indirect allowed energy band gap due to generation of phonons [6].

In addition to photon phonon interaction there are electronic inter band transition-generating an exciton [7,9,10].

An exciton moves through the crystal and transport energy to the atoms. When the transition is accounted for, then excited states occur with their energies in the forbidden gap.

Excitons may be formed by direct photons only [6,11,12]. This probability in the forbidden band gap is represented by

\[
(\alpha h\nu)^{2/3} = A(h\nu - E_g)
\]

\( E_g \) gives direct forbidden band gap.
Excitons may also be formed by photon phonon interaction. The phonon assisted probability or indirect absorption probability in the forbidden gap is represented by

\[(\alpha \ h \ v)^{1/3} = A \ (h \nu - E_g)\]

\(E_g\) gives the indirect forbidden band gap energy.

2.5. DIELECTRIC PROPERTIES.

Tantalum Oxide have rapidly evolved in to an important field of research and development of both basic and applied science with the promise of creating a new generation of advanced micro devices and electronics applications. \(\text{Ta}_2\text{O}_5\) thin films standout as holding the largest promise to potentially replace \(\text{SiO}_2\) in small-scale MIS and MIM capacitor devices. It is a better dielectric material for high-density Dynamic random access memory applications. It has a high dielectric constant (\(e_r \approx 35\)), high refractive index, chemical and thermal stability and compatibility with microelectronic processing \([13,14]\).

Most of the dielectrics are characterized by four factors namely

1. Relative permittivity.

2. Loss tangent.

3. Dielectric strength

4. Dielectric Breakdown.

If \(C_0\) is capacitance of a capacitor with the region between the two conductors with free space and \(C\) is its capacitance when the region is filled with the dielectric then
the ratio \( \frac{C}{C_0} = \varepsilon_r \) is found to be independent of shape or dimensions of the conductor and is solely a characteristic of the particular dielectric medium used.

From the dielectric constant profiles studies Seki et al. [15] pointed out that the crystallographic orientation of the substrate has no influence on homogenous layer formation of the dielectric. They have reported [16] the variation in the dielectric constant with the total thickness of the film.

\[
\varepsilon = \varepsilon_0 \varepsilon_r \text{ is the absolute permittivity of the dielectric medium.}
\]

\[
\varepsilon_0 = 8.854 \times 10^{-12} \text{ F/m} \text{ is the absolute permittivity of free space.}
\]

Dielectric breakdown in materials is an important parameter in expressing capacitor performance. Although an ideal dielectric is expected to behave as an insulator always, in actual practice there is maximum field intensity for every material beyond which damage occurs that results in conduction and breakdown phenomenon. This is expressed by saying that the dielectric loses its insulating property and becomes a conductor after the dielectric breakdown occurs. The magnitude of the electric field at which dielectric exhibits a tendency to breakdown is called the dielectric strength of the material. It is a function of the oxide thickness [17] and is defined as average electric field through the film at a leakage current of \( 1 \times 10^{-7} \text{ A/cm}^2 \). Its dielectric strength depends also on \( \text{Ta}_2\text{O}_3 \) formation temperature [18].

The study of breakdown in thin dielectric film can contribute new ideas in understanding the phenomenon. From the study of discharge of electricity through gases one can understand that in solids also there is a propagating phenomenon in an avalanche
of charge carriers [19]. Such a philosophy is not accepted generally because breakdown to a thermal effect, i.e. the current density even without an avalanche multiplication generates more heat in to the dielectric than the dielectric is able to dissipate to the external surroundings [20]. However the avalanche theory seems to be more appropriate as it gives a better fitting explanation of the experimental results [21].

In solids one kind of charges i.e. the ionic cores are practically motionless. On the other hand the electrostatic potential generated by the ionic cores affects in two ways the motion of the other kind of charge carriers, namely the loosely bound electrons. Due to presence of ionic cores in the lattice sides the electrons exhibit an effective mass different from that of free electrons.

Due to the possibility of inducing lattice vibrations the electron-phonon scattering determines the electron mobility.

The dielectric breakdown depends on the presence of large quantity of loosely bound electrons, which are generally indicated as conduction electrons. But because we deal with insulators the question is in which way these conduction electrons originate? C.Zener [21] proposed an internal emission, which causes electrons to jump from the valence band to the conduction band because of the applied electric field provoking the breakdown in the insulators.

In this context two facts are co-operating to understand the breakdown in dielectrics:
1. The electron density in the conduction band dependent upon an applied electric field.

2. Multiplication of this density because of an avalanche phenomenon. The breakdown should occur when the increase of the energy of all the electrons exceeds the energy lost due to the electron-phonon scattering [22]. This is generally referred to as low energy criteria. But according to Frohlich [23] the electron change very frequently the direction of their motion just because of phonons and the net increase of their energy results to be proportional the second power of their field strength. This is generally indicated as high-energy criterion. Here the break down should satisfy two conditions:

1. The field strength is such that the electrons are accelerated up to the ionization energy of the material.

2. The break down field is the highest one for which a balance between ionizing collisions and the charge recombination is reached.

But low energy criterion and high-energy criterion do not explain any dependence on either dielectric film thickness or the cathode material.

The dielectric strength of a material depends in a complicated fashion on a wide variety of variables such as

1. Nature of the material
2. Temperature
3. Humidity
4. Presence of defects
5. Length of time for which the electric field is applied
6. The magnitude of the electric field

The dielectric phenomena can be described in terms of the field. If the distance between the plates of the capacitor is \(d\) then for an applied potential \(V\), the electric field intensity is

\[ E = \frac{V}{d}. \]

The effect of introducing dielectric onto the capacitor can be understood by considering the effect of the applied electric field on the bound charges in the dielectric [24].

The very low conductivity in a dielectric indicates that for all practical purposes the free charges are absent in the material. The action of the field on the bound charges is to displace them slightly relative to one another. The positive charges are displaced in the direction of the field and the negative charges in the opposite direction. Each atom then acquires an electric dipole moment parallel to the direction of \(E\). This effect is called dielectric polarization denoted by \(P\). It is defined as the induced dipole moment per unit volume.

\[ P \propto E \text{ or} \]

\[ P = \varepsilon_0 E \chi. \]

Where \(\chi\) is called Electrical susceptibility.

The dielectric displacement represents the combined effect of applied electric field and electrical polarization it is denoted by \(D\):

\[ D = \varepsilon_0 E + P \]

\[ D = \varepsilon_0 E + \chi \varepsilon_0 E = \varepsilon_0 E (1 + \chi) \]

\(\varepsilon_0(1 + \chi) = \varepsilon\) is the absolute permittivity of the dielectric material.
\( (1 + \varepsilon) = \varepsilon_r \) is the relative permittivity of the dielectric material or dielectric constant.

Therefore \( D = \varepsilon_r \varepsilon E \).

There are four major types of polarization, which takes place in a dielectric:

1. Electronic polarization which prevails in all dielectrics since it is due to the displacement if the negative electron clouds of each atom from its nucleus. It is given by \( \alpha_e = 4\pi \varepsilon_0 a^3 \). The electronic polarizibility is a function of the atomic radius ‘a’ only and it is independent of temperatures at moderate temperature.

2. Ionic polarization is due to the displacement of adjacent ions of opposite sign and is found only in ionic substances. During chemical bonding the atoms may acquire an excess negative or positive charge from an ionic bond. When an electric field is applied to an ionic crystal Cations and Anions get displaced in opposite directions. The ionic polarisability is due to this shift of ions relative to other oppositely charged neighbours. In an electric field the resultant torque lines up the dipole parallel to the field at absolute zero temperature. The field produces forces on the two charges of opposite sign so that the distance between them is changed by some amount. The balance between the electrostatic force and the inter-atomic force due to stretch or compression gives the value of the change in the distance between two ions of opposite charge. From this change in the distance the ionic polarization and hence ionic dipole moment can be determined. It is
denoted by $\alpha$. Ionic polarizibility is also independent of temperatures at moderate temperatures.

3. Orientation polarization occurs in liquids and solids that have asymmetric molecules whose permanent dipole moments can be aligned by the external field.

The orientation polarization is

$$P_o = N P_p L(x)$$

Where $P_p$ is the dipole moment of Permanent dipoles.

$N$ is the number of permanent dipoles.

$L(x)$ is called the Langevin Function.

If $x$ is very small (atomic dimensions) $L(x) = x/2$ then

$$P_o = (N/3) \left( P_p^2 E / 3 K T \right)$$

$E$ is the external field applied

$K$ is the Boltzmann constant.

The orientation polarization per molecule is

$$\alpha_o = P_p^2 / 3 K T$$

At room temperature the orientation polarization is same as electronic polarization.

4. The polarization depends on the frequency of the applied field. This is called dielectric dispersion, which leads to the complex dielectric constant.

When we consider material subjected to a static electric field (D.C. potential) we define its relative permittivity $\varepsilon_r$. When the capacitor is subjected to an alternating electric field two situations arise.
a. When there is no measurable phase difference between $D$ and $E$ then polarization will be in phase with the applied electric field, then $D = eE$ is the valid relation.

b. When there is a phase difference between $D$ and $E$, the polarization $P$ is not in phase with the applied electric field.

The basic difference between the two situations is that when $P$ is in phase with $E$ no energy is absorbed by the dielectric from the applied electric field. When $P$ is not in phase with $E$, energy is absorbed by the dielectric, which is known as the dielectric loss or the loss factor.

Consider an alternating voltage $E$ applied to a parallel plate capacitor of capacitance $C_0$ with its equivalent resistance $R$ as shown in fig 2.1 The charge on the capacitor at any instant is $Q = C_0 E$ and $E = E_0 e^{j\omega t}$, $\omega = 2\pi f$ (f is the frequency of applied ac voltage)

![Equivalent circuit of a practical capacitor applied with A.C.](image)

*Fig 2.1 Equivalent circuit of a practical capacitor applied with A.C.*
The charging current $I_c = \frac{dq}{dt} = j\omega C_0 E$ and this current leads the applied voltage by $90^\circ$. When the space between the capacitor plates is filled by a dielectric material, the capacitance increases to $C$ and $C = \varepsilon C_0$.

$$\varepsilon = \varepsilon / \varepsilon_0$$

$\varepsilon$ is the absolute permittivity of the dielectric and $\varepsilon_0$ is the absolute permittivity of free space.

Due to presence of dielectric the charge on the capacitor is increased to $Q = C_0 E$. Consequently the charging current is increased to $I_c = j\omega C E = j\omega \varepsilon C_0 E$.

Experimentally it is found [6.12.19] that no dielectric material is a perfect insulator, therefore in addition to $I_c$ which leads $E$ by $90^\circ$ there is a loss current $I'$ in phase with $E$ and of magnitude $I' = G E$, where $G$ is the equivalent conductance of the dielectric. $G$ arises because of finite insulation [resistance due to sources of dielectric loss].

The total current through the capacitor $I = I_c + I' = (j\omega C + G) E$.

This total current deviates from the ideal characteristic of phase and leads the voltage $E$ by a phase angle $\theta < 90^\circ$.

And $\cos \theta = I' / I = G / \sqrt{(G^2 + \omega^2 C^2)}$ is the power factor. Alternatively the behavior may be considered in terms of the loss angle $\delta = (90 - \theta)$ where, $\tan \delta = (I' / I_c) = (G / \omega)$

$$[\tan \delta = (1 / \tan \theta)]$$

is called the tangent loss or loss tangent as represented in fig 2.2.
As a special case in the case of dielectric where the loss current is due only to finite conductivity, the capacitor can be represented by an equivalent capacity in parallel with a resistance $R = 1/G$ and the quantity $\tan\delta \propto 1/f$.

Such a behavior is observed in some materials at low frequencies. However in most dielectric materials the behavior differs from this simple form. The behavior indicates the presence of other sources of dielectric loss. The applied voltage $E = E_0 e^{j\omega t}$ gives the current density $J = \delta D / \partial t$. .... $[D = \varepsilon E]$

$$D = D_0 \cos\alpha t, \text{ therefore } J = -\omega D_0 \sin\alpha t.$$  

but when $D$ and $E$ are out of phase by a quantity $\delta$, $D = D_0 \cos (\omega t - \delta)$. Hence it is useful to use a complex notation

$$D = D_0 e^{j(\omega t - \delta)} \text{ And } E = E_0 e^{j\omega t}.$$
Here \( D = D_0 \cos(\omega t - \delta) \) is the real part of the complex notation of electric induction and 
\( E = E_0 \cos \omega t \) is the real part of the complex voltage.

When the phase difference is independent of \( E \) then the ratio of these complex quantities will give a complex dielectric constant \( \varepsilon^* \).

\[
\varepsilon^* = \frac{D_0 e^{i(\omega t - \delta)}}{E_0 e^{i\omega t}} = \frac{D_0}{E_0} e^{i\delta}
\]

The complex relative permittivity \( \varepsilon^* = \varepsilon' - j \varepsilon'' \).

\( \varepsilon' \) is the real part of this complex notation and \( \varepsilon'' \) is the imaginary part, which represents the dielectric loss factor as shown in fig 2.3

\[
\varepsilon' = \frac{D_0}{E_0} \cos \delta \\
\varepsilon'' = \frac{D_0}{E_0} \sin \delta
\]

\[
\therefore \frac{\varepsilon''}{\varepsilon'} = \tan \delta \text{ [ the tangent loss] and }
D_0/E_0 = \sqrt{(\varepsilon'')^2 + (\varepsilon')^2}.
\]

The total charging current \( I = j\omega \varepsilon^* C_0 E \)

\[
I = (j\omega \varepsilon' + \omega \varepsilon'') E C_0
\]

The equivalent conductance \( G = \omega \varepsilon'' C_0 \) and the capacitance \( C = \varepsilon' C_0 \).

The real dielectric constant \( \varepsilon_r \) describes the dielectric property of the material at frequency \( f \).
The power loss = $\pi f E^2 \varepsilon' \tan \delta$.

The analysis indicates that dielectric materials are electrical insulators yet susceptible to polarization in the presence of an electric field. The polarization phenomena accounts for the ability of the dielectrics to increase the charge storing capability of capacitors, the efficiency of which is expressed in terms of a dielectric constant. Polarization results from the inducement by or orientation with the electric field of atomic or molecular dipoles. Not all types of polarization present in a particular dielectric. For alternating electric fields whether a specific polarization type contributes to the total polarization and dielectric constant depends on the frequency of the applied voltage. In the presence of an alternating electric field with each direction reversal the dipoles attempt to reorient with the field, a process requiring some finite time. For each polarization mechanism some minimum reorientation time exists, which depends on the ease with which the particular dipoles are capable of realignment. The reciprocal of this minimum reorientation time is
referred to as relaxation frequency. When the period of applied voltage is much larger than the relaxation time of a polarization process, polarization is essentially complete at any instant during each cycle. The charging current is $90^\circ$ advanced in relation to the voltage so that no electrical energy is lost during charging. When the period of the applied voltage is much shorter than the relaxation time for a polarization process, the process does not occur at all. Here again charging current is $90^\circ$ advanced of the applied voltage. When the period is in the same range of relaxation time resonance occurs. Here the current leads the voltage by $(90-\delta)$. $\delta$ is called loss angle and $\tan\delta$ is taken as a measure of the electrical loss.

A dipole cannot keep shifting orientation direction when the frequency of the applied field exceeds its relaxation frequency and therefore do not make a contribution to the dielectric constant. When the frequency exceeds this limiting value there is an abrupt drop in the dielectric constant. Each polarization ceases to function when the applied frequency exceeds its relaxation frequency [25.26].

2.6 CONDUCTION PHENOMENA IN DIELECTRICS

Tantalum oxide has excellent chemical stability and a large dielectric constant compared with silicon oxide. Ta$_2$O$_5$ films have been studied for applications such as capacitors of dynamic random access memories. However Ta$_2$O$_5$ films tends to exhibit more leakage current than SiO$_2$ or Si$_3$N$_4$ films. Quite frequently post deposition annealing in an oxidizing ambient have been suggested by many authors to reduce the leakage current in the investigation of Ta$_2$O$_5$ deposition.
The problem of leakage current and dielectric breakdown in insulating films has been under discussion since a long time that many books, reviews and research literature are available on this subject.

In an ideal insulator the conductance is assumed to be zero. Real insulators show carrier conduction when the temperature or electric field is sufficiently high. In MIS configuration the applied field (voltage /cm) will partly appear across the insulator and partly across the silicon surface. The applied voltage \( V' = V_i + \psi_s \), where \( V_i \) is the potential across the insulator

\[
V_i = E_i d,
\]

where 'd' is the thickness of the insulator.

\[
V_i = Q_s d / \varepsilon_i
\]

where \( Q_s \) is the total charge per unit area in the region.

\[
V_i = Q_s / C_i
\]

where \( C_i = \varepsilon_i A / d \), and \( A = 1 \text{ cm}^2 \).

The total capacitance of MIS system is a series combination of \( C_i \) due to insulating film and \( C_d \) due to SiO\(_2\) on the silicon surface (depletion layer).

The net capacitance \( C = C_i C_d / C_i + C_d \text{ Fcm}^2 \).

For a given insulator thickness 'd' the value of \( C_i \) is constant and corresponds to maximum capacitance of the system. The capacitance \( C_d \) depends on the voltage \( C_d = \varepsilon_s / L_D \).

where \( L_D \) is extrinsic Debye length.

Since \( E_i \varepsilon_i = E_s \varepsilon_s \)

\[
E_i = E_s \left[ \varepsilon_s / \varepsilon_i \right] \text{ and } \varepsilon_s = \text{ Absolute permittivity of silicon.}
\]
The electric field for silicon at avalanche break down is about $0.3\text{MVcm}^{-1}$ [27].

The corresponding field in the oxide film is about $1\text{MVcm}^{-1}$.

At this strength of the field the conductance is much higher in $\text{Ta}_2\text{O}_5$ than in $\text{SiO}_2$.

Beyond this field the current in the dielectric increases monotonically indicating several conduction phenomenon, namely

1. Schottky barrier controlled conduction.
2. Poole Frankel hopping conduction.
3. Bulk limited space charge conduction.

In Schottky emission process, thermionic emission across the metal insulator surface is responsible for carrier transport. The Poole Frankel emission is due to the field enhanced thermal excitation of trapped electrons in to the conduction band. The tunnel emission is caused by the field ionization of trapped electrons in to the conduction band or by electrons tunneling from the metal fermi energy in to the insulator conduction band. It has strongest dependence on the applied voltage but is essentially independent of the temperature.[28]

The space charge limited current results from a carrier injected in to the insulator where no compensating charge is present. The current for the unipolar trap free case is proportional to the square of the applied voltage. At low voltage and high temperature current is carried by thermally excited electrons hopping from one excited state to the next. This mechanism yields an ohmic characteristic exponentially dependent on the temperature.
Generally the dc ionic conductivity in insulators during the moment of the application of the external electric field is observed to be very small because ions cannot be readily injected in to or extracted from the insulator. Once the injection is initiated positive and negative space charges will buildup near the semi conductor-insulator interface causing a distortion of the potential distribution.

For a given insulator each conduction process may dominate in certain voltage ranges. The processes are also not exactly independent of one another. The SiO$_2$ depletion layer has the lowest conductance at a given field. At 6 MVcm$^{-1}$ and at room temperature the current density in SiO$_2$ layer is about 40 pAcm$^2$ that is many orders of magnitude lower than that in Ta$_2$O$_5$ thin film.
REFERENCES


4. ASTM X-Ray Powder Data No.25-932.

5. ASTM X-Ray Powder Data No.18-1303.


