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Direct extraction of the electron tunneling effective mass in ultrathin SiO₂

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Electron transport in ultrathin $(t_{ox} < 40 \text{ Å}) \text{ Al/SiO}_2/n-\text{Si}$ structures is dominated by direct tunneling of electrons across the SiO₂ barrier. By analyzing the tunneling currents as a function of the SiO₂ layer thickness for a comprehensive set of otherwise identical samples, we are able to extract an effective mass for the tunneling electron in the SiO₂ layer. Oxide films 16–35 Å thick were thermally grown *in situ* in a dry oxygen ambient. The oxide thicknesses were determined by capacitance–voltage measurements and by spectroscopic ellipsometry. The tunneling effective mass was extracted from the thickness dependence of the direct tunneling current between an applied voltage of 0 and 2 V, a bias range that has not been previously explored. Employing both a parabolic and a nonparabolic assumption of the $E - \kappa$ relationship in the oxide forbidden gap, we found the SiO₂ electron mass to be $m_P^* = 0.30 \pm 0.02m_e$, and $m_{NP}^* = 0.41 \pm 0.01m_e$, respectively, independent of bias. Because this method is based on a large sample set, the uncertainty in the mass determination is significantly reduced over prior current-voltage fitting methods. © 1996 American Institute of Physics. [S0003-6951(96)04644-X]

The properties of silicon dioxide (SiO₂) have been studied since ancient times, but never more intensely than in the past three decades. In metal/oxide/semiconductor (MOS) transistors, the ability to decrease the oxide thickness has allowed device sizes to be reduced while still maintaining high current drive. Oxide thicknesses in the range 50–100 Å are commonplace today in manufacturing, and research into sub-50 Å oxides has intensified. Below 50 Å, the quantum mechanical tunneling current becomes a limiting leakage component in MOS technology, and an enabling element in resonant tunneling and light-emitting silicon devices.^{1,2} Toward this end it is important to have reliable measurements of the basic tunneling properties of ultrathin SiO₂, particularly the barrier height and the effective mass.

Values for the tunneling effective mass in SiO₂ are typically obtained by current-voltage (I-V) measurements.^{1,3-6} The effective mass is obtained by fitting the I-V measurements to analytic expressions, which are not applicable over a wide bias or oxide thickness range.^{3,6} In the present paper, we employ a direct approach to extract the effective mass for tunneling in SiO₂. By characterizing a set of nine different samples with oxide thicknesses in the range 16-35 Å, we are able to observe the exponential dependence of the direct tunneling current on oxide thickness and determine the effective mass and its dependence on device bias. A similar method has been used by Maserjian⁷ to investigate the energymomentum $(E - \kappa)$ dispersion relationship in the SiO₂ forbidden gap. However, in Maserjian's paper, there exists significant scatter in the extracted value of the effective mass for low applied bias corresponding to tunneling of electrons with energies up to 1 eV higher than the conduction band of the Si substrate. This low-bias regime is extremely important for the design of scaled MOS devices and resonant tunneling devices. In the present paper, we are able to determine, with a high degree of precision, the effective mass of the tunneling electrons at low applied biases, corresponding to electrons tunneling with energies from 0 to 2 eV above the Si conduction band edge.

An expression that is well suited for the analysis of the thickness dependence of the tunneling current is obtained from Simmons' treatment of a similar problem in metal/insulator/metal structures.³ From Simmons' paper, the forward tunneling current density for an applied bias smaller than the barrier height can be represented as

$$t_{\rm ox}^2 = J_0 \, \exp(-2\,\kappa t_{\rm ox}),\tag{1}$$

where t_{ox} is the oxide thickness, and κ is the magnitude of the electron wave vector in the oxide band gap. The prefactor J_0 , derived by Simmons for a symmetric structure with metal electrodes, does not enter into our analysis. Clearly, Simmons' expression for J_0 falls short of a complete description of the current in MOS structures, where one needs to take into account important details such as the different densities of states in the two electrodes as well as the oxide barrier. For precisely this reason, it is incorrect to use Simmons' expression to fit the amplitude of the tunneling current in MOS structures, i.e., the entire I-V characteristic for a single sample, to extract the electron effective mass, and may explain the large error bars associated with previous determination of the tunneling effective mass using such a technique.⁸ However, in the present work, we analyze the change in the tunneling current as a function of thickness, which only requires the portion of Simmons' expression that is derived from basic quantum mechanical considerations, i.e., reflections across a trapezoidal energy barrier, independent of electrode band structure. From the exponential dependence of the product Jt_{ox}^2 on t_{ox} , we can determine κ . The effective mass can then be extracted from κ by using either a parabolic relationship,

$$\kappa = \left(\frac{2m_P^*q[\Phi_B - (V_{\rm ox}/2)]}{\hbar^2}\right)^{1/2},$$
(2)

or a nonparabolic relationship,

$$\kappa = \left[\frac{2m_{NP}^{*}q[\Phi_{B} - (V_{\text{ox}}/2)]}{\hbar^{2}} \left(1 - \frac{[\Phi_{B} - (V_{\text{ox}}/2)]}{E_{G}}\right)\right]^{1/2}, \quad (3)$$

where m_P^* is the effective mass in the parabolic $E - \kappa$ approximation Eq. (2), m_{NP}^* is the effective mass in the nonpa-

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rabolic (two-band) $E - \kappa$ approximation Eq. (3), $q\Phi_B$ is the Al-SiO₂ energy barrier height, V_{ox} is the voltage dropped across the oxide, and E_G is the oxide band gap. We assume that the barrier has an average height of $q(\Phi_B - V_{\text{ox}}/2)$, after Simmons.

For our analysis we need to know only two important oxide parameters: (i) The barrier height $q\Phi_B$, which we assume to be 3.17 eV after the work of Maserjian⁹ and (ii) the thickness of the oxide t_{ox} , which we determine by both capacitance–voltage (C-V) and ellipsometric measurements. The value for the oxide voltage may be assumed to be equal to the applied voltage, or may be determined more accurately by including the surface band bending, which in turn is obtained from the C-V data after Berglund.¹⁰ The difference in the extracted value of the effective mass is less than 3% between the two approaches, and therefore, to keep our analysis simple, we assume that the applied bias is equal to V_{ox} .

The oxides were grown on nominally flat *n*-type Si(100) wafers with $\rho = 0.01 - 0.02 \Omega$ cm. A thermal cleaning process was used for *in situ* surface preparation under ultrahigh vacuum (UHV) conditions with a base pressure of 7×10^{-11} Torr. The oxides were grown in a 400 Torr dry O₂ ambient (samples were transferred under UHV). Diodes were fabricated with electron-beam evaporated Al contacts, and I-V and C-V measurements were performed on devices with areas spanning four orders of magnitude in current (15, 150, and 1500 μ m diameter). The measured quantities were very reproducible and scaled linearly with the device area, thereby showing excellent uniformity of the oxide layers.

Capacitance-voltage measurements were performed on an HP 4275 LCR meter at 10 kHz. Figure 1 shows the capacitance of the nine samples as a function of applied bias from 0 to 2 V. For our bias polarity, an applied positive voltage to the top Al electrode results in an accumulation in the Si. Capacitance-voltage data through the full two-volt range are obtained for all but the thinnest oxide sample, which is measured only to 0.3 V, limited by the large direct tunneling current through the 16 Å oxide. We determine the oxide capacitance from the C-V measurements in the degenerate accumulation regime, after a method described by Maserjian et al.¹¹ Assuming a bulk dielectric constant for the SiO₂ of ϵ_{ox} = 3.9, we can determine the oxide thickness t_{ox} from the oxide capacitance. For the sample with the thinnest oxide where the C-V data are limited, we estimate a t_{ox} value of 16.5 Å from the zero-bias capacitance, a value which agrees well with our analysis of the tunneling current measured in these structures, and also correlates with the ellipsometric measurement. A comparison of the oxide thicknesses as determined from spectroscopic ellipsometry and C-V measurements is shown in the inset of Fig. 1. We find that the oxide thickness obtained from the C-V data is approximately 3–5 Å larger than the ellipsometric value. This discrepancy is not unusual and may be attributed to the electron wave function in the Si that is peaked away from the oxide barrier, thereby increasing the effective thickness of the SiO₂ layer as measured by C-V.¹² For our analysis, we use the thickness determined from the C-V data, because both the C-V and I-V measurements are performed on the



FIG. 1. Capacitance-voltage (C-V) measurements in the accumulation region for the nine samples studied. The capacitance for the thinnest oxide cannot be measured above about 0.3 V because of large tunneling currents. The numbers to the right of the curves represent the oxide thickness, which is determined by C-V after the procedure used by Maserjian *et al.* (see Ref. 11) for all but the thinnest oxide. The inset shows a comparison of the oxide thicknesses as measured by C-V and ellipsometry.

same device. This provides a better local value for the oxide thickness compared to the ellipsometric value. An advantage of analyzing the *change* in the tunneling current as function of thickness is that a systematic error of 5 Å in the oxide thickness for our samples would change the extracted value of κ by only 2%.

Current–voltage measurements were performed using an HP4155 semiconductor parameter analyzer. The current measured in the thickest oxide sample in the low voltage (<0.7 V) range is limited by the sensitivity of the instrument. Figure 2 shows the I-V data in the direct tunneling regime for all nine samples measured on a diode with a diameter of 150 μ m. The direct tunneling current is a very sensitive function of the oxide thickness, and is observed to increase over seven orders of magnitude for a decrease in the oxide thickness from 30 to 16 Å. Note that the curves for all the samples are "parallel," indicating that the samples are identical in their electron transport properties. The key point is that the major difference in the I-V curves is in the magnitude of the tunneling current, which is a direct consequence of the different oxide layer thicknesses.

An interesting qualitative aspect of the data in Figs. 1 and 2 is the "correspondence" between the I-V and C-Vmeasurements. From the relative magnitudes, one can clearly identify the C-V curve that corresponds to the I-V curve for the same sample. Inasmuch as the C-V data are used to extract a t_{ox} value for the oxide, such a correspondence suggests that we may also be able to infer a thickness directly from the magnitude of the tunneling currents measured in ultrathin oxides. In the final analysis, the tunneling current is the quantity that interests us most, and is very useful for determining thicknesses in the regime, where the C-V measurements are unreliable as a result of the large tunneling currents.

Figure 3 is a plot of the product Jt_{ox}^2 as a function of t_{ox} at different bias points for eight of the nine samples. The data for the thickest oxide are not included because its tunneling current is too low to measure accurately below 0.7 V.



FIG. 2. Oxide thickness dependence of the current–voltage characteristics for nine $Al/SiO_2/n$ -Si MOS structures with a diameter of 150 μ m. Numbers to the right of the curves are the oxide thickness in Angstroms.

The currents for the eight samples fit an exponential dependence on thickness over six orders of magnitude, in excellent agreement with the tunneling current expression in Eq. (1).

Assuming a thick-oxide barrier height of 3.17 eV^9 and using Eqs. (1)–(3) we can extract the effective mass of the tunneling electron at each bias point. Figure 4 is a plot of the electron effective mass in the SiO₂ extracted from the thickness dependence of the tunneling currents at various bias points in the direct tunneling regime, using both the parabolic $E - \kappa$ dispersion [Eq. (2); m_P^*], and the nonparabolic dispersion [Eq. (3); m_{NP}^*]. We obtain a value of $m_P^* = 0.30$ $\pm 0.02m_e$, and $m_{NP}^* = 0.42 \pm 0.01m_e$, over the bias range measured. It is important to note that the effective mass is approximately constant over the bias range studied. The parabolic value is in good agreement with the mass obtained by fits of the tunneling I-V characteristic by Depas et al.⁵ $(0.28-0.31m_e)$, J. Maserjian⁹ $(0.27\pm0.05m_e)$, and Hiroshima et al.³ $(0.33 \pm 0.08 m_{e})$. The mass obtained from assuming a nonparabolic dispersion is in excellent agreement with Maserjian's value of $0.42m_e$ for higher bias voltages.⁷ Clearly, care must be taken in modeling the direct tunneling current to use the appropriate mass for the dispersion relationship assumed in the oxide forbidden gap. The fact that



FIG. 3. Exponential dependence of the direct tunneling current on the thickness t_{ox} of the SiO₂ insulating layer at four different bias voltages for eight Al/SiO₂/*n*-Si MOS structures. The lines represent an exponential fit to the data spanning six orders of magnitude.



FIG. 4. The tunneling effective mass for the electron in the SiO₂ layer extracted from the fit shown in Fig. 3 assuming both a parabolic E-k (m_P^*) and a nonparabolic $E-\kappa$ dispersion (m_{NP}^*) in the oxide, see Eqs. (2) and (3).

 m_P^* and m_{NP}^* extracted using this simple procedure are essentially independent of the applied bias, and that the data are obtained from I-V curves measured from eight different samples, with t_{ox} ranging from 16.5 to 35 Å, gives better confidence in the value obtained for the effective mass of tunneling electrons in the SiO₂ barrier.

A closer inspection of the dependence of the effective mass on bias in Fig. 4 shows that m_P^* and m_{NP}^* both increase slightly with applied bias (about 3% from 0 to 2 V). A more accurate analysis that includes the effect of band bending in the Si accumulation layer corrects the extracted value of the effective mass in the desired manner, making the data in Fig. 4 flatter, independent of applied bias. However, such a calculation does not add any new physics to our analysis, and only changes the value of the effective mass by less than 3% at 2 V. From the fit to our data, we find that the nonparabolic $E - \kappa$ dispersion provides a more accurate description of the bands in the oxide forbidden gap. This is consistent with the observations of Maserjian for tunneling electrons with energies closer to the conduction band edge of the SiO₂.⁷

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