Distribution of potential barrier height local values at Al-SiO$_2$ and Si-SiO$_2$ interfaces of the metal-oxide-semiconductor structures

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Abstract. In this work studies of barrier height local values are presented. Distribution of the gate-oxide $E_{BG}(x, y)$ and semiconductor-oxide $E_{BS}(x, y)$ barrier height local values have been determined using the photoelectric measurement methods. Two methods were used to obtain the local values of the barrier heights: modified Powell-Berglund method and modified Fowler method. Both methods were modified in such a way as to allow determination of the $E_{BG}(x, y)$ and $E_{BS}(x, y)$ distribution over the gate area using a focused UV light beam of a small diameter $d = 0.3$ nm. Measurements have been made on a series of Al-SiO$_2$-Si(n$^+$) MOS structures with semitransparent ($t_{Al} = 35$ nm) square aluminum gate ($1 \times 1$ mm$^2$). It has been found that the $E_{BG}(x, y)$ distribution has a characteristic dome-like shape, with highest values at the center of the gate, lower at the gate edges and still lower at gate corners. On the contrary, the $E_{BS}(x, y)$ distribution is of a random character. Also, in this paper, both barrier height measurements have been compared with the photoelectric effective contact potential difference measurements which are reflected in the $E_{CPD}$ distribution. These results show good agreement between distribution of the barrier heights $E_{BG}(x, y)$ and $E_{BS}(x, y)$ measurements and independently determined shape of the effective contact potential difference $\phi_{MS}(x, y)$ distribution.

Key words: barrier height, effective contact potential difference, MOS system.

1. Introduction

It has been observed for several years in our laboratory that local values of the effective contact potential difference (ECPD or $\phi_{MS}$) in Al-SiO$_2$-Si structures have a characteristic shape of distribution over the gate area [1,2]. An example of such a distribution shape is shown Fig. 1. In this figure the experimentally determined $V^0_{G}(\zeta)$ distribution is shown, where $V^0_{G} = \phi_{MS} + C$ and $C$ is a constant (see e.g. [3]). Hence, the shape of $\phi_{MS}$ distribution over the gate area is identical with the shape of $V^0_{G}$ distribution, shown in Fig. 1.

Mechanical stress in a MOS structure is known to influence its electrical parameters [4, 5]. One of these parameters is the effective contact potential difference $\phi_{MS}$. The influence of mechanical stress on the $\phi_{MS}$ value of a MOS structure was quantitatively estimated [6] and it was shown that the mechanical stress has a dominating influence on the shape of the $\phi_{MS}$ distribution (among others by showing the influence of aluminum gate thickness on this shape). Hence, other factors which may cause non uniform distributions of $\phi_{MS}$ (such as non uniform distribution of electric field, due to the edge effect or to the surface roughness) are not considered in this article.

It is also known that mechanical stress is non uniformly distributed under the metal gate of a MOS structure [5, 7–9] and that it changes rapidly in the vicinity of the gate edges (Fig. 2).

Assuming, that changes in the $\phi_{MS}$ value are proportional to the changes in mechanical stress under the gate of the MOS structure, a model of the $\phi_{MS}$ distribution over the gate area was developed and verified experimentally [1,2]. A typical distribution of $\phi_{MS}$ local values over the square gate area, calculated using this model is shown in Fig. 3. In this figure we see the highest values in the center of the gate, lower values at the gate edges and lowest at the corners.

As shown in the next section, the $\phi_{MS}$ value depends directly on the difference of potential barrier heights $E_{BG}$ and $E_{BS}$. Hence, one or both barrier heights must have distributions which are reflected in the $\phi_{MS}$ distribution over the gate area.

Fig. 1. Typical dependence of the $(\phi_{MS} + C)$ voltage measured at the wavelength $\lambda = 244$ nm on the position in Al-SiO$_2$-Si(n$^+$) structures with aluminum gate thickness $t_{Al} = 35$ nm and SiO$_2$ layer thickness $t_{OX} = 60$ nm. The direction is either (1) along the diagonal of the square gate, or (2) through the centre of the square gate and parallel to its edges.

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It was the purpose of this research to prove that, as expected, it is the gate-dielectric barrier height distribution \( E_{BG}(x, y) \), which determines the shape of the \( \phi_{MS}(x, y) \) distribution. To do this, we modified the barrier height measurements methods of Powell-Berglund and of Fowler, used these modified methods to determine distributions of both barrier heights \( E_{BG}(x, y), E_{BS}(x, y) \) and compared these results with independently measured \( \phi_{MS}(x, y) \) distributions.

![Fig. 2. The expected one-dimensional distribution of stress \( \sigma_{OX}(z) \) in the oxide layer under the aluminum gate](image)

![Fig. 3. Two-dimensional distribution of \( \phi_{MS}(x, y) \) calculated using model after Ref. 1 for MOS structures with square gates of side length \( L = 1 \text{ mm} \)](image)

### 2. Theory

The internal photoemission phenomena may be observed in a MOS structure with a semitransparent gate, illuminated by UV radiation. The UV radiation absorbed in the electrodes (the gate or the substrate) causes excitation of some electrons. If these electrons acquire sufficient energy to surmount the potential barrier at the electrode-dielectric interface, they may pass into the insulator giving rise to a photocurrent which can be measured in the external circuit. This photocurrent \( I_P \) is a function of the barrier height \( E_B \) which electrons have to surmount, as well as of the wavelength \( \lambda \) of UV light illuminating the structure and the gate potential \( V_G \). The band diagram of the MOS system is shown in Fig. 4.

![Fig. 4. Band diagram of the MOS system, at arbitrary gate potential \( V_G \). \( E_{BG}, E_{BS} \) are potential barrier heights at gate-dielectric and semiconductor-dielectric interfaces, respectively](image)

Balancing the potentials on both sides of the dielectric layer yields:

\[
\phi_M - V_G = \chi - \phi_I - \phi_S + \frac{E_G}{2q} + \phi_F. \tag{1}
\]

where: \( \phi_M \) – the barrier height at the gate-dielectric interface, \( V_G \) – gate potential, \( \chi \) – the electron affinity of the silicon substrate at the interface, \( \phi_I, \phi_S \) – the potential drop in the dielectric and at the semiconductor surface, \( E_G/2q \) – the voltage equivalent of half energy bandgap in the semiconductor, \( q \) – the electron charge, \( \phi_F \) – the Fermi level.

The definition of the effective contact potential difference \( \phi_{MS} \) offers the possibility of a comparison between the difference of internal photoemission barrier heights from both sides of the dielectric and the value of \( \phi_{MS} \). The effective contact potential difference \( \phi_{MS} \) is defined as [10]:

\[
\phi_{MS} = \phi_M - \chi = \frac{E_B - E_{BS} + E_G}{2q} + \phi_F. \tag{2}
\]

The value of \( \phi_{MS} \) given by (2) depends on the doping density of the substrate (the \( \phi_F \) value). Sometimes it is more convenient to use the value of the reduced effective contact potential difference (RECPD or \( \phi_{MS}^* \) factor), defined as:

\[
\phi_{MS}^* = \phi_{MS} - \chi \tag{3}
\]

or

\[
\phi_{MS}^* = \phi_{MS} + \frac{E_G}{2q} + \phi_F. \tag{4}
\]

The \( \phi_{MS}^* \) value depends on the barrier heights on both sides of the dielectric and does not depend on the doping concentration in the substrate.

Using the band diagram shown in Fig. 4, one finds that:

\[
\phi_{MS}^* = \phi_M - \chi = \frac{1}{q} (E_{BG} - E_{BS} + E_G). \tag{5}
\]
Hence, using Eqs (1–4), comparisons can be made between the independently measured values of $\phi_{MS}$ and values of $E_{BG}$ and $E_{BS}$, if the $\phi_F$ and $E_G$ values are known.

The experimentally determined $I_P = f(V_G, \lambda)$ characteristics can be used to determine the individual barrier heights ($E_{BG}$ and $E_{BS}$) by the well known Powell-Berglund [11–13] and Fowler [14,15] methods. An example of such $I_P = f(\lambda)$ characteristics taken for the $E_{BS}$ barrier height determination is shown in Fig. 5.

It is well known [10], that the gate voltage $V_G$ is a sum of three components:

$$V_G = V_I + V_S + \phi_{MS} \quad (6)$$

where: $V_I$ – the voltage drop in dielectric and $V_S$ – the semiconductor surface potential.

The band diagram of the MOS system for $V_G = V_{G0}$ is shown in Fig. 6. In this case the situation when voltage drop in dielectric $V_I = 0$ (flat band in dielectric) and semiconductor surface potential $V_S$ is equal $V_{S0}$ takes place. Hence, it results from Eq. (6) and Fig. 6 that:

$$V_{G0} = V_{S0} + \phi_{MS} \quad (7)$$

where: $V_{S0}$ – the semiconductor surface potential for $V_G = V_{G0}$.

Measuring $I_P = f(V_G)$ characteristics for different (values (Fig. 7) and choosing the one which is symmetrical with respect to the $I_P = 0$ point, the value of gate voltage $V_G = V_{G0}$, at which $V_I = 0$ can be determined [3]. This can be done with an accuracy of the order of $\pm 1 \text{ mV}$ [16].

Having found $V_{G0}$, one still has to find $V_{S0}$, to determine $\phi_{MS}$ from Eq. (7). $V_{S0}$ can be determined in a separate measurement (e.g. from the value of the MOS capacitance $C$ at $V_G = V_{G0}$), or it can be made negligible in comparison with $\phi_{MS}$ (e.g. by using heavily doped substrate MOS structures). These two approaches allow the determination of $\phi_{MS}$, with $\pm 10 \text{ mV}$ accuracy, or better [3].

The principle of the recently developed modification of the photoelectric $E_{BG}$ and $E_{BS}$ measurement method is illustrated in Fig. 8.

Barrier heights were measured by both methods: modified Powell-Berglund method and modified Fowler method. The modifications of both methods consisted in using a UV light
3. Experimental details

In this work measurements were made on Al-SiO$_2$-Si capacitors with semitransparent ($t_{Al} = 35$ nm) square (1 $\times$ 1 mm$^2$) gate. Phosphorus doped n$^+$ substrates ($\rho = 0.015$ $\Omega$cm) of <100> orientation were used to simplify interpretation of the photoelectric measurements, as discussed in [1,3]. Wafers were thermally oxidized at temperature $T = 1000^\circ$C, in dry oxygen, to grow a SiO$_2$ layer of thickness $t_{OX} = 60$ nm. Although SiO$_2$ layers of current technological interest are thinner than $t_{OX} = 3$ nm, we used thicker oxides to optimize the sensitivity of the applied photoelectric methods.

Oxidized wafers were subsequently annealed in nitrogen for $t = 10$ min and $t = 120$ min, at $T = 1050^\circ$C. The post metalization annealing was carried out for $t = 20$ min, at $T = 450^\circ$C in forming gas atmosphere. Photoelectric measurements of barrier heights were made after all the structures were checked for gross defects, such as non negligible leakage currents, ionic instability, low breakdown voltage of the SiO$_2$ layer, etc., and the defective structures were eliminated.

The absolute accuracy of $E_{BG}$ and $E_{BS}$ determination is estimated to be $\pm 50$ meV. However, the relative accuracy in determining the changes of $E_{BG}$ and $E_{BS}$ in consecutive measurements (in different places over the gate area) is better and is estimated to be $\pm 10$ meV.

4. Results and discussion

Measurements of local $E_{BG}$ and $E_{BS}$ barrier heights were made by both modified Powell-Berglund and (for comparison) by the modified Fowler method, in nine locations over the gate area (as shown in Fig. 8), on each of the 26 MOS structures on one silicon wafer.

The so determined values were averaged in such a way that average local $E_{BG}$ and $E_{BS}$ values were determined for each of the nine positions over the gate area and then were connected by smooth (3rd order polynomial) lines to obtain approximate distributions of barrier heights over the entire gate area of the MOS structure.

Such distributions of the averaged values are shown in Figs. 9a and 9b for measurements made by the modified Powell-Berglund method and in Figs. 10a and 10b for measurements made by the modified Fowler method.

Figure 9a and 10a show that averaged $E_{BG}(x, y)$ distribution has a dome-like shape and the difference between maximum $E_{BG\max}$ and minimum $E_{BG\min}$ local barrier height values over the gate area, $(E_{BG\max} - E_{BG\min})$ remains relatively large (68 or 45 meV) in comparison with averaged $E_{BS}(x, y)$ distribution, shown in Fig. 9b and 10b, which has a random character and a smaller $E_{BS\max} - E_{BS\min}$ difference (18 or 10 meV). Moreover, this difference shows a decreasing tendency with the increasing number of MOS structures measured and taken into account in the averaging process.

The $E_{BG\max} - E_{BG\min}$ difference is called the amplitude of the $E_{BG}$ distribution, similarly $E_{BS\max} - E_{BS\min}$ is called the amplitude of the $E_{BS}$ distribution. It is clearly seen that the amplitude of $E_{BG}$ distribution is c.a. 4 times larger than the amplitude of the $E_{BS}$ distribution.

\[
\frac{E_{BG\max} - E_{BG\min}}{E_{BS\max} - E_{BS\min}} \approx 4
\]
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There are slight differences between averaged distributions obtained by both measurement methods (compare Fig. 9a with Fig. 10a, and Fig. 9b with 10b), which are due to measurement inaccuracies by both methods, but the general features of averaged $E_{BG}(x,y)$ and $E_{BS}(x,y)$ distributions do not depend on the measurement method applied.

On the other hand, the $V_{GO}$ voltage ($V_{GO} \approx \phi_{MS}$ in this case) also has a characteristic dome-like shape of distribution over the gate area with local $V_{GO}$ values being highest in the middle of the gate, lower at the gate edges, and lowest at gate corners. Fig. 11 shows the measured and averaged $V_{GO}(x,y)$ distribution over the gate area.

To simplify explanation of the obtained results we propose the following symbols for the $\phi_{MS}$ (or RECPD) value:

- $\phi_{MS}^*(1)$ – the reduced effective contact potential difference determined applying Eq. (4) in which $\phi_{MS}$ values measured by the photoelectric method [3] are used,
- $\phi_{MS}^*(2)$ – the reduced effective contact potential difference calculated (Eq. 5) using the $E_{BG}$ and $E_{BS}$ values measured by both modified Powell-Berglund and modified Fowler methods.

Subtracting Eq. (3) from Eq. (4) we have:

$$\phi_{MS}^*(1) - \phi_{MS}^*(2) = \phi_{MS} - \phi_{M} + \frac{E_{G}}{2q} + \phi_{F} = R. \quad (9)$$

The $R$ factor should be equal to 0 for ideally accurate measurements. Otherwise we consider $R$ to stand for the error of the barrier height measurement (since we know that $\phi_{MS}$ is measured much more accurately [3,9]). The value of $R$ higher than 10 mV means that at least one of the considered barrier heights was measured inaccurately.

The averaged $\phi_{MS}^*(2)(x,y)$ distribution over the gate area is similar to the $V_{GO} \approx \phi_{MS}$ distribution shown in Fig. 11, just shifted vertically according to Eq. (4).

Figure 12 shows averaged $\phi_{MS}^*(2)(x,y)$ distribution for the modified Powell-Berglund method (Fig. 12a) and for the modified Fowler method (Fig. 12b) over the gate area.

In Fig. 12 characteristic dome-like shape of the $\phi_{MS}^*(2)(x,y)$ distribution over the gate area for both measurement methods can be observed. There are slight differences between $\phi_{MS}^*(2)$ distributions determined by modified Powell-Berglund and by modified Fowler method, as can be seen in Fig. 12a and 12b. These differences are due to the inaccuracies of both barrier height measurement methods.

The differences between $\phi_{MS}^*(1)$ and $\phi_{MS}^*(2)$ values (calculated by Eq. (9)) for the modified Powell-Berglund method and modified Fowler method on each position over the gate area are given in Table 1.

<table>
<thead>
<tr>
<th>Positions over the gate area</th>
<th>R [mV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Powder-Berglund</td>
<td>20</td>
</tr>
<tr>
<td>Fowler</td>
<td>49</td>
</tr>
</tbody>
</table>

Table 1

Values of the measurement error $R$
The positive value of the measurement error $R$ may be explained by too low a value of the $E_{BG}$ barrier height or too high a value of the $E_{BS}$ barrier height. The opposite applies when $R < 0$.

Good agreement between the $\phi_{MS}^*(1)(x, y)$ and $\phi_{MS}^*(2)(x, y)$ values has been observed for measurements made by modified Powell-Berglund method ($R_{\text{max}} = 20$ mV at gate corner – position 1, $R_{\text{min}} = 1$ mV at gate edges – position 6). The modified Fowler method compares unfavourably with the modified Powell-Berglund method. The values of error $R$ for each of the nine positions over the gate area (about 40–50 mV) are much higher than respective values for the modified Powell-Berglund method. Hence, it is clearly seen that the complexity of the modified Fowler method is not balanced by higher measurement accuracy, while the simple modified Powell-Berglund method yields relatively accurate measurement results.

In Table 2 are given the average values of $R$ (in [mV]) for analogous positions over the gate area.

In case of the measurements made by both methods the highest values of $R$ at gate corners, lower values at gate edges and lowest value at the center of the gate can be observed.

To confirm the results reported above, a similar investigation was made using the UV light beam of a smaller diameter $d = 0.25$ mm. This allowed to find local barrier heights values in 16 different positions over the gate area (instead of 9 positions, as shown in Fig. 8). Measurements were made on 30 MOS structures, on one silicon wafer (which, however, was differently processed than the wafer used in previously described measurements) and the averaging procedure was the same as described above.
5. Conclusions

The lateral distribution of local $E_{BG}$ and $E_{BS}$ barrier height values over the gate area of a MOS structure were studied. Measurements were made on two series of 26 and 30 Al-SiO$_2$-Si capacitors. Two photoelectric measurement methods were used in this investigation: modified Powell-Berglund method and modified Fowler method. The modifications of these methods consisted in applying a focused UV light beam (diameter $d = 0.3$ and 0.25 mm) which allowed measurements to be made in 9 and 16 different locations over the gate area. It was found that $E_{BG}$ barrier height has a characteristic dome-like shape of distribution, with highest values in the middle of the gate, lower at gate edges, and lowest at gate corners. On the other hand, the $E_{BS}$ barrier height distribution has a random character and differences between highest and lowest values of $E_{BS}$ (so-called amplitude) for any of the measured MOS structures are much smaller than the respective differences in $E_{BG}$ values.

The dome-like shape of $E_{BG}(x, y)$ distribution is identical with the shape of independently (and much more accurately) measured distributions of $\phi_{MS}(x, y)$ over the gate area. This proves that, as expected, the shape of the $\phi_{MS}$ distribution results directly from the distribution of gate-dielectric barrier height $E_{BG}(x, y)$ over the gate area. We ascribe the dome-like shape of the $E_{BG}$ distribution to the non uniform distribution of mechanical stress at the gate-dielectric interface in a MOS structure.

REFERENCES


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