Paper

Investigation of barrier height distributions over the gate area of Al-SiO_2-Si structures

Krzysztof Piskorski and Henryk M. Przewłocki

Abstract—Distributions of the gate-dielectric $E_{BG}(x,y)$ and semiconductor-dielectric $E_{BS}(x,y)$ barrier height values have been determined using the photoelectric measurement method. Modified Powell-Berglund method was used to measure barrier height values. Modification of this method consisted in using a focused UV light beam of a small diameter $d = 0.3$ mm. It was found that the $E_{BG}(x,y)$ distribution has a characteristic dome-like shape which corresponds with the independently determined shape of the effective contact potential difference $\phi_{MS}(x,y)$ distribution. On the other hand, the $E_{BS}(x,y)$ distribution is of a random character. It is shown that the $E_{BG}(x,y)$ distribution determines the shape of the $\phi_{MS}(x,y)$ distribution. The model of the E_{BG} and E_{BS} barrier height distributions over the gate area has been proposed.

Keywords*— *barrier height, effective contact potential difference, MOS system.

1. Introduction

The present work is a logical continuation of our previous research (see, e.g., [1–4]) concerning the distribution of electrical parameters over the gate area of Al-SiO_2-Si structures. It has been experimentally proved that the effective contact potential difference (ECPD or ϕ_{MS}) and zero photocurrent gate voltage V_G^0 have a characteristic dome-like shape distribution over the gate area. An example of such a distribution is shown in Fig. 1. The distribution of V_G^0 obtained experimentally (see, e.g., [3, 4]) in two different directions (along the diagonal and through the center of the square gate) shows the highest values at the center of the gate and lowest values at the gate corners.

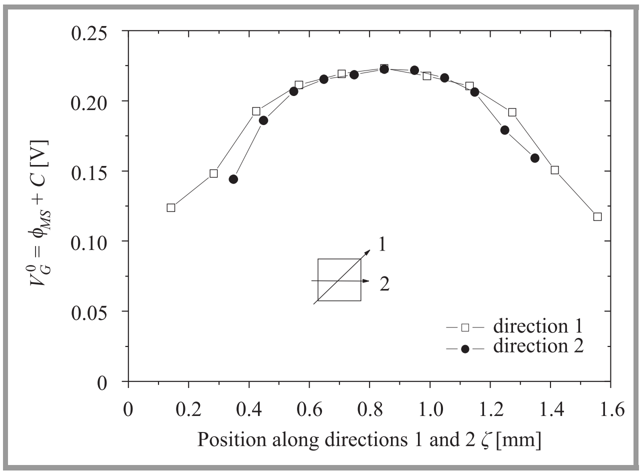

Fig. 1. Typical dependence of the V_G^0 voltage measured at the wavelength $\lambda = 244$ nm on the position in Al-SiO_2-Si(n^+) structures with aluminum gate thickness $t_{Al} = 35$ nm and SiO_2 layer thickness $t_{ox} = 60$ nm. The direction is either Eq. (1) along the diagonal of the square gate, or Eq. (2) through the center of the square gate and parallel to its edges.

We ascribe the characteristic shape of this distribution to the distribution of mechanical stress which is present in the oxide layer under the gate in the MOS system [5–8]. This non-uniform distribution of the mechanical stress is shown in Fig. 2.

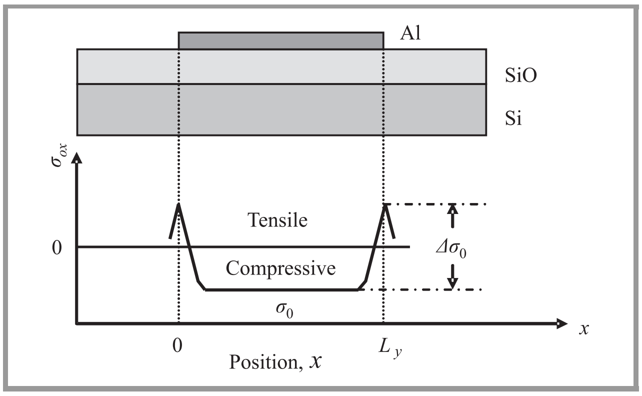

Fig. 2. A qualitative one-dimensional distribution of stress $\sigma_{ox}(x)$ in the oxide layer under the Al gate.

Assuming that changes in V_G^0 and ϕ_{MS} values are proportional to changes in mechanical stress σ under the gate, a model of $\phi_{MS}(x,y)$ distribution was developed and confirmed experimentally [3]. A typical distribution of ϕ_{MS} local values over the square gate area, calculated using this model is shown in Fig. 3. It is clearly seen in Fig. 3 that the $\phi_{MS}(x,y)$ distribution has a dome-like shape, with the highest values at the center of the gate, lower at the gate edges and still lower at gate corners.

The ECPD depends directly on the difference $E_{BG} - E_{BS}$ of barrier heights at both sides of the dielectric, as discussed in the next section. Hence, one or both of these barriers must have distributions which result in the characteristic $\phi_{MS}(x,y)$ distribution. Since it is the gate that causes the non-uniform distribution of mechanical stress in the oxide, it is more likely that the gate-dielectric E_{BG} barrier height has the decisive influence on the shape of $\phi_{MS}(x,y)$ distribution.

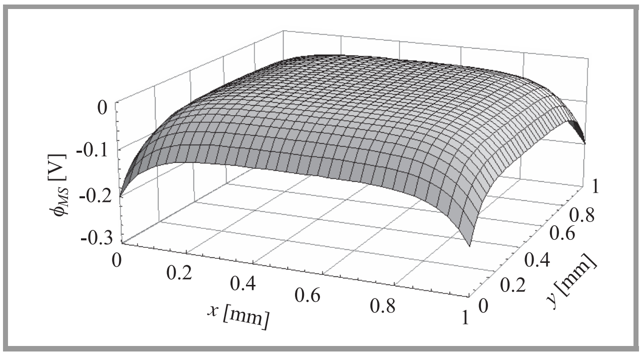

Fig. 3. Example of two-dimensional distribution of $\phi_{MS}(x, y)$ calculated using model [3, 4] for MOS structures with square gates of side length $L = 1$ mm.

The aim of this investigation was to determine the distributions of both E_{BG} and E_{BS} barrier height local values over the gate area and to find out how the individual barrier heights influence the ϕ_{MS} distribution. Moreover, barrier height measurement results have been compared in this work with independently determined ϕ_{MS} local values, to estimate the accuracy of barrier height determination. A model (similar to the above mentioned ϕ_{MS} distribution model) has also been applied in this work to the $E_{BG}(x, y)$ and $E_{BS}(x, y)$ distributions over the gate area.

2. Theory

The barrier height measurements were performed using internal photoemission phenomena, which can be observed in a MOS structure with a semitransparent gate under illumination by UV light. The UV radiation absorbed in both electrodes (gate or substrate) may cause excitation of some electrons. When the energy of the excited electrons is sufficient to surmount the potential barrier at the gate-dielectric or semiconductor-dielectric interface the photocurrent flow takes place. This photocurrent is a function of the barrier height E_B, the wavelength λ of UV light illuminating the structure and the gate potential V_G and can be measured in the external circuit, as shown in Fig. 4. In this figure the measurement system with MOS structure illuminated by UV light beam is schematically illustrated. The beam may be focused in nine different positions over the gate area. In Fig. 5 the band diagram of the MOS system is shown.

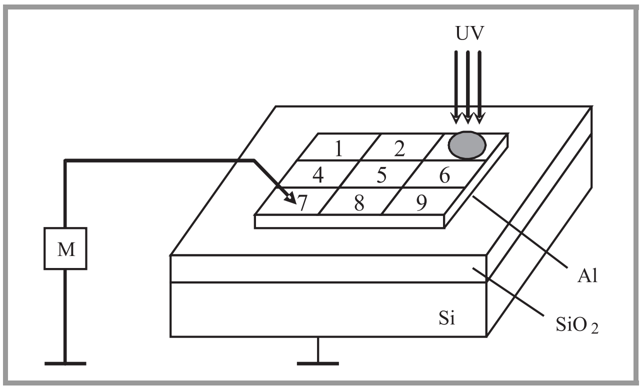

Fig. 4. The measurement system: the MOS structure with semitransparent Al gate is illuminated at 9 different locations over the gate area by a focused light beam. The photocurrent is measured in the external circuit M.

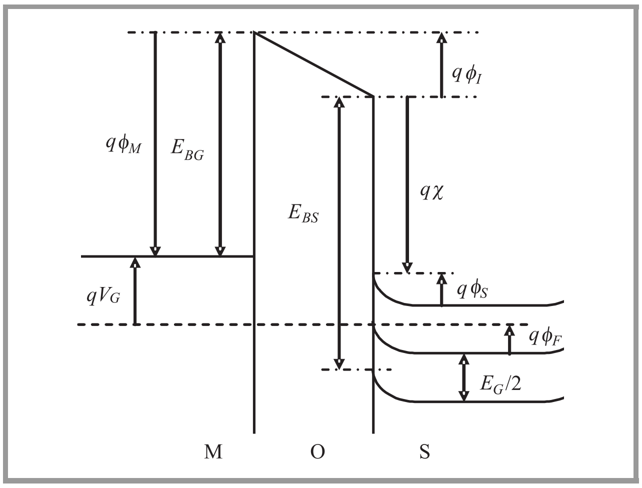

Fig. 5. Band diagram of the MOS system. E_{BG}, E_{BS} are potential barrier heights at gate-dielectric and semiconductor-dielectric interfaces, respectively.

Adding up all potentials on both sides of the dielectric layer leads to a formula (1):

$$\phi_M - V_G = \chi - \phi_I - \phi_S + \frac{E_G}{2q} + \phi_F \,, \tag{1}$$

where: ϕ_M – the barrier height at the gate-dielectric interface, V_G – gate potential, χ – the electron affinity of the silicon substrate at the interface, ϕ_I, ϕ_S – the potential drop across the dielectric and at the semiconductor surface, $E_G/2q$ – the voltage equivalent of half energy band gap in the semiconductor, q – the electron charge, ϕ_F – the Fermi potential.

The effective contact potential difference (ECPD or ϕ_{MS}) is defined as [9]:

$$\phi_{MS} \stackrel{def}{=} \phi_M - \left(\chi + \frac{E_G}{2q} + \phi_F\right). \tag{2}$$

Sometimes it is more convenient to use the value of the reduced effective contact potential difference (RECPD or ϕ^*_{MS}), defined as:

$$\phi^*_{MS} = \phi_M - \chi \tag{3}$$

or

$$\phi^*_{MS} = \phi_{MS} + \frac{E_G}{2q} + \phi_F \,. \tag{4}$$

It is clearly seen from Eq. (3) that the ϕ^*_{MS} value depends only on the barrier heights on both sides of the dielectric and does not depend on the doping concentration in the substrate (while the ϕ_{MS} value depends on it through the ϕ_F value).

The definition of ECPD, given by Eq. (2), allows a comparison to be made between the measured ϕ_{MS} values (by the photoelectric method [2]) and the independently measured values of both barrier heights (E_{BG} and E_{BS}). This can be done by comparing two ϕ^*_{MS} values, namely:

– the $\phi^*_{MS}(1)$ value calculated using Eq. (4) and the ϕ_{MS} value determined directly by the photoelectric method, and
– the $\phi^*_{MS}(2)$ value calculated using [13, 14]:

$$\phi^*_{MS}(2) = \frac{1}{q}\left(E_{BG} - E_{BS} + E_G\right) \quad (5)$$

with the values of E_{BG} and E_{BS} barrier heights measured using the modified Powell-Berglund method [10–14].

The R value defined as:

$$R = \phi^*_{MS}(1) - \phi^*_{MS}(2) \quad (6)$$

is an indicator of the accuracy of barrier height measurement. This is so because both the ϕ_{MS} (measured by the photoelectric method [2]) and the ϕ_F value (determined using capacitance voltage, $C(V_G)$ characteristics) needed to calculate $\phi^*_{MS}(1)$, are determined with high accuracy – better than ± 10 mV in both cases, while the barrier height measurements are known to be less accurate [15]. Obviously, the value of R decreases with improved accuracy of the measurements.

3. Experimental

Measurements were made on Al-SiO_2-Si MOS structures with semitransparent ($t_{Al} = 35$ nm) square gates (1×1 mm^2). To simplify interpretation of the photoelectric measurements [2], in this work the phosphorus doped n^+ substrates ($\rho = 0.015\,\Omega$cm) of $< 100 >$ orientation were used. After an initial hydrogen-peroxide-based cleaning sequence, the wafers were thermally oxidized at 1000°C in oxygen to grow silicon-dioxide layers of with the thickness of approximately 60 nm, and subsequently annealed in nitrogen for 10 min at 1050°C. It is obviously known, that current technological interest consists in measurements of oxide layers thinner than 3 nm, but in this case thicker oxides were used to optimize the sensitivity and accuracy of the applied photoelectric methods [2]. The frontside metalization was carried out in a thermal evaporator to the Al thickness of 35 nm. Postmetalization annealing was carried out at 450°C for 20 min in the forming gas atmosphere.

Photoelectric measurements of the barrier heights were made using the modified Powell-Berglund method. The modification of this method consisted in using a diameter of UV light beam ($d = 0.3$ mm) that was small in comparison with the dimension of the side length of the Al gate (1 mm). Hence, it was possible to scan the whole gate area and to measure local values of barrier heights (E_{BG} and E_{BS}), on both interfaces of the dielectric.

The 26 MOS capacitors were used in this investigation. On each of these capacitors local barrier heights were determined in 9 different locations, as illustrated in Fig. 4. The local values of barrier heights determined in this way were connected by 3rd order polynomial lines to obtain approximate distributions of barrier height over the entire gate area.

The results of barrier height measurements were compared with ϕ_{MS} measurements, as described in Section 2.

Based on measurements results, models have been developed of distributions of both barrier heights (E_{BG}, E_{BS}) over the gate area, as well as that of RECPD (ϕ^*_{MS}) values. The parameters of these models were fitted to obtain good agreement between measured and calculated distributions.

4. Results and discussion

Averaged distributions of E_{BG} and E_{BS} are shown in Fig. 6, while an averaged distribution of V^0_G is shown in Fig. 7.

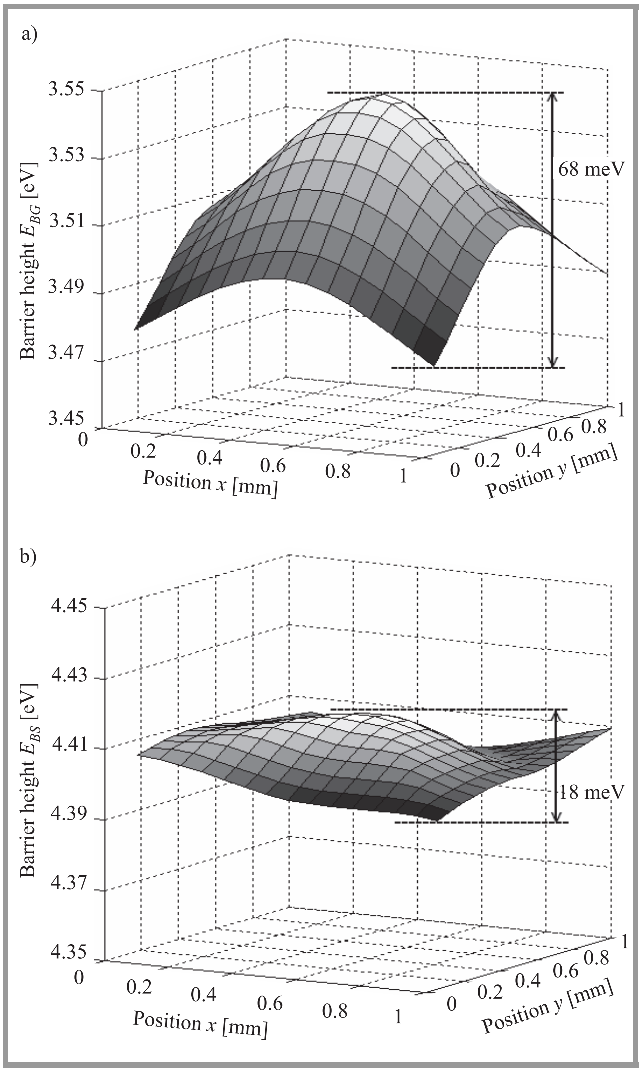

Fig. 6. Averaged two-dimensional distribution of: (a) E_{BG} and (b) E_{BS} barrier heights measured using modified Powell-Berglund method for 26 MOS structures. Average E_{BG} and E_{BS} values were found for each of the 9 locations over the gate area (shown in Fig. 4) and used to determine distributions shown in the figure.

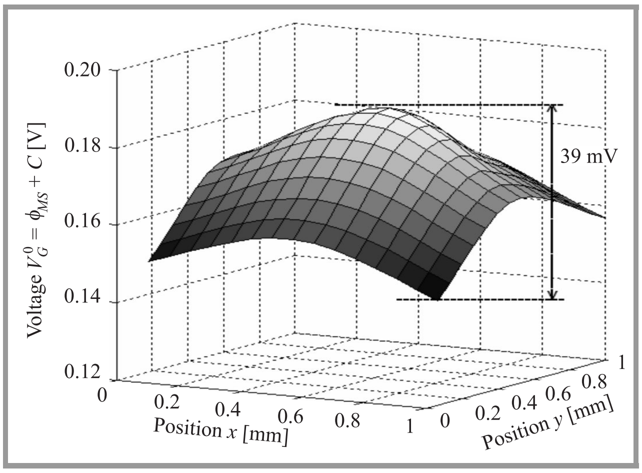

Fig. 7. Averaged two-dimensional distribution of V_G^0 voltage values measured for 26 MOS structures. Average V_G^0 values for the same wavelength $\lambda = 242$ nm were found for each of the 9 locations over the gate area (shown in Fig. 4) and used to determine the distribution shown in the figure.

In Figs. 6a and 7 it is seen that averaged E_{BG} and V_G^0 distributions have a characteristic dome-like shape with the highest values at the center of the square gate and lowest values at gate corners. On the other hand an averaged E_{BS} distribution is practically uniform, with random departures from uniformity. The averaged departures from the uniform distribution of E_{BS} decrease with the number of structures taken into account in the averaging process. Defining the amplitude A as the difference between the maximum and minimum local values of the same parameter over the gate area (e.g., $A(E_{BG}) = E_{BG\max} - E_{BG\min}$), one finds that the amplitude of E_{BG} distribution $A(E_{BG})$ is about four times larger than the amplitude $A(E_{BS})$ of the E_{BS} distribution ($A(E_{BG}) \approx 4A(E_{BS})$). This means that the distribution of the gate-dielectric barrier height $E_{BG}(x, y)$ has the decisive influence on the $\phi_{MS}(x, y)$ distribution.

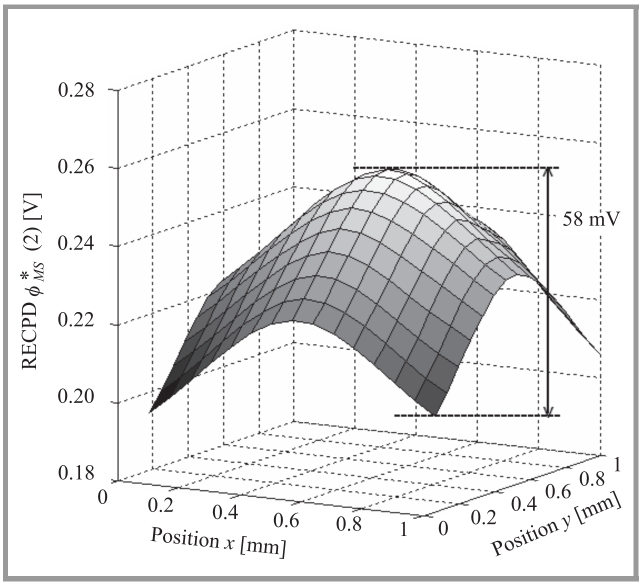

Fig. 8. Averaged two-dimensional distribution of $\phi^*_{MS}(2)$ calculated using E_{BG} and E_{BS} values for 26 MOS structures. Average $\phi^*_{MS}(2)$ values were found for each of the 9 locations over the gate area (shown in Fig. 4) and used to determine distributions shown in the figure.

Using Eq. (5) the average distribution of $\phi^*_{MS}(2)$ over the gate area was calculated and plotted in Fig. 8. This distribution has a similar shape to the distributions of the E_{BG} (Fig. 6) and the V_G^0 (Fig. 7) with the highest values at the gate center and lowest values at gate corners. It is well known [2] that the shape of $\phi^*_{MS}(1)$ distribution is the same as the shape of V_G^0 distribution, shifted by a constant value C.

Using Eq. (6) R values were obtained at each of nine positions over the gate area and are given in Table 1.

Table 1
Values of measurement errors R at the 9 positions over the gate area

Position (as indicated in Fig. 4)	1	2	3	4	5	6	7	8	9
R [mV]	20	1	9	13	–2	1	15	1	18

The values given in Table 1 are relatively small (we consider them as indicators of barrier height measurement accuracy). The accuracy of the both barrier height measurements is very good in the middle of the square gate (−2 mV, negative sign means that E_{BS} value is too low in comparison with E_{BG} value or that E_{BG} value is too high in comparison with E_{BS} value). There are larger differences between $\phi^*_{MS}(1)$ and $\phi^*_{MS}(2)$ at gate corners (the average value of R for four equivalent positions is 15 mV) and gate edges (4 mV is the average R value for four equivalent positions).

The model which has been applied to the ϕ_{MS} distribution [3, 4] can be also used to describe distributions of E_{BG}, $\phi^*_{MS}(1)$ and $\phi^*_{MS}(2)$. This model for the one-dimensional distribution $K(x)$ of the parameter K is given by the formula:

$$K(x) = K_0 + \Delta K \cdot \left[e^{\frac{x}{L}} + e^{\frac{a-x}{L}} \right], \qquad (7)$$

where: K_0 – value of K parameter far away from gate edges, ΔK – deviation of $K(x)$ from K_0, L – characteristic length of $K(x)$ distribution, a – side length of the square gate.

The predictions of the model are in good agreement with experimental results obtained on MOS structures with square gates used in this investigation. The model values at the gate center – K_0 were fitted to those obtained from the measurements. Values of all the parameters at gate corners were fairly close to the measured values.

Using the model based on Eq. (7), two-dimensional $E_{BG}(x, y)$ distribution was calculated and is shown in Fig. 9. The parameters used in model calculations are listed below the plot. The flat $E_{BS}(x, y)$ distribution can also be expressed in terms of the model Eq. (7), with the parameters: $E_{BS0} = 4.405$ eV, $\Delta E_{BS} = 0$ eV, $L = 0$ mm.

The RECPD distributions of $\phi^*_{MS}(1)$ and $\phi^*_{MS}(2)$ calculated using the model based on Eq. (7) are shown in Fig. 10.

In both cases the K_0 parameter of the model was so chosen as to obtain the same ϕ^*_{MS} value at the center of the gate as that obtained from measurements. Parameters used in model calculations are indicated below the diagrams. Clearly, $\phi^*_{MS}(2)$ values are lower than $\phi^*_{MS}(1)$ at the gate

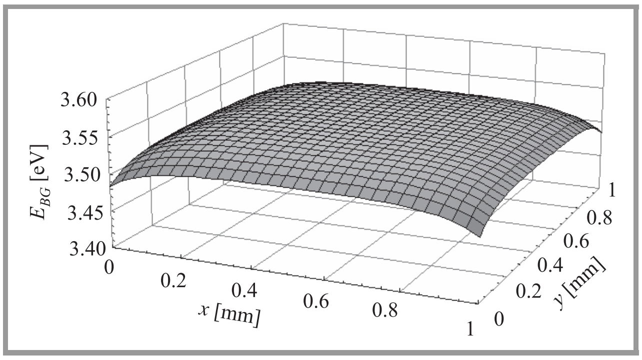

Fig. 9. Two-dimensional distribution of E_{BG} barrier height values calculated using the model based on formula (7). Model parameters: $E_{BG0} = 3.545$ eV, $\Delta E_{BG} = -0.061$ eV, $L = 0.1$ mm, $a = 1$ mm.

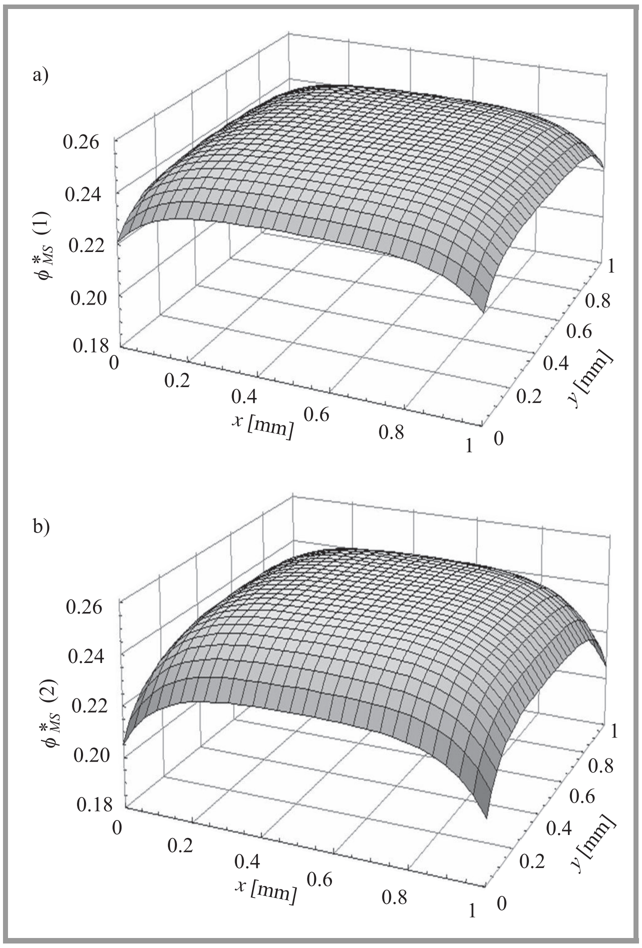

Fig. 10. Two-dimensional distributions of: (a) $\phi^*_{MS}(1)$ and (b) $\phi^*_{MS}(2)$ reduced effective contact potential difference values calculated using the formula (7). Model parameters: (a) $\phi^*_{MS0}(1) = 0.253$ V, $\Delta\phi^*_{MS}(1) = -0.032$ V, $L = 0.1$ mm, $a = 1$ mm; (b) $\phi^*_{MS0}(2) = 0.255$ V, $\Delta\phi^*_{MS}(2) = -0.05$ V, $L = 0.1$ mm, $a = 1$ mm.

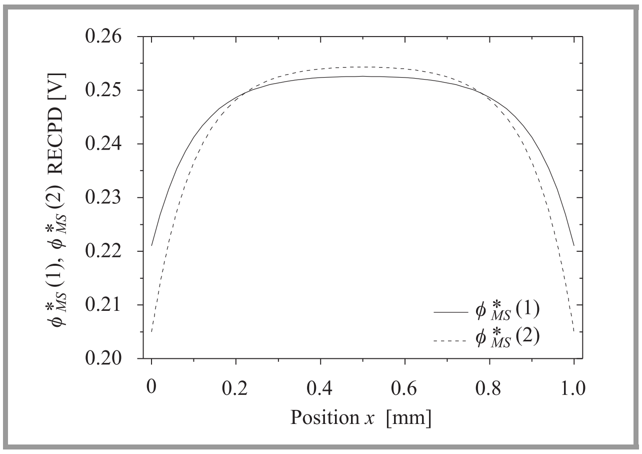

Fig. 11. Comparison of the $\phi^*_{MS}(1)$ (solid line) and $\phi^*_{MS}(2)$ (dashed line) distributions calculated using the model.

corners, as reflected in the $\Delta\phi^*_{MS}$ values ($|\Delta\phi^*_{MS}(2)| > |\Delta\phi^*_{MS}(1)|$. This is demonstrated more clearly in the one-dimensional distributions of $\phi^*_{MS}(1)$ and $\phi^*_{MS}(2)$ shown in Fig. 11.

5. Conclusions

Distributions of E_{BG} and E_{BS} barrier heights, V_G^0 voltage as well as RECPD ($\phi^*_{MS}(1)$ and $\phi^*_{MS}(2)$) over the gate area were studied. Measurements were made on a series of 26 Al-SiO_2-Si(n^+) MOS capacitors on one silicon wafer. Barrier heights were measured by modified Powell-Berglund method using a UV light beam of small diameter. This allowed the gate area to be scanned with the light beam and to measure local barrier height values at nine different positions over the gate area. It was found that E_{BG}, V_G^0, $\phi^*_{MS}(1)$ and $\phi^*_{MS}(2)$ values have a characteristic dome-like shape, with the highest values at the gate center, lower at gate edges and still lower at gate corners. On the other hand, E_{BS} barrier height distribution is essentially uniform, with random departures from uniformity.

The accuracy of both barrier height measurements was checked by comparing the $\phi^*_{MS}(1)$ value (determined using the ϕ_{MS} measured by the photoelectric method) with the value of $\phi^*_{MS}(2)$ (obtained from E_{BG} and E_{BS} measurements). It has been shown that the difference R between these values is very small (2 mV) at the center of the gate and becomes larger ($\sim$ 15 mV) at the corners of the square gate. These results (as well as the results of other experiments not reported in this paper), allow the accuracy of the measurement of local barrier height values by the modified Powell-Berglund method to be estimated. Our (rather conservative) estimation is that the possible measurement error ΔE_B does not exceed $\pm$50 meV in this case.

It was found that models of 2D distributions, similar to the model previously developed for $\phi_{MS}(x, y)$ distribution, can be successfully applied to other parameters – in particular to $E_{BG}(x, y)$ and $\phi^*_{MS}(2)(x, y)$ distributions.

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