ELECTRON TECHNOLOGY
Internet Journal
ISSN 1897-2381
http://www.ite.waw.pl/etij/

DISTRIBUTION OF POTENTIAL BARRIER HEIGHT LOCAL VALUES AT Al-SiO$_2$ AND Si-SiO$_2$ INTERFACES OF THE METAL-OXIDE-SEMICONDUCTOR (MOS) STRUCTURES

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Received November 8, 2004; modified December 17, 2004; published December 23, 2004

ABSTRACT

Using the photoelectric measurement methods distributions have been determined of the gate-dielectric $E_{BG}(x, y)$ and semiconductor-dielectric $E_{BS}(x, y)$ barrier height values in square gate (1 x 1 mm^2) Al-SiO$_2$-Si(n$^+$) structures. Measurements have been made on a series of 26 MOS capacitors with semitransparent gates (t_{Al} = 35 nm), on one silicon wafer. Barrier heights were measured using the modified Powell-Berglund and the modified Fowler methods. Measurement methods were modified in such a way as to allow determination of $E_{BG}(x, y)$ and $E_{BS}(x, y)$ distributions, as described in the text. It has been found that the $E_{BG}(x, y)$ distribution has a characteristic dome-like shape which is identical with the independently determined shape of the effective contact potential difference $\phi_{MS}(x, y)$ distribution. The $E_{BS}(x, y)$ distribution is of a random character and differences between highest and lowest values of E_{BS} for any of the measured capacitors are much smaller than the respective differences in E_{BG} values. These results show that it is the gate-dielectric barrier height distribution $E_{BG}(x, y)$ which causes the dome-like shape of the $\phi_{MS}(x, y)$ distribution, observed for several years in our laboratory. This finding supports our hypothesis that the characteristic $\phi_{MS}(x, y)$ distribution over the gate area of Al-SiO$_2$-Si structures results from the mechanical stress distribution under the gate electrode.

1. Introduction

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

As discussed in [1], we attribute this characteristic distribution to the mechanical stress in metal-oxide-semiconductor system which is also known [4–6] to be non-uniformly distributed under the gate. With this assumption in mind and assuming that changes in ϕ_{MS} value are proportional to the changes in mechanical stress σ, a model of ϕ_{MS} distribution over the gate area was developed and thoroughly verified experimentally [1]. A typical distribution of ϕ_{MS} local values over the square gate area, calculated using this model is shown in Fig. 2.

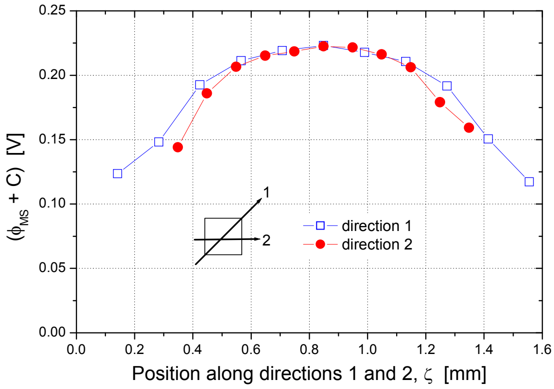

Fig. 1 Typical dependence of the (ϕ_{MS} + C) voltage measured at the wavelength λ = 244 nm on the position in Al-SiO$_2$-Si(n$^+$) structures with aluminum gate thickness t_{Al} = 35 nm and SiO$_2$ layer thickness t_{OX} = 60 nm. The direction is either (*1*) along the diagonal of the square gate, or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

As shown in the next section, the ϕ_{MS} value depends directly on the difference of potential barrier heights $E_{BG} - E_{BS}$, where E_{BG}, E_{BS} are respectively the barrier heights at gate-dielectric and semiconductor-dielectric interfaces. Hence, one or both of these barrier heights must have distributions which are reflected in the ϕ_{MS} distribution over the gate area. If the barrier height distribution is indeed caused by the mechanical stresses under the gate, as we assume, one would expect that it is the E_{BG} distribution which primarily determines the distribution of ϕ_{MS} over the gate area.

It is the purpose of this work to determine the distributions of both E_{BG} and E_{BS} over the gate area and to find out how they influence the ϕ_{MS} distribution.

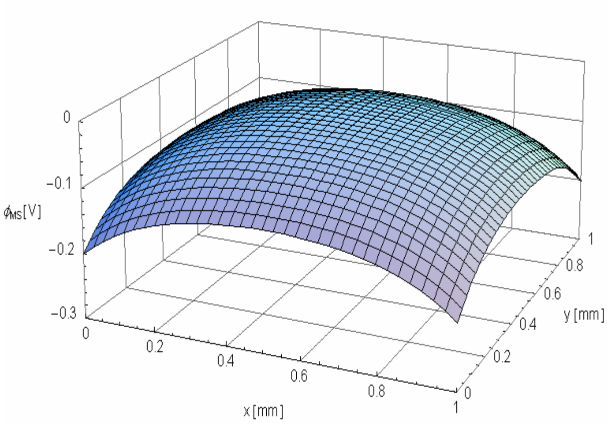

Fig. 2. Two-dimensional distribution of $\phi_{MS}(x, y)$ calculated using model [1] for MOS structures with square gates of side length $L = 1$ mm.

2. Theory

The band diagram of the MOS system is shown in Fig. 3.

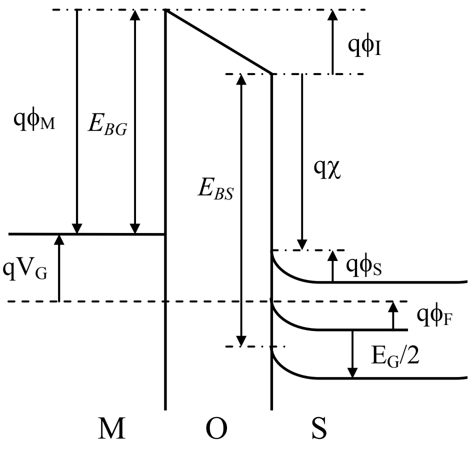

Fig. 3. Band diagram of the MOS system, at arbitrary gate potential V_G. E_{BG}, E_{BS} are potential barrier heights at gate-dielectric and semiconductor-dielectric interfaces, respectively.

The effective contact potential difference (ECPD or ϕ_{MS}) is defined as (see e.g. [7]):

$$\phi_{MS} \overset{\text{def}}{=} \phi_M - \left(\chi + \frac{E_G}{2q} + \phi_F \right) \tag{1}$$

where: ϕ_M is potential barrier height for internal photoemission from metal to dielectric (in V), χ is electron affinity at semiconductor-dielectric interface (in V), E_G is band gap energy (in J), q is electron charge (in C), ϕ_F is Fermi level in semiconductor (in V), as shown in Fig. 3.

The value of ECPD given by Eq. (1) depends on the doping density of the substrate (through the ϕ_F value). Sometimes it is more convenient to use the value of the reduced effective contact potential difference (RECPD or ϕ^*_{MS} factor), defined as:

$$\phi^*_{MS} = \phi_M - \chi \, . \tag{2}$$

It is clear from definition (2) that ϕ^*_{MS} value depends on the barrier heights on both sides of the dielectric and does not depend on the doping density in the substrate.

Using the band diagram shown in Fig. 3, one finds that:

$$\phi^*_{MS} = \phi_M - \chi = \frac{1}{q}(E_{BG} - E_{BS} + E_G) \, . \tag{3}$$

Hence, making use of Eqs (1)–(3), comparisons can be made between the independently measured values of ϕ_{MS} and values of E_{BG} and E_{BS}, if the ϕ_F and E_G values are known.

The individual barrier height values (E_{BG} and E_{BS}) can be determined making use of the internal photoemission phenomena which take place when a MOS structure, with semitransparent gate is 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 pass into the conduction band of the dielectric 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 the electrons have to surmount, as well as of the wavelength λ of UV light illuminating the structure and of the gate potential V_G. The experimentally determined $I_P = f(V_G, \lambda)$ characteristics can be used to determine the E_{BG} and E_{BS} barrier heights by the well known Powell-Berglund [8–10], [12] and Fowler [11], [12] methods.

3. Experimental details

Measurements were made on Al-SiO$_2$-Si(n$^+$) structures with square (1 x 1 mm^2) Al gates of thickness t_{Al} = 35 nm. Phosphorus doped n$^+$ substrates (ρ = 0.015 Ω·cm) of (100) orientation were used to simplify interpretation of the photoelectric measurements, as discussed in [1], [3]. After the initial cleaning sequence, wafers were thermally oxidized at temperature T = 1000°C, in dry oxygen, to grow a SiO_2 layer of thickness t_{OX} = 60 nm. Although much thinner oxides are of current technological interest, thicker oxides were used to optimize the sensitivity of photoelectric methods [3]. Oxidized wafers were subsequently annealed in nitrogen for t = = 10 min, at T = 1050°C. Frontside metalization was carried out by thermal evaporation and was patterned by photo- lithography. Backside oxide was etched off prior to backside metalization. The post metalization annealing was carried out for t = 20 min, at T = 450°C in the 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. Barrier heights were measured by two classical – but modified – methods, the Powell-Berglund method [8–10], [12] and the Fowler method [11], [12]. These methods were modified in such a way as to determine the distributions of barrier heights over the gate area of the MOS structure. The modification consisted in using a UV light beam of a fairly small diameter d = 0.3 mm. This diameter is much larger than the diameter of the light beam used to obtain results shown in Fig. 1, but it is smaller than the side length of the Al gates. Hence, using this light beam it was possible to measure the local values of both gate-dielectric E_{BG} and semiconductor-dielectric E_{BS} barrier heights (by both methods), in nine different locations over the gate area, as illustrated in Fig. 4.

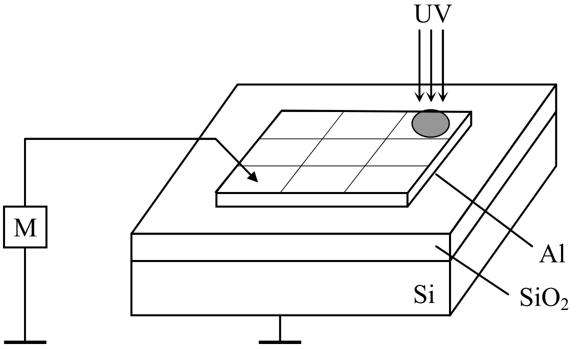

Fig. 4. The measurement system: the MOS structure with a semi-transparent square gate of side length L = 1 mm is illuminated in 9 different locations over the gate area by a focused UV light beam. The photocurrent is measured in the external circuit M.

The so determined local values of barrier heights were then connected by smooth (3rd order poly-nomial) lines to obtain approximate distributions of barrier heights over the entire gate area of the MOS structure, as discussed in the next section.

The absolute accuracy of E_{BG} and E_{BS} determination is estimated to be ± 50 mV. 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 much better and is estimated to be ± 10 mV.

4. Results and discussion

Typical distributions of E_{BG} and E_{BS} barrier height values determined as described above, for one individual MOS structure, are shown in Fig. 5a and 5b. As shown in these figures, both barrier heights have non-uniform distributions over the gate area. However, the amplitude of E_{BG} changes over the gate area is significantly larger than the corresponding amplitude of E_{BS} changes. The amplitude is defined here as the difference between the maximum and the minimum values of the local barrier heights found over the gate area. It has also been noticed that the dome-like shape of the $E_{BG}(x, y)$ distribution is observed in all the measured MOS structures, while the shape of the $E_{BS}(x, y)$ distribution is different for different MOS structures and is of a random character. To prove that indeed the E_{BG} distribution has a regular and reproducible dome-like shape and that the distribution of E_{BS} is of a random character, the following experiment was made.

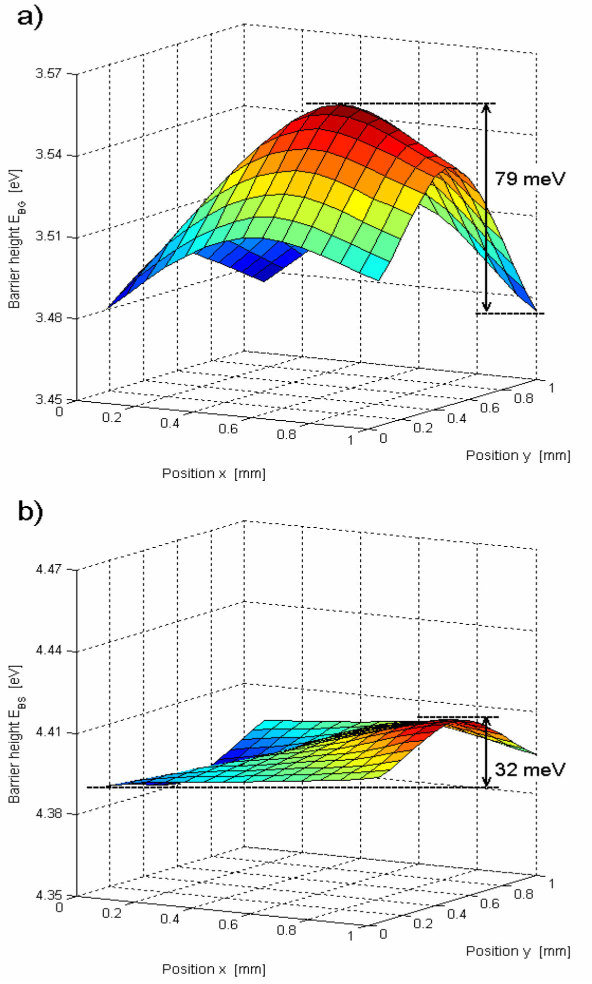

Fig. 5. Two-dimensional distribution of a) E_{BG} and b) E_{BS} barrier height calculated using Powell-Berglund method for 1 MOS structure with a square gate of side length L = 1 mm.

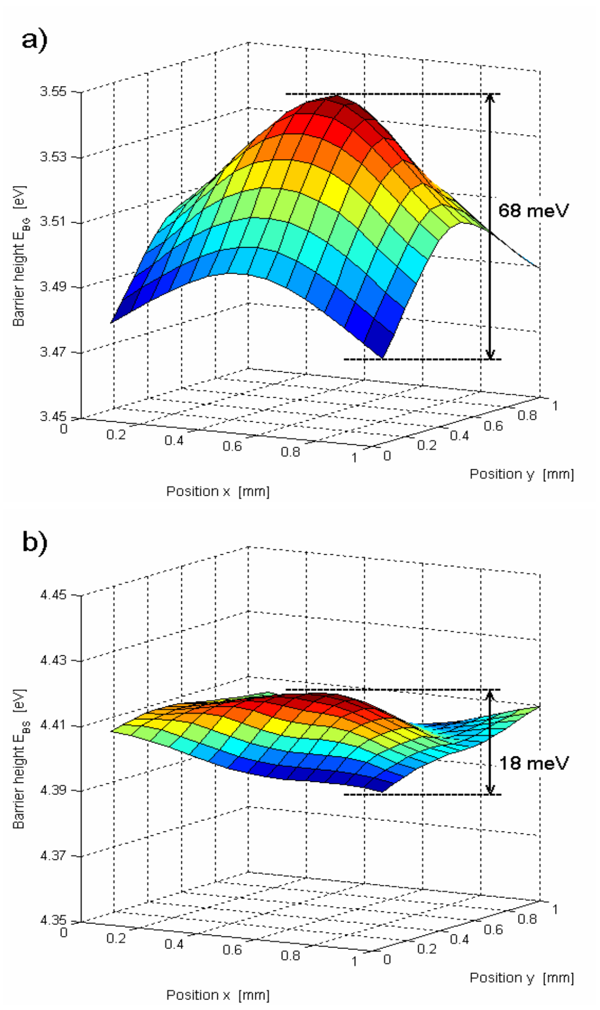

Fig. 6. Averaged two-dimensional distribution of a) E_{BG} and b) E_{BS} barrier heights measured using Powell-Berglund method for 26 MOS structures. Average E_{BG} and E_{BS} values were found for each of the 9 locations over the gate area (shown in Fig. 4) and used to determine distributions shown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

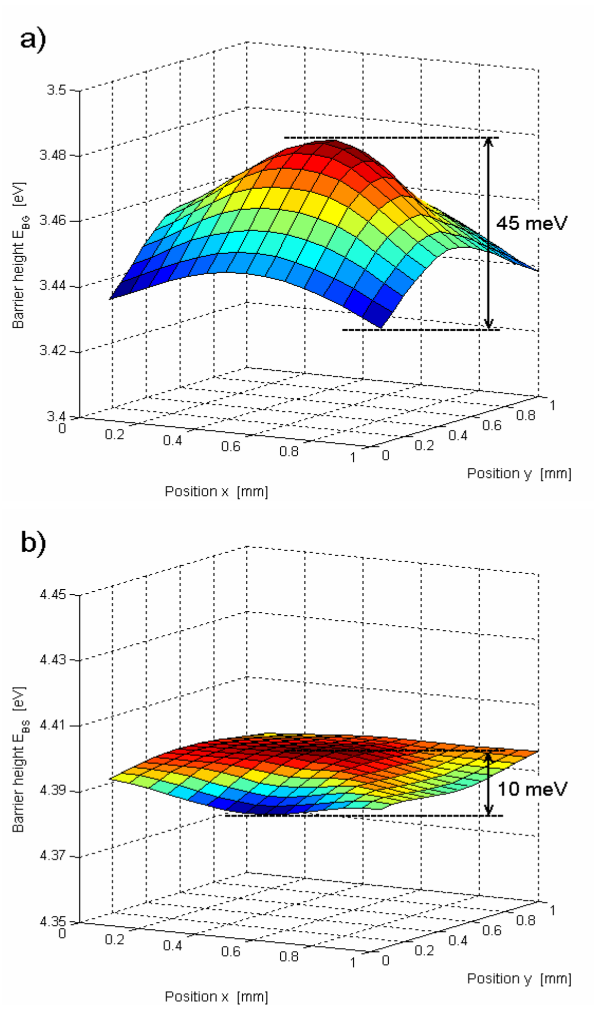

Fig. 7. Averaged two-dimensional distribution of a) E_{BG} and b) E_{BS} barrier heights measured using Fowler method for 26 MOS structures. Average E_{BG} and E_{BS} values were found for each of the 9 locations over the gate area (shown in Fig. 4) and used to determine distributions shown in the figure.

Measurements of local E_{BG} and E_{BS} barrier heights were made by both Powell-Berglund and (for comparison) by the Fowler method, in nine locations (as shown in Fig. 4), 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. The so obtained distributions of the averaged values are shown in Figs. 6a and 6b for measurements made by the Powell-Berglund method and in Figs. 7a and 7b for measurements made by the Fowler method.

Figures 6a and 7a show that the averaged $E_{BG}(x, y)$ distribution retains its dome-like shape and the amplitude of the distribution remains relatively large (68 or 45 meV). On the contrary, the amplitudes of the averaged $E_{BS}(x, y)$ distributions, shown in Fig. 6b and 7b are smaller than corresponding amplitudes observed for individual MOS structures. Moreover, these amplitudes show a decreasing tendency with the increasing number of MOS structures measured and taken into account in the averaging process.

There are slight differences in the averaged distributions obtained for measurements by the Powell-Berglund and by the Fowler methods (compare Fig. 6a with Fig. 7a and Fig. 6b with Fig. 7b) which are due to the measurement inaccuracies by both methods. Nevertheless, the general features of averaged E_{BG} and E_{BS} distributions determined using both methods are the same.

5. Conclusions

In this paper results have been presented of photoelectric barrier height measurements made on a series of 26 Al-SiO$_2$-Si(n$^+$) capacitors on one silicon wafer. Both the gate-dielectric (E_{BG}) and semiconductor-dielectric (E_{BS}) barrier heights were measured using the modified Powell-Berglund and the modified Fowler method. The modifications of these methods consisted in applying a focused UV light beam (diameter d = 0.3 mm) which allowed measurements to be made in nine locations over the gate area. As a result, approximate distributions of $E_{BG}(x, y)$ and $E_{BS}(x, y)$ have been found.

It has been shown that $E_{BG}(x, y)$ distribution has a characteristic dome-like shape, with the highest E_{BG} values at the central part and lowest values at the corners of a square aluminum gate. The shape of $E_{BS}(x, y)$ distribution is of a random character and the amplitude of this distribution is much smaller. The dome-like shape of the $E_{BG}(x, y)$ distribution is identical with the shape of independently (and much more accurately) measured distributions of $\phi_{MS}(x, y)$ over the gate area (see Fig. 1). This proves that, as expected, the shape of the $\phi_{MS}(x, y)$ distribution results directly from the distribution of gate-dielectric barrier height $E_{BG}(x, y)$ over the gate area. This result lends support to our hypothesis that it is the mechanical stress under the gate which causes the characteristic $\phi_{MS}(x, y)$ distribution over the gate area in Al-SiO_2-Si structures.

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