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Lateral distribution of Schottky barrier height: a theoretical approach

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The effect of the metal, semiconductor and interface parameters on the Schottky barrier height is analysed in order to determine whether the lateral distribution of the barrier height obeys a normal or the lognormal law. It is found that the fluctuations of some parameters result in a normal lateral distribution, while the fluctuations of the others yield a lognormal lateral distribution of the Schottky barrier height. It is shown that the only available experimental barrier height distribution may be explained by a superposition of two lognormal distributions.

1. Introduction

It is well known that Schottky junctions are often inhomogeneous laterally. Several models have been proposed for the barrier height (BH) distribution (D) in these junctions, and so for the explanation of the electrical characteristics obtained[1–19]. Most of the authors explained the experimental results by a parallel connection of two or more phases with different BHs[1–16]. Others assumed a continuous variation of the BH, and proposed the normal (Gaussian) D to describe it[17–19].

Recently the present author showed that several features of the capacitance–voltage characteristics obtained for an Au/n-GaAs Schottky contact might be equally explained by either the normal or the lognormal lateral D of the BH[20]. In this paper the effect of the metal, semiconductor and interface parameters on the Schottky BH is analysed in order to determine whether the lateral D of the BH obeys the normal or the lognormal law.

2. Theoretical analysis

Applying the interfacial layer model to Schottky junctions, the BH may be described by the following expressions:

$$Q_{i0}(\phi^n_{b0}) - \varepsilon_0\varepsilon_i(\phi_M - X - \phi^n_{b0})/\delta + [2\varepsilon_0\varepsilon_s q N_D(\phi^n_{b0} - \phi_n - kT/q)]^{1/2} = 0 \quad (1)$$

for the n-type[21], and

$$Q_{i0}(\phi^p_{b0}) + \varepsilon_0\varepsilon_i(E_g/q - \phi_M + X - \phi^p_{b0})/\delta - [2\varepsilon_0\varepsilon_s q N_A(\phi^p_{b0} - \phi_p - kT/q)]^{1/2} = 0 \quad (2)$$

for the p-type[22] junctions. Here $Q_{i0}(\phi^n_{b0})$ and $Q_{i0}(\phi^p_{b0})$ represent the equilibrium interface charge as single-valued functions of the equilibrium potential BHs (not reduced by the image force lowering) ϕ^n_{b0} and ϕ^p_{b0}, ε_0 is the dielectric constant of the vacuum, ε_i and ε_s are the relative dielectric constants of the interfacial layer and of the semiconductor, respectively, ϕ_M is the metal work function, X is the electron affinity of the semiconductor, E_g is the band gap, δ is the thickness of the interfacial layer, q is the elementary charge, N_D and N_A are the donor and acceptor concentrations in the semiconductor, respectively, ϕ_n is the energy difference between the conduction band edge and the Fermi-level, while ϕ_p is the energy difference between the valence band edge and the Fermi-level in the semiconductor.

For each actual Schottky junction the only variables in these expressions are the equilibrium BHs ϕ^n_{b0} and ϕ^p_{b0}, respectively. The interfacial layer model, and so equations (1) and (2), may be applied to intimate Schottky junctions as well. For these junctions the interfacial layer thickness should be considered as the depth of the centroid of the interface charge from the metal/semiconductor interface.

From equations (1) and (2), it can be seen that the Schottky BH is determined by the metal work function, the electron affinity, the band gap, the doping concentration, the thickness and dielectric constant of the interfacial layer, and the $Q_{i0}(\phi^n_{b0})$ or $Q_{i0}(\phi^p_{b0})$ function, i.e. by the interface state energy D spectrum and the fixed interface charge. The effect of these parameters on the Schottky BH may be analysed by the differentiation of equations (1) and (2) according to these parameters. It is expedient to divide the equilibrium interface charge into two parts before differentiation:

$$Q_{i0} = Q_{is0} + Q_{if} \quad (3)$$

where Q_{is0} is the equilibrium charge in interface states and Q_{if} is the fixed interface charge.

The resultant partial derivatives of the BH are presented in Table 1. The specific capacitances which figure in Table 1 are defined as follows: c_{is} is that of interface states:

$$c_{is} = dQ_{i0}/d\phi^n_{b0} = q^2 D_s \quad (n\text{-type}) \quad (4a)$$

Table 1. Partial derivatives of the equilibrium barrier height according to the parameters of the metal, semiconductor and interface

Parameter	Derivative: n-type	p-type
ϕ_M	$\frac{c_{il}}{\Sigma c}$	$-\frac{c_{il}}{\Sigma c}$
X*	$-\frac{c_{il}+c_{is}}{\Sigma c}$	$\frac{c_{il}+c_{is}}{\Sigma c}$
E_g*	0	$\frac{1}{q}\cdot\frac{c_{il}+c_{is}}{\Sigma c}$
N_D, N_A	$-\frac{\phi^n_{b0}-\phi_n}{N_D}\cdot\frac{c_{s0}}{\Sigma c}$	$-\frac{\phi^p_{b0}-\phi_p}{N_A}\cdot\frac{c_{s0}}{\Sigma c}$
ε_s	$-\frac{\phi^n_{b0}-\phi_n-kT/q}{\varepsilon_s}\cdot\frac{c_{s0}}{\Sigma c}$	$-\frac{\phi^p_{b0}-\phi_p-kT/q}{\varepsilon_s}\cdot\frac{c_{s0}}{\Sigma c}$
Q_{if}	$-\frac{1}{\Sigma c}$	$\frac{1}{\Sigma c}$
δ	$\frac{\phi^n_{b0}-(\phi_M-X)}{\delta}\cdot\frac{c_{il}}{\Sigma c}$	$\frac{\phi^p_{b0}-(E_g/q-\phi_M+X)}{\delta}\cdot\frac{c_{il}}{\Sigma c}$
ε_i	$-\frac{\phi^n_{b0}-(\phi_M-X)}{\varepsilon_i}\cdot\frac{c_{il}}{\Sigma c}$	$-\frac{\phi^p_{b0}-(E_g/q-\phi_M+X)}{\varepsilon_i}\cdot\frac{c_{il}}{\Sigma c}$

* Obtained with the assumption that interface states are bound to the vacuum level.

$$c_{is} = -\mathrm{d}Q_{i0}/\mathrm{d}\phi^p_{b0} = q^2 D_s \quad (p\text{-type}) \tag{4b}$$

where D_s is the interface state density, c_{il} is the specific capacitance of the interfacial layer:

$$c_{il} = \varepsilon_0\varepsilon_i/\delta \tag{5}$$

and c_{s0} is the specific capacitance of the depletion layer:

$$c_{s0} = \{\varepsilon_0\varepsilon_s q N_D/[2(\phi^n_{b0}-\phi_n-kT/q)]\}^{1/2} \quad (n\text{-type}) \tag{6a}$$

$$c_{s0} = \{\varepsilon_0\varepsilon_s q N_A/[2(\phi^p_{b0}-\phi_p-kT/q)]\}^{1/2} \quad (p\text{-type}) \tag{6b}$$

while

$$\Sigma c = c_{is}+c_{il}+c_{s0} \tag{7}$$

The lateral inhomogeneity of the BH may be connected with the variation of all of the above parameters as well as with the surface roughness, crystal defects, etc. The effect of the latter parameters on the local electric field D may be considered as an equivalent change in the dopant concentration.

The probability function for the normal D of the BH is well known[17–19]:

$$f(\phi_{b0}) = \frac{1}{(2\pi)^{1/2}\sigma_a}\exp\left[-\frac{(\phi_{b0}-\phi_{b0a})^2}{2\sigma_a^2}\right] \tag{8}$$

where σ_a is the algebraic standard deviation of the BH, and ϕ_{b0a} is its algebraic mean value. This D is symmetrical with respect to the low and high BHs.

In the case of the lognormal D, not the BH, but its logarithm, obeys the normal D. The probability function of the BH for the three-parameter form of the lognormal D[23] is

$$f(\phi_{b0}) = \frac{1}{(2\pi)^{1/2}(\phi_{b0}-\phi_{b0m})\sigma_g} \times \exp\left[-\frac{\{\ln[(\phi_{b0}-\phi_{b0m})/(\phi_{b0g}-\phi_{b0m})]\}^2}{2\sigma_g^2}\right] \tag{9}$$

Here σ_g is the geometric standard deviation (the algebraic standard deviation of ln ϕ_{b0}), ϕ_{b0g} is the geometric mean value, and ϕ_{b0m} the minimal possible value of the BH. This D has a longer tail towards high BHs.

It is an interesting—and important for the discussion of the experiments—property of the lognormal D that the median coincides with the geometric mean value, while for the normal D it coincides with the algebraic mean value.

A variate obeys the normal D, if its fluctuations due to the effect of different parameters are independent of its actual value. If the fluctuations depend on the actual value of the variate, the variate obeys the lognormal D[23]. On the basis of the partial derivatives presented in Table 1, one can conclude that the lateral fluctuations of the fixed interface charge, of the metal work function, of the electron affinity and of the band gap of the semiconductor result in a normal lateral D of the BH, as the partial derivatives obtained for these quantities do not depend on the value of the BH. On the other hand, the fluctuations of the thickness and of the dielectric constant of the interfacial layer, and the fluctuations of the dielectric constant and of the doping concentration of the semiconductor (including other effects mentioned above which distort the potential D) result in a lognormal D of the Schottky BH, as the partial derivatives obtained for these quantities depend on the BH. It may be shown that the change in the interface state energy D spectrum also results in a normal D of the BH[24].

This means that (i) the BH may obey both the normal and the lognormal *D*, and also their several superpositions, and (ii) knowing the BH *D*, one can distinguish between these two groups of the influencing parameters.

3. Comparison with experiments

To the best of the present author's knowledge, there are only two works presenting experimental lateral *D* data of Schottky BH obtained by ballistic electron emission microscopy (BEEM) in Au/CdTe[25] and PtSi/Si[26] Schottky junctions. Unfortunately, the probability function obtained of the BH for the Au/CdTe junction is too rough for a detailed analysis (it contains 15 data only).

The experimental BH *D* obtained in PtSi/n-Si Schottky junctions[26] is presented in Figure 1. The experimental probability function presented contains 300 measured BH values. Unfortunately these values were obtained on six different diodes, which were prepared in a similar way, but had different thickness of the PtSi layer in the range of 3–20 nm. The cumulative presentation of the data for six diodes makes analysis of the *D* spectrum rather difficult.

It is clear that no single normal *D* may be fitted to the experimental results presented in Figure 1. The attempt at fitting a single lognormal *D* has not been successful either. But a superposition of two lognormal *D*s (one with 2/3 intensity and large scatter, the other with 1/3 intensity and small scatter) may be fitted well, as is also presented in Figure 1. The parameters resulting in a good fit presented in Figure 1 are as follows: $\phi_{b0m} = 0$ for the both components, $\sigma_g = 0.17$ V and $\phi_{b0g} = 0.95$ V for the component with 2/3 intensity, while $\sigma_g = 0.04$ V and $\phi_{b0g} = 0.87$ V for the component with 1/3 intensity.

The experimental data suggest the presence of two other peaks at barrier height values of about 0.83 and 0.98 V which may be connected with the specific features of the individual diodes. On the other hand, these apparent peaks may also be connected with the large scatter of the probability density due to the relatively small number of measurements.

The difference between the geometric means of the two fitting components may also be connected with the properties of the individual diodes, or, more likely, with the presence of two dominating parallel phases with different mean BH values in most of the diodes. Thus, the properties of the individual diodes themselves may be connected to the presence of two parallel phases with different relative ratios of their area. The presence of two parallel phases was obtained earlier in PtSi/Si junctions prepared in a similar way[27]. Epitaxial PtSi grains were observed by transmission electron microscopy and X-ray photoelectron spectroscopy surrounded with amorphous PtSi in the layers studied with thickness below 8 nm, and with polycrystalline PtSi in the thicker layers. The authors themselves concluded[26] that some feature of the transmission probability results obtained in the diodes discussed here, 'may be related to the change from predominantly amorphous to polycrystalline structure as the film thickness increases'.

The scatter and the median values of the barrier height were also presented for all of the diodes[26]. The median (i.e. the geometric mean for the lognormal *D*) for four of the diodes with PtSi thicknesses below 20 nm was in the range of 0.86–0.90 V, while it was about 0.98 V for the two diodes with thicker PtSi layers which exhibited the highest scatter. These median values are in agreement with the geometric means obtained by the fitting of the two components.

Therefore the resultant lateral *D* of the BH in the diodes studied may be due to the presence of two parallel phases: an amorphous phase and a polycrystalline phase.

Finally, it should be mentioned that the lognormal *D* is very frequent in nature in general[23], and also in the condensed matter, in particular in amorphous materials[28,29].

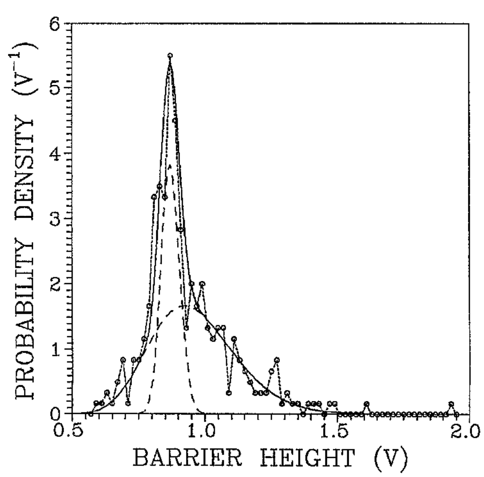

Figure 1. The potential barrier height distribution obtained in PtSi/n-Si Schottky junctions by BEEM measurements[26] (dots and dotted line), and the fitted superposition (solid line) of two lognormal distributions (dashed lines).

4. Conclusions

It has been shown that the lateral fluctuations of the fixed interface charge, the interface state density, the metal work function, the semiconductor electron affinity and the band gap result in a normal lateral *D* of the Schottky BH, while the fluctuations in the interfacial layer thickness, the dielectric constant of the interfacial layer and the semiconductor, and the fluctuations in the doping concentration result in a lognormal *D* of the BH.

It has also been shown that the BH *D* of PtSi/n-Si Schottky junctions obtained by BEEM technique[26] may be explained by a superposition of two lognormal *D*s which may be connected with an amorphous and a polycrystalline phase of the PtSi layer.

Note added in proof

Since the submission of this paper, several experimental lateral Ds of Schottky BH have been presented[30–32] that seem to be in agreement with the conclusions of the above analysis.

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