Numerical study of electrical transport in inhomogeneous Schottky diodes

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The Poisson equation together with the drift-diffusion equations have been used to simulate both forward and reverse $I-V$ and $C-V$ characteristics of inhomogeneous Schottky diodes. The barrier height distribution has been modeled by a single Gaussian. It is shown that the $I-V$ and $C-V$ curves and consequently extracted apparent Schottky diode parameters depend only slightly, if at all, on a lateral correlation between the single barrier patches in the structure for larger dimension of patches. The apparent barrier height of ordered structures differ only in several thousandths of volt from that of uncorrelated barrier patches. Very small differences were also found between the currents through the diodes with large inhomogeneities and nanosize inhomogeneities. The numerical results show that there is almost no dependence of the current on a pinch-off effect of electric potential. The diminishing of a drift part of the total current in the area of pinched-off potential is probably compensated by a greater diffusion current in the region. Consequently, very small and not unambiguous differences were found between the so called interacting and noninteracting diodes and this division is, according to the above results, questionable. © *1999 American Institute of Physics.* [S0021-8979(99)02203-3]

I. INTRODUCTION

In spite of a great deal of attention devoted to understanding physical and electronic properties of metal semiconductor contacts, there are still many inconsistencies between the data measured on experimental structures and their theoretical interpretation. The currently established model connects the responsibility for the magnitude of a Schottky barrier height (SBH) with electron states present at the metal semiconductor interface. Physical approaches usually assume a uniform crystallographic and also electronic structure up to the interface. In recent years, a number of papers was published which not only admit that it might not be true but also provide indications that inhomogeneity of the interface may significantly influence electrical characteristics of the structures.

The Schottky contacts are usually characterized by electrical techniques, most often by $I-V$ or $C-V$ measurements. Both techniques are differently sensitive to possible occurrence of inhomogeneities at the Schottky contact. As the current of the Schottky diode depends exponentially on the barrier height, inhomogeneities and especially small patches with a lower SBH in the contact strongly influence the resulting apparent SBH. On the other hand, SBHs calculated from the $C-V$ measurement have a tendency to be an average value of the SBHs of patches present in the contact, and in most cases they are higher than the SBH extracted from $I-V$ measurements.

There have been many attempts to study these effects theoretically and to simulate the influence of inhomogeneities on $I-V$ and $C-V$ measurements. Ohdomari and Tu[1] prepared and analyzed parallel Schottky contacts consisting of PtSi and NiSi with fixed ratios of contact areas. They used the approach of independent diodes, i.e., they assumed that the single patches are large or at least comparable with the space charge layer width to allow for neglecting of their mutual interaction.

Freeouf *et al.*[2] simulated $I-V$ and $C-V$ curves of the two mixed-phase contacts with the two SBHs using a finite element device analysis program that simultaneously solved Poisson's equation and the current continuity equations in two dimensions.

A similar study was carried out by Sullivan *et al.* in Ref. 3 where the authors inserted a small patch with a lower SBH into otherwise homogeneous contact with a larger SBH. They discussed various anomalous behavior observed in the Schottky barriers, such as the ideality factor greater than unity, various temperature dependence of the ideality factor, and strongly bias-dependent reverse characteristics.

The most consistent theory of real Schottky contacts has been worked out by Tung.[4,5] The dominant role in his theory plays the potential pinch-off effect which should block the low barrier channel by the high potential surrounding of the high-barrier region. At some critical size, there is already no potential pinch-off. The critical size depends on the low barrier height patch size, the Schottky barrier height difference, the doping concentration, the temperature, etc. He showed that the nanometer scale inhomogeneities influence $I-V$ curves very significantly. His theoretical model based on the electric potential contours near the interface is prevalently used for the explanation of electrical properties of Schottky contacts.[6–9] This model confirms formerly accepted division of inhomogeneous diodes into interacting and noninteracting[1,2] according to the absolute dimension of the inhomogeneity comparing to the semiconductor depletion width.

A simulation of $I-V$ curves of Schottky contacts with a Gaussian barrier height distribution (BHD) of SBH with different standard deviations together with the influence of series resistance was performed in Ref. 10. It was shown that increasing the standard deviation and decreasing the temperature results in lowering the apparent SBH and in increasing the ideality factor. The approach used enables one to divide the diode into a great number of homogeneous diodes with different barrier heights and series resistances connected in parallel. However, it is unable to take into account mutual interaction of the diodes, which is directly connected to the pinch-off effect and which should influence electrical characteristics of the diode. The same approach was also used in Refs. 11 and 12.

The simulation procedure was reverted in Ref. 13 where a method was developed for the extraction of the parameters of the Gaussian BHD from an $I-V$ curve of an inhomogeneous diode. The limitation for the barrier height changes which are supposed to be in a scale larger than the depletion region width is also valid there.

$C-V$ curves of Schottky contacts with the Gaussian BHD and without limitation of noninteracting diodes were also modeled for both reverse and forward biases.[14] The $C-V$ curves of inhomogeneous diodes were found to be very similar to the homogeneous ones with the same SBH as the mean barrier height of the BHD for inhomogeneous diodes.

II. NUMERICAL MODEL

To overcome the limitations of the approach of noninteracting diodes, it is necessary to generate $I-V$ and $C-V$ curves from more general equations describing electrical transport in semiconductor structures. We have to use Poisson's equation together with the drift and diffusion equations

$$\begin{aligned} &\Delta\varphi = -(q/\epsilon_s)(p-n+N_d), \\ &\frac{\nabla\cdot\mathbf{J}_n}{q} = U, \quad \mathbf{J}_n = q(-\mu_n n\nabla\varphi + D_n\nabla n), \\ &\frac{\nabla\cdot\mathbf{J}_p}{q} = -U, \quad \mathbf{J}_p = q(-\mu_p p\nabla\varphi - D_p\nabla p), \end{aligned} \tag{1}$$

where φ is the electrostatic potential, q is the elementary charge, ϵ_s is the permittivity of the semiconductor, p and n are the hole and the electron densities, respectively, μ_n, μ_p, D_n, D_p, and $\mathbf{J}_n$, $\mathbf{J}_p$ are, respectively, the mobilities, diffusion coefficients, and current densities of electrons and holes, and U is the net recombination rate. The mobilities were considered to be constant in the whole bias range used and the values were $\mu_n = 1500\ \mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}$ and $\mu_p = 500\ \mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}$. The net recombination was considered to be zero.

Mayergoyz[15] and Korman and Mayergoyz[16] developed an iterative technique for solving the discretized steady-state semiconductor equations which used Gummel's block iteration technique[17] for decoupling the Poisson's and electron-hole continuity equations. The method has an advantage of being globally convergent, and the approach does not require the solution of simultaneous algebraic equations. The method utilizes the Slotboom variables (exponential quasi-Fermi potentials) u and ν, which are defined as

$$\begin{aligned} &n = n_i u \exp(q\varphi/kT), \quad u = \exp(-q\psi_n/kT), \\ &p = n_i \nu \exp(-q\varphi/kT), \quad \nu = \exp(q\psi_p/kT), \end{aligned} \tag{2}$$

where n_i is the intrinsic carrier concentration, and ψ_n and ψ_p are the electron and hole quasi-Fermi potentials. The solution of these equations gives the concentration of electrons and holes throughout the whole structure for every bias applied to the diode. Using Eqs. (1), we calculated the current flowing through the structure. The solution of the drift-diffusion equations together with Poisson's equation also allows for the simultaneous simulation of $C-V$ curves of the diodes. The differential capacitance was calculated according to Ref. 14.

The differential form of these equations inherently incorporates the influence of the pinch-off effect. Extracting the apparent barrier height from simulated reverse parts of C^2-V curves offers the possibility to evaluate the influence of inhomogeneities on a difference between the φ_{I-V} and φ_{C-V} which is almost always observed in experimental practice. To describe completely the influence of the barrier heights inhomogeneities on electrical characteristics, one should study a three-dimensional system the solution of which, however, would require too long CPU time even for relatively thin meshes. Nevertheless, physically equivalent results can be obtained with a two-dimensional mesh assuming only a one-dimensional distribution of barrier height inhomogeneities. The barrier height does not change in the perpendicular direction. We simulated an inhomogeneous Schottky diode by a Gaussian BHD in two modifications. In the first case, the particular barrier heights adjoin those barrier heights in space which they adjoin also in the electrostatic potential distribution, i.e., there exists a high level of correlation between local patches and their position at the metal semiconductor interface. In the second case, the barrier heights from the potential distribution were distributed in space randomly by a random number generator—the two random variables—the barrier height and its position were supposed to be independent, i.e., there was no correlation between the local barrier height and its placement in the diode. In this case, the potential differences between neighboring patches are, on the average, higher, and one could expect a more pronounced influence of the pinch-off effect on $I-V$ curves.

The set of semiconductor equations was discretized by a standard five-point finite difference scheme. The limitation of the CPU time led to a mesh with $40\times n$ points (40 points in the direction of the current flow and n points along the inhomogeneous barrier). The number of mesh points parallel to the BHD n was varied in order to change the dimension of the barrier height inhomogeneity and to explore its influence on the apparent barrier height.

In order to solve the system of equations, it is necessary to formulate boundary conditions for the potential and quasi-Fermi potentials. The Schottky boundary conditions were used for the metal semiconductor interface, i.e., the quasi-Fermi levels of electrons and holes coincide at the interface with the Fermi level of the metal. For the ohmic contact, the charge neutrality was considered besides the thermodynamic

TABLE I. Apparent parameters of the Si Schottky diode with the dimensions 10 μm×0.1 m calculated from simulated $I-V$ and $C-V$ curves with the mesh consisting of 40×90 points. The mean barrier height is $\varphi_0=0.5$ V.

Mean barrier height (V)	Diode dimensions	Standard deviation (V)	N_D (cm^{-3})	$\Phi_{I-V,\mathrm{CORR}}$ (V) ideality coeff. series resistance (Ω)	$\Phi_{I-V,\mathrm{RAND}}$ (V) ideality coeff. series resistance (Ω)	$\Phi_{C-V,\mathrm{CORR}}$ (V)	$\Phi_{C-V,\mathrm{RAND}}$ (V)
0.5	10 μm×0.1 m	0.04	10^{15}	0.420	0.419	0.488	0.496
				1.382	1.364		
				1.03×10^{-1}	1.03×10^{-1}		
			10^{17}	0.360	0.357	0.485	0.485
				1.138	1.142		
				1.19×10^{-4}	1.20×10^{-4}		
		0.08	10^{15}	0.368	0.368	0.482	0.499
				2.541	2.462		
				8.39×10^{-2}	8.22×10^{-2}		
			10^{17}	0.307	0.301	0.480	0.480
				1.378	1.386		
				1.26×10^{-4}	1.29×10^{-4}		

equilibrium, i.e., the potential of the ohmic contact was given as

$$\varphi=V_e+\frac{KT}{q}\ln\left(\frac{N_d}{2n_i}+\sqrt{\left(\frac{N_d}{2n_i}\right)^2+1}\right), \tag{3}$$

where V_e is the external voltage and the second term is the built-in voltage.

III. RESULTS AND DISCUSSION

The set of inhomogeneous Si (silicon material constants were taken) Schottky diodes with different parameters was calculated. The distribution of the barrier height inhomogeneities was assumed to be a single Gaussian. The combinations of the two different mean barrier heights 0.5 and 0.7 V, two standard deviations 0.04 and 0.08 V, and the two different doping concentration (10^{15} and 10^{17} cm^{-3}) were used as input parameters. The doping concentration influences the series resistance but should also play a decisive role in the pinch-off effect.[3] The diode thicknesses were chosen to be 2.5 μm for the doping concentration 10^{15} cm^{-3} and 0.25 μm for 10^{17} cm^{-3}. At these dimensions, the thicknesses of the depletion layer and the quasineutral part of the semiconductor are comparable. The barrier height intervals used for the mean barrier height 0.5 V were from 0.406 to 0.579 V for the standard deviation $\sigma=0.04$ V and from 0.338 to 0.648 V for $\sigma=0.08$ V. The barrier height intervals used for the mean barrier height 0.7 V were 0.614–0.786 and 0.545–0.855 V, respectively. Because of the fact that the barrier height interval for the current integration was limited, very high and very low SBHs (in spite of the influence of the latter on the current) with the Gaussian probabilities lower than the reciprocal of the belonging number of mesh lines had to be omitted.

For each structure, $I-V$ and $C-V$ curves were simulated for the case with highly correlated barrier patches and the same was done also for the diode with the same parameters but laterally uncorrelated—randomized—barrier patches. These two situations are the extreme cases. In reality one can expect some lateral correlation because of physical and chemical conditions which control the Schottky barrier formation and which are expected to change continuously at the interface.

From each simulated $I-V$ curve, the Schottky diode parameters—apparent barrier height, ideality coefficient, and series resistance—were evaluated by the method for the parameter extraction for sharp barrier height described in Ref. 13. The barrier heights were also calculated from $C-V$ curves. The results for the structures with the dimensions 10 μm×0.1 m, where the BHD were divided by 90 points (30 different barrier height patches from the BHD with three points per patch) and a mean barrier height 0.5 V are shown in Table I. The numerical results for the same structures but the mean barrier height 0.7 V are in Table II. The typical dimension of the patch is 112 nm. The electrical characteristics were calculated also for the same diode area but the dimensions 1 mm×1 mm for comparison. The division of the mesh was the same as by smaller structures. Here the typical patch dimension was 11.2 μm. A cross comparison in Table II shows almost no differences between small and large diodes and between correlated and uncorrelated ones. Simulated $I-V$ and C^2-V curves for one of the structures for both mean barrier heights used are in Figs. 1–4. It is seen that there are practically no differences between the extracted parameters for correlated and randomized barrier height patches.

The barrier heights from the C^2-V simulation are slightly below the mean barrier height for every parameters combination and certainly, as often met in practice, above the apparent barrier height from $I-V$ simulation. We may conclude that the diodes with the patch dimensions greater than 112 nm and the above parameters behave as fully noninteracting ones, i.e., there is no influence of the pinch-off effect.

In order to describe every barrier height more faithfully, we increased the number of mesh points for a single patch to 6 for the structure with the mean barrier height 0.7 V, standard deviation 0.08 V, and the doping concentration 10^{15} cm^{-3}. In order to get an acceptable CPU time, we diminished the number of different barrier heights in BHD to

TABLE II. Apparent parameters of the Si Schottky diode with the dimensions 10 μm×0.1 m and 1 mm×1 mm calculated from simulated $I-V$ and $C-V$ curves with the mesh consisting of 40×90 points. The mean barrier height is $\varphi_0=0.7$ V.

Mean barrier height (V)	Diode dimensions	Standard deviation (V)	N_D (cm^{-3})	$\Phi_{I-V,\mathrm{CORR}}$ (V) ideality coeff. series resistance (Ω)	$\Phi_{I-V,\mathrm{RAND}}$ (V) ideality coeff. series resistance (Ω)	$\Phi_{C-V,\mathrm{CORR}}$ (V)	$\Phi_{C-V,\mathrm{RAND}}$ (V)
0.7	10 μm×0.1 m	0.04	10^{15}	0.621	0.620	0.697	0.697
				1.074	1.080		
				1.30×10^{-1}	1.24×10^{-1}		
			10^{17}	0.554	0.555	0.687	0.687
				1.057	1.062		
				1.49×10^{-4}	1.48×10^{-4}		
		0.08	10^{15}	0.568	0.567	0.686	0.700
				1.150	1.182		
				1.72×10^{-1}	1.35×10^{-1}		
			10^{17}	0.508	0.503	0.680	0.680
				1.076	1.076		
				2.38×10^{-4}	2.24×10^{-4}		
	1 mm×1 mm	0.04	10^{15}	0.622	0.619	0.690	0.690
				1.077	1.081		
				1.31×10^{-1}	1.33×10^{-1}		
			10^{17}	0.560	0.557	0.690	0.690
				1.054	1.055		
				1.51×10^{-4}	1.55×10^{-4}		
		0.08	10^{15}	0.568	0.563	0.683	0.683
				1.168	1.177		
				1.67×10^{-1}	1.70×10^{-1}		
			10^{17}	0.508	0.503	0.682	0.682
				1.077	1.079		
				2.39×10^{-4}	2.43×10^{-4}		

18. The mesh had 108 points for the barrier height division and the elemental patch was ~93 nm long for 10 μm×0.1 m and 9.3 μm for 1 mm×1 mm geometry. Resulting barrier height for the structures with small and large barrier height patch were 0.568 and 0.565 V and ideality factors 1.17 and 1.18, respectively. It is seen that the differences between the apparent barrier heights and ideality factors are in spite of the remarkable difference between the potential contours (Figs. 5 and 6) very small and practically negligible.

The second set of diodes had the dimensions 1 μm×1 m with 30 points parallel to the barrier height change (Table III). The typical dimension of the patch was 34 nm. The differences between the extracted parameters for the correlated and uncorrelated structures are now greater than for the previous structures, especially for the diodes with 0.08 V standard deviation of the barrier height but no unambiguous trend for the apparent barrier height related to the correlation of the barrier height patches was found. The considerations taking into account the pinch-off effect which should have greater impact in randomized structures lead to the expectations of lower apparent barrier heights for correlated structures. In those diodes there are in average smaller differences between the neighboring barrier heights and consequently the smaller impact of pinch-off effect. This theory works

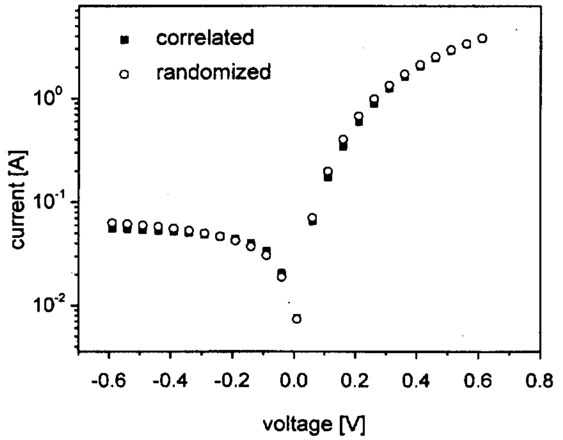

FIG. 1. $I-V$ curves of the Si Schottky diode with the mean barrier height $\varphi_0=0.5$ V, standard deviation $\sigma=0.08$ V, $N_D=10^{15}$ cm^{-3}, and the dimensions 10 μm×0.1 m.

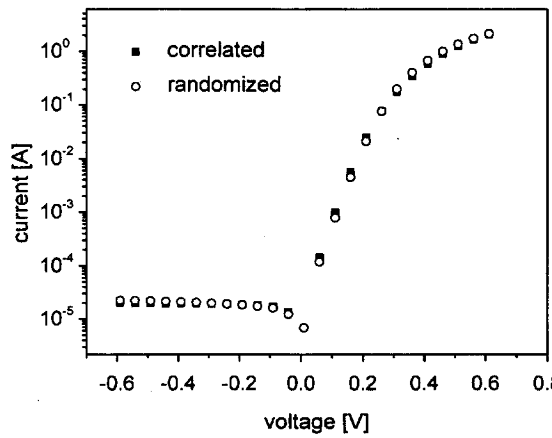

FIG. 2. $I-V$ curves of the Si Schottky diode with the mean barrier height $\varphi_0=0.7$ V, standard deviation $\sigma=0.08$ V, $N_D=10^{15}$ cm^{-3}, and the dimensions 10 μm×0.1 m.

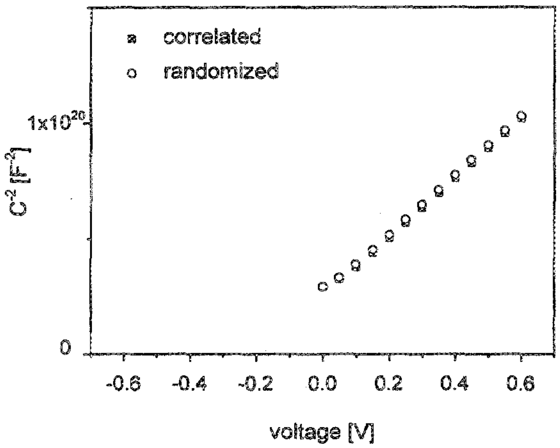

FIG. 3. $C^{-2}-V$ curves of the Si Schottky diode with the mean barrier height (a) $\varphi_0=0.5$ V, standard deviation $\sigma=0.08$ V, $N_D=10^{15}$ cm^{-3}, and the dimensions 10 μm×0.1 m.

well for the diodes where the standard deviation of the barrier height is 0.08 V, the doping concentration 10^{15} cm^{-3}, i.e., where the doping concentration is low enough and the barrier height interval is relatively high. Ideality factors for these diodes, especially for the one with the mean barrier height 0.5 V, are higher than for other structures, which is the tax paid for the consideration of strongly inhomogeneous diode as a homogeneous one.

For other structures, we got opposite results. But it is necessary to say that the differences between correlated and randomized structures are relatively small. Generally, the apparent barrier heights differ only in the third decimal place, maximum difference is ~0.02 V for the structures with $\sigma=0.08$ V.

In order to go further towards the lower patch dimensions and to compare our results with the ones published in Refs. 3–9, we made calculations also for the diode dimensions 0.4 μm×2.5 m, where 0.4 μm has been divided by 21 points of mesh. The patch dimension in that case was 20 nm. The potential distribution in the structure without external bias is in Fig. 7. The places where the potential is pinched

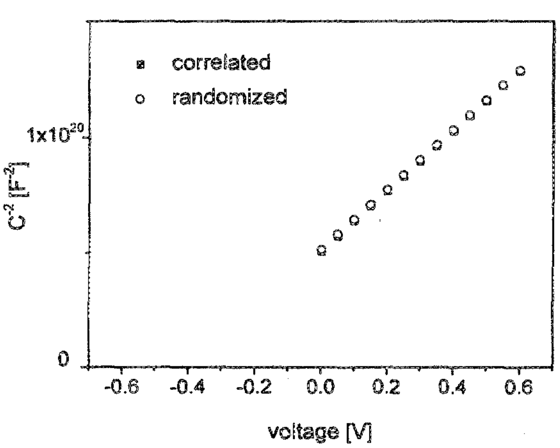

FIG. 4. $C^{-2}-V$ curves of the Si Schottky diode with the mean barrier height $\varphi_0=0.7$ V, standard deviation $\sigma=0.08$ V, $N_D=10^{15}$ cm^{-3}, and the dimensions 10 μm×0.1 m.

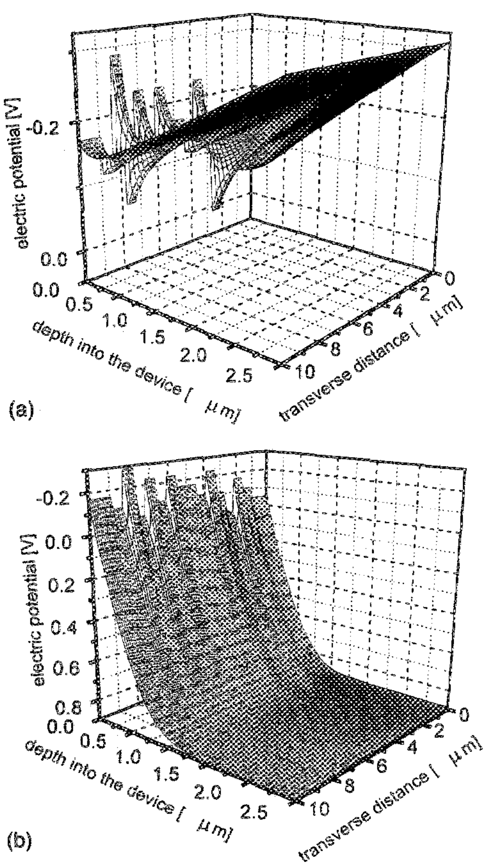

FIG. 5. Numerically calculated potential distribution of the structure with the dimensions 10 μm×0.1 m, the mean barrier height 0.7 V, standard deviation 0.08 V, the doping concentration 10^{15} cm^{-3}, and (a) 0.6 V in forward bias and (b) 0.6 V in reverse bias.

off are clearly seen. For comparison with the so-called noninteracting diodes, there are also results for the structures with the same area and the same mesh division, but the diode dimensions 1 mm×1 mm. The patches in both structures were again equally laterally randomly distributed. The results of the simulation are in Table IV. Remarkably higher apparent barrier is observed only for the structure with $N_D=10^{15}$ cm^{-3} and $\sigma=0.08$ V (Figs. 8 and 9). For smaller σ, the difference in barrier heights has even opposite sign. The results are again not unambiguous and the differences between the barrier heights again small. They are considerable only for the structure with extreme parameters from the point of view of inhomogeneity.

The barrier heights from the C^2-V simulations are very close to the mean barrier heights (weighted average in our case) and are greater than the appropriate barrier heights from the $I-V$ curves. This fact is very well known from the measurement on experimental structures. Also the difference between the barriers for correlated and the uncorrelated structure are very low.

Ideality factors are relatively close to unity and the differences between the appropriate curves are small again. In general, the ideality coefficient grows with increasing standard deviation of the BHD.

Only small differences in the series resistance between the diodes with correlated and uncorrelated local barrier

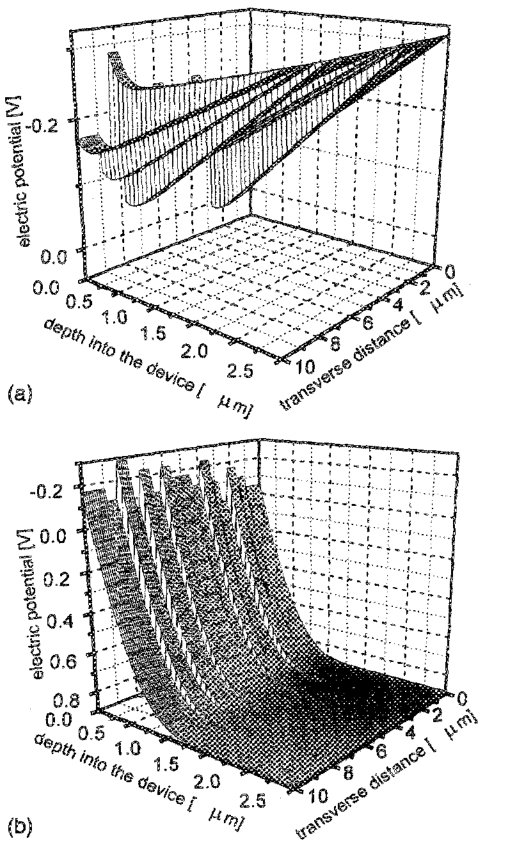

FIG. 6. Numerically calculated potential distribution of the structure with the dimensions 1 mm×1 mm, the mean barrier height 0.7 V, standard deviation 0.08 V, the doping concentration 10^{15} cm^{-3}, and (a) 0.6 V in forward bias and (b) 0.6 V in reverse bias.

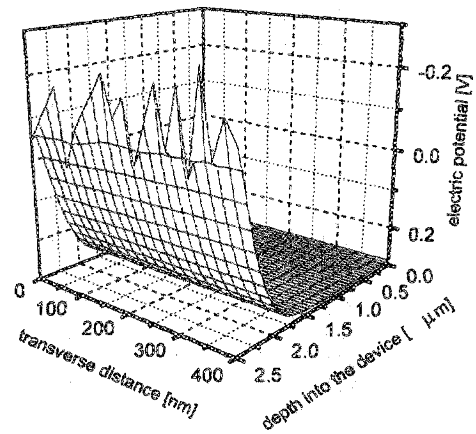

FIG. 7. Numerically calculated potential distribution of the structure with the dimensions 0.4 μm×2.5 m, the mean barrier height 0.7 V, standard deviation 0.08 V, and the doping concentration 10^{15} cm^{-3} without external bias.

heights are a measure of the integrity of the whole simulation process.

To the accuracy of our method, the extracted apparent barrier parameters are in average almost the same for the diodes with a relatively large typical inhomogeneity dimension and for the diodes where the typical barrier patch dimension is smaller than the depletion region width. The main result which can be extracted from the calculations is that for the inhomogeneous barrier height with a Gaussian BHD (and probably also for other type of distributions[18,19]) and a moderate standard deviation of the barrier height there is practically no influence of the pinch-off effect on the current.

TABLE III. Apparent parameters of the Si Schottky diode with the dimensions 1 μm×1 m calculated from simulated $I-V$ and $C-V$ curves with the mesh consisting of 40×30 points. The mean barrier height is $\varphi_0=0.5$ V and $\varphi_0=0.7$ V.

Mean barrier height (V)	Diode dimensions	Standard deviation (V)	N_D (cm^{-3})	$\Phi_{I-V,\mathrm{CORR}}$ (V) ideality coeff. series resistance (Ω)	$\Phi_{I-V,\mathrm{RAND}}$ (V) ideality coeff. series resistance (Ω)	$\Phi_{C-V,\mathrm{CORR}}$ (V)	$\Phi_{C-V,\mathrm{RAND}}$ (V)
0.5	1 μm×1 m	0.04	10^{15}	0.430	0.428	0.499	0.511
				1.210	1.355		
				1.09×10^{-1}	1.05×10^{-1}		
			10^{17}	0.370	0.358	0.484	0.495
				1.103	1.133		
				1.25×10^{-4}	1.23×10^{-4}		
		0.08	10^{15}	0.391	0.410	0.484	0.499
				1.631	1.626		
				1.06×10^{-1}	9.70×10^{-2}		
			10^{17}	0.327	0.305	0.470	0.485
				1.221	1.338		
				1.41×10^{-4}	1.29×10^{-4}		
0.7	1 μm×1 m	0.04	10^{15}	0.630	0.625	0.684	0.697
				1.063	1.109		
				1.28×10^{-1}	1.18×10^{-1}		
			10^{17}	0.562	0.552	0.682	0.695
				1.071	1.079		
				1.40×10^{-4}	1.36×10^{-4}		
		0.08	10^{15}	0.586	0.599	0.683	0.700
				1.180	1.190		
				1.27×10^{-1}	1.14×10^{-1}		
			10^{17}	0.523	0.504	0.668	0.687
				1.062	1.091		
				2.25×10^{-4}	1.80×10^{-4}		

TABLE IV. Apparent parameters of the Si Schottky diode with the dimensions 0.4 μm×2.5 m and 1 mm×1 mm calculated from simulated $I-V$ and $C-V$ curves with the mesh consisting of 40×21 points. The mean barrier height is $\varphi_0=0.7$ V.

Mean barrier height (V)	Diode dimensions	Standard deviation (V)	N_D (cm^{-3})	$\Phi_{I-V,\mathrm{SMALL}}$ (V) ideality coeff. series resistance (Ω)	$\Phi_{I-V,\mathrm{LARGE}}$ (V) ideality coeff. series resistance (Ω)	$\Phi_{C-V,\mathrm{SMALL}}$ (V)	$\Phi_{C-V,\mathrm{LARGE}}$ (V)
0.7	0.4 μm×2.5 m	0.04	10^{15}	0.620	0.614	0.701	0.687
	1 mm×1 mm			1.119	1.087		
				1.19×10^{-1}	1.43×10^{-1}		
			10^{17}	0.549	0.553	0.685	0.683
				1.088	1.057		
				1.34×10^{-4}	1.17×10^{-4}		
		0.08	10^{15}	0.610	0.577	0.703	0.691
				1.195	1.157		
				1.13×10^{-1}	1.82×10^{-1}		
			10^{17}	0.521	0.518	0.701	0.689
				1.122	1.072		
				1.61×10^{-4}	2.61×10^{-4}		

From a diffusion theory point of view, the driving force for the current are the gradients of the electron and hole quasi-Fermi levels. The decrease of the drift current near the interface due to the pinch-off effect is compensated by the diffusion of the free charge carriers. They have higher concentration gradients in those regions in order to come up with the large side potential gradients.

That is why there is no necessity to divide the Schottky diodes into interacting and noninteracting ones because their electrical characteristics are, in principle, the same. The other implication from these considerations is that there is no possibility to realize switching of the current by lateral connecting of diodes connected in parallel. The same current is flowing through the set of diodes whether they are laterally connected or not. The total current flowing through the structure is determined only by the barrier height distribution and bias voltage. The influence of the pinch-off effect occurs only at extreme conditions—low doping concentration of the semiconductor, high standard deviation of the barrier height, i.e., high potential steps at the border of two patches, and certainly, nanosize dimensions of the low barrier patches.

We should note that the absolute value of the apparent barrier heights are somewhat lower than one could expect and they are for relatively strongly inhomogeneous structures lower than the lowest local barrier height at the interface. That is why we tested our algorithm with one-dimensional (homogeneous) structure. If we take the homogeneous barrier height 0.7 V as an input for drift-diffusion approximation, we get 0.674 V for extracted barrier height and the value 1.042 for ideality factor, i.e., the apparent barrier height calculated through the least-squares fit for thermionic emission are slightly lower. However, this fact does not influence the main trends which are important for the conclusions concerning the deformation of the parabolic shape of the potential and the pinch-off effect.

IV. CONCLUSION

We have shown by the diffusion approach that, in principal, almost the same current is flowing through the so-called interacting and noninteracting inhomogeneous

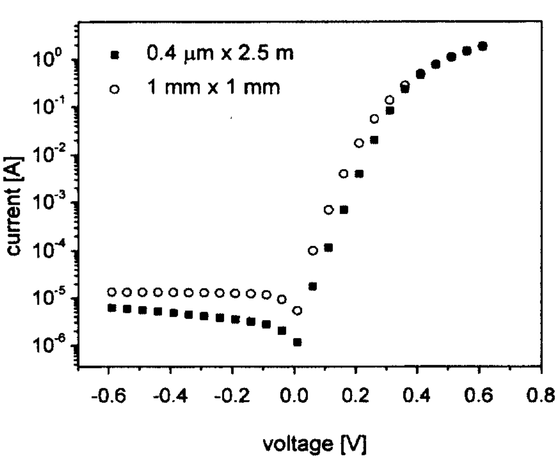

FIG. 8. $I-V$ curves of the Si Schottky diode with the mean barrier height $\varphi_0=0.7$ V, standard deviation $\sigma=0.08$ V, $N_D=10^{15}$ cm^{-3}, and the dimensions 0.4 μm×2.5 m and 1 mm×1 mm.

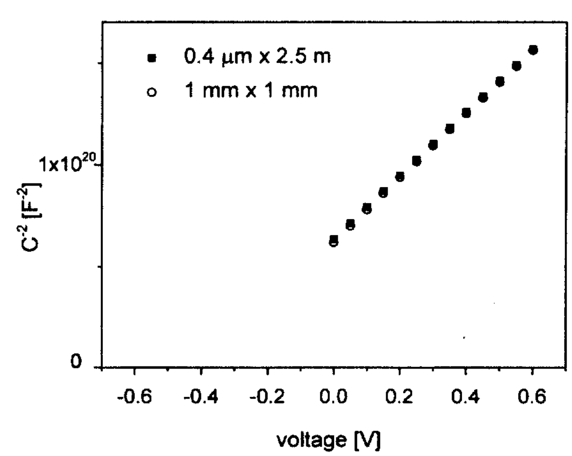

FIG. 9. $C^{-2}-V$ curves of the Si Schottky diode with the mean barrier height $\varphi_0=0.7$ V, standard deviation $\sigma=0.08$ V, $N_D=10^{15}$ cm^{-3}, and the dimensions 0.4 μm×2.5 m and 1 mm×1 mm.

Schottky diodes with Gaussian BHD. The apparent barrier height parameters differ also in negligible manner. Remarkable influence was found only for the structure with extreme parameters (low doping concentration, relatively high standard deviation of barrier height, nanosize patch dimensions). Consequently, there is no need for dividing the diodes with a moderate degree of inhomogeneity (standard deviation of barrier height) into interacting and noninteracting ones. The decrease of the drift part of the current in the neighborhood of pinch-off area is probably compensated by an enhancement of the diffusion current in that region. Side interconnections between the diodes do not influence remarkably the diode current in a longitudinal direction.

ACKNOWLEDGMENT

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Comment on ''Numerical study of electrical transport in homogeneous Schottky diodes'' [J. Appl. Phys. 85, 1935 (1999)]

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In a recent article [J. Appl. Phys. **85**, 1935 (1999)], Osvald simulated forward and reverse current–voltage and capacitance–voltage characteristics of inhomogeneous Schottky barrier (SB) diodes and concluded that the currents flowing in interacting and noninteracting inhomogeneous SBs were largely identical. This Comment points out the inappropriateness of some of the conditions chosen for these simulations which likely has rendered that conclusion untenable. © *2000 American Institute of Physics.* [S0021-8979(01)00101-3]

In a recent article,[1] Osvald simulated forward and reverse current–voltage and capacitance–voltage characteristics of inhomogeneous Schottky barrier (SB) diodes and concluded that the currents flowing in interacting and noninteracting inhomogeneous SBs were largely identical. This conclusion was in direct conflict with a host of earlier publications.[2–4] The purpose of this Comment is to offer a likely explanation of this apparent disagreement. Electron transport at inhomogeneous SB has been treated theoretically and shown to depend on the lateral length scale with which the SB height (SBH) varies.[2] In particular, it has been shown that for SBH varying in one dimension (termed the ''strip'' geometry, which is the geometry used in Ref. 1), a critical width of the strip exists

$$L_{\mathrm{crit}}=\frac{2W\Delta}{\pi V_{\mathrm{bb}}}, \tag{1}$$

where W is the depletion region width, Δ is the difference between the SBH of the low-SBH strip and an ''average SBH,'' and V_{bb} is the band bending for a SB with the ''average SBH.'' When SBH varies on a length scale longer than the critical width $L>L_{\mathrm{crit}}$, the electronic transport to different SB areas is largely independent, and can be described by a ''parallel conduction'' model.[5] The above is the condition called ''noninteracting'' in Ref. 1, as opposed to the more interesting ''interacting'' case which occurs when the SBH varies on a small length scale, $L<L_{\mathrm{crit}}$. Then, the conduction paths in front of the low-SBH strips are partially pinched off, leading to various phenomena which have been observed routinely from real SBs for several decades, although not necessarily interpreted correctly until recently.[2] The most notable of these phenomena is an ideality factor which significantly exceeds unity. The validity of the concept of saddle-point potential (pinch off) and the rest of the analytic theory[2] was convincingly demonstrated in numerical simulations, which simultaneously solved drift-diffusion equations and Poisson's equation,[3] and in numerous experiments involving inhomogeneous SBHs.[4] A parameter $\Omega=(L\Delta/2\pi W V_{\mathrm{bb}})^{1/2}$ has been shown to be an adequate measure of the degree of pinch off of low SBH regions in the strip geometry.[2] The larger Ω is, the less ''ideal'' the current will appear to be; yet the smaller Ω is, the more the total current will depart from that predicted by the parallel conduction model.[5]

In Osvald's simulations Gaussian distributions of SBH, centered around 0.5 and 0.7 V and with σ of 0.04 and 0.08 V, were assumed for two semiconductor (n-Si) doping levels, 10^{15} and $10^{17}\ \mathrm{cm}^{-3}$. The width of the individual strip was varied from 20 nm to 1.1 μm. A simple calculation using Eq. (1) shows $L_{\mathrm{crit}}<20$ nm for all the inhomogeneous SBs simulated on $10^{17}\ \mathrm{cm}^{-3}$ Si. Since the narrowest strips used in these simulations is 20 nm, all of the simulations on $10^{17}\ \mathrm{cm}^{-3}$ substrate pertain to noninteracting SBH. It is thus expected that these diodes give largely identical results, as was indeed revealed by the actual simulations.[1] On $10^{15}\ \mathrm{cm}^{-3}$ Si, L_{crit}s are longer (see Table I) and pinch off is expected from inhomogeneous SBH consisting of 33 and 20 nm wide strips, as used in Osvald's simulations.[1] The same analysis (Table I), however, reveals that, for low-SBH strips of these dimensions, the location of the saddle point is ~15–32 nm away from the metal–semiconductor (MS) interface. Since the size of the vertical mesh chosen for Osvald's simulations was 62.5 nm, the first mesh point is placed at twice or more the distance of the saddle point away from the MS interface. With such a coarse mesh, a proper description of the rapid potential variation near the saddle point is not possible. The effect of potential pinch off could

TABLE I. Relevant parameters for inhomogeneous SBH strips used in Osvald's simulations on $10^{15}\ \mathrm{cm}^{-3}$ Si, calculated at zero bias using the analytic theory.[a] Ω and the saddle-point position z_{sad} were calculated for $L=20$ nm and $L=33$ nm. The standard deviation σ has been used as the SBH difference (Δ) in these calculations.

SBH (V)	σ (V)	V_{bb} (V)	W (μm)	L_{crit} (nm)	Ω 20 nm	Ω 33 nm	z_{sad} (nm) 20 nm	z_{sad} (nm) 33 nm
0.5	0.04	0.231	0.549	60.5	0.032	0.041	17.4	22.3
	0.08	0.231	0.549	121.0	0.045	0.058	24.6	31.6
0.7	0.04	0.431	0.75	44.3	0.020	0.025	14.9	19.1
	0.08	0.431	0.75	88.6	0.028	0.036	21.0	27.0

[a]See Ref. 2.

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be significantly underestimated or even completely missed, as a result. To avoid grid-related artifacts, it is important for simulations to be performed on a grid size of which any further refinement has been shown to lead to no or little change in the physical quantities calculated. All the results reported from our numerical simulations[3] were calculated under conditions where possible grid-related effects were specifically looked for and found to be absent. Mesh sizes as small as 0.5–1 nm were often used near locations expected of rapid potential variations.[3] The effect of potential pinch off was clearly demonstrated in those earlier simulations.[3]

There may be other problems with Osvald's calculations. The potential contours shown in Fig. 6 of Ref. 1 contain sharp kinks and corners throughout the space charge region. Such a potential distribution is obviously unphysical as it does not satisfy Poisson's equation. This likely points to problems with the algorithm used in these simulations.[1] How severely Osvald's simulations have been affected by the mesh size or the apparent nonconformality with Poisson's equation is unclear. What seems clear is that the conclusion drawn from that study, namely that potential pinch off does not affect the electron transport at inhomogeneous SBHs,[1] is erroneous.

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Response to "Comment on 'Numerical study of electrical transport in inhomogeneous Schottky diodes' " [J. Appl. Phys. 88, 7366 (2000)]

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In his comment [J. Appl. Phys. **88**, 7366 (2000)] Tung brings into question the appropriateness of some of the simulation conditions used in J. Appl. Phys. **85**, 1935 (1999) and the conclusion taken from the results. This Response explains that the differences in the conclusions between our work and the work of Sullivan *et al.* [J. Appl. Phys. **70**, 7403 (1991)] are caused by the differences in the parameters of the inhomogeneous structures described. It is also shown that the numerical experiments made by Sullivan *et al.* [J. Appl. Phys. **70**, 7403 (1991)] were done for special diode parameters, and they probably did not support such general conclusions as were made. © *2000 American Institute of Physics.* [S0021-8979(01)00201-8]

First it is necessary to say that in principle there is no controversy between our results and those of Sullivan *et al.*[1] and Tung,[2] although our study was done for more general diode parameters, and were not specified to maximize the influence of the pinch-off effect on a diode current. From this point of view it is likely that the conclusions of Ref. 1 concerning the pinch-off effect influence on the current flowing through inhomogeneous Schottky diodes, are probably more general than the input parameters used in the simulation would support.

The objections of Tung are concentrated in two points: a coarse mesh was possibly used, and the nonconformality of the potential contours with the Poisson equation. In his comment[3] Tung took as the Schottky barrier height (SBH) difference Δ a value of the standard deviation σ (0.04 and 0.08 V) to calculate the critical strip width and the saddle-point location of our SBH distributions. But the standard deviation is not a relevant value for this case. For the pinch-off observation the actual SBH difference is important. The largest possible SBH differences between the neighboring patches used in our calculations were 0.17 and 0.31 V for σ=0.04 and 0.08 V, respectively. The neighboring barriers with Δ>0.2 V are depicted in our figures of the potential contours for σ=0.08 V. This means that the critical strip widths should be more than 2.5 times greater and also the saddle points should be placed at a larger distance than stated by Tung.[3] But there still remains the problem of the applicability of the analytical theory, which assumes a small low-SBH patch in a large homogeneous background, to our structures that contain parallel diode strips with the same or comparable areas. Figures 5 and 6 of Ref. 4 clearly demonstrate the difference between the potential curves for relatively great strip and mesh dimensions. But for the development of the pinch-off effect it was necessary to decrease the strip dimensions.

By diminishing the patch area dimension to 20 nm in Fig. 7 of Ref. 4, we clearly demonstrated several visible saddle points, and for this case the barrier height increase was also reported (especially for $N_D = 10^{15}\ \mathrm{cm}^{-3}$). Repeating this simulation for a mesh size three times lower (20 nm) in the direction of the current flow brought no further substantial change of the apparent parameters.

The second objection addressed the "nonconformality" of the potential distribution. One should realize that what is seen in the figure is the visualization of the results of numerical calculations, i.e., the solutions found only for discrete points were connected by the straight lines in the figure. The measure of the sharpness of the kinks and corners depends only on the density of mesh points used and is not the result of the apparent nonconformality with Poisson's equation. Similar potential curves with sharp corners are shown, e.g., in Figs. 4 and 5 of the pioneering work of Freeouf *et al.*[5] This is practically the same objection as the first one, and has nothing to do with the algorithm itself and should not contradict it.

The numerically determined current–voltage (I–V) plots presented in Fig. 19 of Ref. 1 represent the low-SBH patch in a uniform background region. It is worth mentioning that the radius of the low-SBH patch used for the I–V curves calculation (0.1 μm) is about four to five times greater than the mostly used radii for the pinch-off effect demonstration (~0.02–0.026 μm) in the same article. The low-SBH patch area is hence 16–25 times greater but with the simultaneous diminishing of the pinch-off influence on the whole current at those dimensions. Throughout the whole article only one doping concentration $-1\times10^{16}\ \mathrm{cm}^{-3}$ was used. For a lower doping concentration the series resistance begins to influence the diode current already at very low forward voltages, and for the doping concentration of $1\times10^{17}\ \mathrm{cm}^{-3}$ the influence of the pinch-off effect already diminishes. The range of the pinch-off influence study seems too limited to support a new general theory of the current transport in Schottky diodes.

The concept of Sullivan *et al.*[1] simulations is significantly different from ours. Our diodes represent a mixture of different but largely comparable SBHs with comparable areas. The SBH differences between neighboring patches are much lower than those in Ref. 1 even for uncorrelated local barrier patches. The probability of finding a low-barrier patch with an SBH of about 0.4 V is low for our SBH distributions, and the probability that the neighboring patch has an SBH of 0.7 V or higher is even lower (hence such neighboring pairs did not occur in our simulated structures). Then is can be expected that the results for the special structures studied in Ref. 1 would be more sensitive to the pinch-off effect than our structures with the normal SBH distribution.

Sullivan *et al.*[1] made their simulations for a set of inhomogeneity parameters for which the influence of the pinch-off effect was maximized. However, for SBH inhomogeneities with moderate parameters and doping concentrations out of the $10^{16}\ \mathrm{cm}^{-3}$ range the influence of the pinch-off effect is suppressed by the series resistance for lower doping concentrations or by screening for higher doping concentrations. There is also experimental evidence of a failure of using the pinch-off phenomenon for explaining I–V curves of real Schottky diodes.[6]

We certainly agree that further refinement of the mesh size could enhance slightly the differences between the large and the small structures but the conclusion remains the same. Remarkable influence of the pinch-off effect is to be expected only for the ''defect'' structures which contain a great number of neighboring patches with a large SBH difference and small areas of low-SBH patches. The influence of the pinch-off effect is very low for the structures with the statistical SBH distribution that is common in experimental practice.

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