Journal of Applied Physics

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

Cite as: Journal of Applied Physics **88**, 7366 (2000); https://doi.org/10.1063/1.1324996
Submitted: 11 January 2000 • Accepted: 22 September 2000 • Published Online: 28 November 2000

R. T. Tung

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

R. T. Tung[a)]
Lucent Technologies Bell Labs, 600 Mountain Avenue, Murray Hill, New Jersey 07974

(Received 11 January 2000; accepted for publication 22 September 2000)

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. [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

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

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 $L>L_{\text{crit}}$, 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, $L<L_{\text{crit}}$. 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 $\Omega=(L\Delta/2\pi WV_{\text{bb}})^{1/2}$ 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} cm^{-3}. The width of the individual strip was varied from 20 nm to 1.1 μm. A simple calculation using Eq. (1) shows $L_{\text{crit}}<20$ nm for all the inhomogeneous SBs simulated on 10^{17} cm^{-3} Si. Since the narrowest strips used in these simulations is 20 nm, all of the simulations on 10^{17} 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} 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} 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.

[a)]Electronic mail: rtt@lucent.com

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.

[1] J. Osvald, J. Appl. Phys. **85**, 1935 (1999).
[2] R. T. Tung, Phys. Rev. B **45**, 13509 (1992).
[3] J. P. Sullivan, R. T. Tung, M. R. Pinto, and R. W. Graham, J. Appl. Phys. **70**, 7403 (1991).
[4] Recent examples include A. Olbrich *et al.*, J. Appl. Phys. **83**, 358 (1998); T. Clausen and O. Leistiko, Appl. Surf. Sci. **123/124**, 567 (1998); F. E. Jones *et al.*, J. Appl. Phys. **86**, 6431 (1999).
[5] I. Ohdomari and K. N. Tu, J. Appl. Phys. **51**, 3735 (1980).