Microelectronic Engineering 86 (2009) 117–120

Contents lists available at ScienceDirect

Microelectronic Engineering

journal homepage: www.elsevier.com/locate/mee

Temperature dependence of barrier height parameters of inhomogeneous Schottky diodes

J. Osvald *

Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 841 04 Bratislava, Slovakia

ARTICLE INFO

Article history:
Received 15 July 2008
Received in revised form 19 September 2008
Accepted 10 October 2008
Available online 18 October 2008

PACS:
73.30.+y
73.40.Ei
73.40.Ns

Keywords:
Schottky diode
Ideality factor
Barrier height

ABSTRACT

We have shown by numerical simulations of *I–V–T* curves that the ideality factor of inhomogeneous Schottky diodes does not increase for decreasing temperature to such extent as is commonly observed for Schottky diodes in experiment. The main consequence of such a result is that in spite of the fact that the barrier height inhomogeneities fullfil the conditions for barrier height lowering for decreasing temperature they might not be a general or the only reason for occuring of this effect in experimental structures. We found out much slower ideality factor temperature dependence than reported in the literature and the dependence was even not monotonous for simulation conditions used. We conclude that some other reason as barrier inhomogeneity is responsible for ideality factor temperature dependence.

1. Introduction

It has been known for a long time that the Schottky barrier height is temperature dependent. The Schottky barrier height is practically always lower for lower temperatures. The changes are more significant at very low temperatures. On the other hand the ideality factor of the diodes simultaneously increases with decreasing temperature [1–3]. The standard thermionic emission theory assumes the barrier height independent of the temperature and that is why it fails to explain this result. Researchers obviously try to find some explanation of this observation. Several theories were developed to explain this contradiction. The changes found in experimental diodes are usually higher than expected dependence of the band gap. According to some authors the reason that could be responsible for the above temperature dependence of apparent barrier height and ideality factor could be the existence of a generation-recombination current in the structure [4–7]. Chattopadhyay et al. [8] studied transport mechanism in Pt/*p*-strained – Si Schottky diodes at low temperatures (95–150 K). They also found the above mentioned temperature dependence of the barrier height and ideality factor and they meant that the measured current was a combination of the thermionic current and the recombination current. The same meaning was expressed in [9] where Au/GaN diodes were studied. On the other hand there are works that concluded [10,11] that this might not be the case.

Many times the barrier height inhomogeneity concept is chosen for an explanation of the barrier height temperature dependence. For lower temperatures the lower barrier patches carry a larger fraction of the current because of the exponential temperature dependence of the current through these patches. The resulting apparent barrier height is then lower for lower temperature. This hypothesis is very often used non-critically without experimental confirmation of real barrier inhomogeneities in the diode.

Linear dependence of the barrier height on the ideality factor was found in [12] on Au/*n*-GaAs Schottky diodes on *n*-Ge. Almost the same dependence of the barrier height on the temperature and increase of ideality factor with decreasing temperature on H-terminated Sn/*p*-Si (100) Schottky contacts was explained by the Gaussian distribution of barrier heights [13]. Barrier height inhomogeneity was also used for an explanation of *I–V–T* characteristics of metal/GaN Schottky diodes in [14], Ni/nGaAs [15], Ni/n-6H-SiC [16], and Ag/p-SnSe diodes [17].

We tried to verify in this article by simulation of *I–V* characteristics of inhomogeneous Schottky diodes by different approaches

* Tel.: +421 2 5477 5816.
E-mail address: elekosva@savba.sk

0167-9317/$ - see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.mee.2008.10.006

whether the simultaneous barrier height increase and ideality factor decrease is consistent with the drift-diffusion or thermionic conduction theory or is a result of the presence of other conduction mechanism(s) in the structures.

2. Numerical model

Silicon with its material parameters was chosen for simulating diode characteristics. We used two physical concepts for Schottky diodes *I–V* characteristics generation.

2.1. Drift-diffusion approximation

The first one was the drift-diffusion approximation. The method enables to calculate electrical characteristics of inhomogeneous diodes. The temperature interval in which *I–V* characteristics were studied was 100–300 K with the step of 50 K. Three equations – Poisson and continuity equations for electrons and holes were solved simultaneously

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

where φ is the electrostatic potential, q is the elementary charge, ε_s is the dielectric constant of semiconductor, n and p are the electron and hole densities, respectively, μ_n, μ_p, D_n, D_p and J_n, J_p are respectively the mobilities, diffusion coefficients and the current densities of electrons and holes, and U is the net recombination rate. The net recombination was considered to be zero.

The model takes into account also the temperature dependence of intrinsic carrier concentration which was given by [18]

$$N_i = 1.4\times10^{15}T^{\frac{3}{2}}\exp\left(-\frac{1850}{T}\right) \tag{2}$$

and the temperature dependence of electron and hole mobilities [19]

$$\begin{aligned} \mu_n &= 0.1448\left(\frac{300}{T}\right)^{2.33} \\ \mu_p &= 0.0473\left(\frac{300}{T}\right)^{2.23}. \end{aligned} \tag{3}$$

The diode was assumed to be inhomogeneous in one dimension while in the second dimension the barrier height was constant. The structure then consists of sufficiently long 333 nm wide ribbons with the constant barrier height in each small ribbon. In the drift-diffusion approximation we have simulated *I–V–T* curves of the diode with the doping concentrations $N_d = 10^{15}$ cm^{-3} and for $N_d = 10^{17}$ cm^{-3}. The substrate thickness was 2.5 and 0.5 μm, respectively. The barrier height distribution used was of Gaussian type with the mean barrier height $\overline{\varphi} = 0.7$ V and the standard deviation of the distribution was $\sigma = 0.08$ V.

2.2. Thermionic emmision model

We have used also thermionic emission model of current transport for generation of *I–V* curves. Two modifications of characteristics simulations according to the series resistance incorporation are possible [20]. In the first one no spreading of the current in the semiconductor substarate was assumed and the current density in the structure was simulated by the expression

$$I = \int_0^{2\bar{\phi}} A^{**}T^2\rho(\phi)\exp(-q\phi/kT)\{\exp[q(V - r(\phi)i/kT] - 1\}d\phi, \tag{4}$$

where $\rho(\varphi)$ is Gaussian barrier height distribution, r is the specific series resistance in Ωcm^2, $i(\varphi)$ is the current density in the infinitesimal diode patch. We assumed that the barrier patches up to the barrier heigh 2 $\overline{\phi}$ contribute to the total current flowing through the diode.

In the second one it was assumed that the current is totally spread in the semiconductor substrate and thence the single small diodes in the structure have the same series resistance. Now the current density is simulated according to the expression

$$I = \int_0^{2\bar{\phi}} A^{**}T^2\rho(\phi)\exp(-q\phi/kT)\{\exp[q(V - RI)/kT] - 1\}d\phi. \tag{5}$$

The mean barrier height was again $\overline{\varphi} = 0.7$ V and the standard deviation of the distribution is $\sigma = 0.08$ V as for the case of drift-diffusion approximation.

I–V curves were again calculated for the temperatures from 100 to 300 K. From such generated *I–V* curves the apparent barrier height parameters were extracted as the diodes were homogeneous and the diode current density was determined by the thermionic expression

$$I = A^{**}T^2\exp\left(-\frac{q\varphi}{kT}\right)\left[\exp\left(\frac{q(V - RI)}{nkT}\right) - 1\right]. \tag{6}$$

Three diode parameters – barrier height ϕ, ideality factor n and series resistance R_S were then extracted from simulated curves by the least square fit approach [21].

3. Results and discussion

I–V curves generated by the drift-diffusion approximation for the doping concentration concentration Nd = 10^{15} cm^{-3} are in Fig. 1. The curves for concentration Nd = 10^{17} cm^{-3} have similar shape and are not shown. The currents for different temperatures do not converge to the same value in forward bias because the series resistance is realized only by the semiconductor bulk resistance that decreases with increasing temperature. Extracted apparent barrier height monotonically increased with increasing temperature as expected for both doping concentrations used (Table 1). For lower doping concentration $N_d = 10^{15}$ cm^{-3} ideality factor increases with increasing temperature but the differences between ideality factors for different temperatures are relatively small, much smaller than the ones observed in experimental practice. For higher doping concentration $N_d = 10^{17}$ cm^{-3} the ideality factor

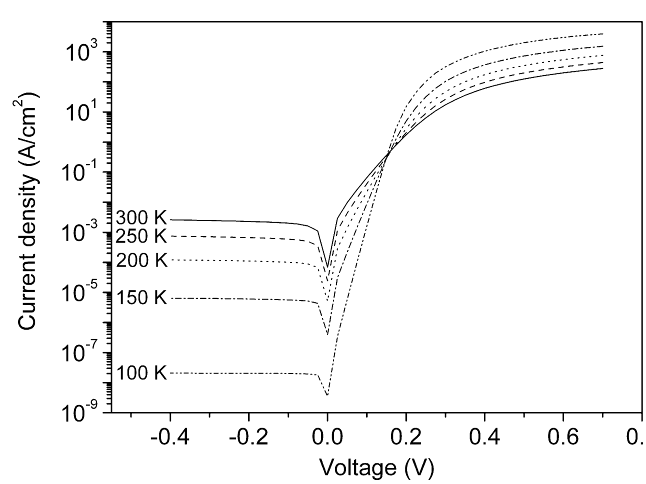

Fig. 1. Simulated *I–V–T* curves for Schottky diodes on Si with the doping concentration $N_D = 10^{15}$ cm^{-3}, $\overline{\varphi} = 0.7$ V, and $\sigma = 0.08$ V.

Table 1
Dependence of extracted apparent barrier height parameters of the Si Schottky diodes *I–V* curves calculated for the doping concentrations $N_D = 1\times10^{15}$ cm^{-3} and N_D = 1x10^{17} cm^{-3} and for various temperatures. The substrate thickness was 2.5 and 0.5 μm, respectively. The input values for *I-V* curve generation were $\bar{\varphi}$ = 0.7 V, σ = 0.08 V.

$N_D = 1\times10^{15}$ cm^{-3}				$N_D = 1\times10^{17}$ cm^{-3}		
T (K)	φ_{ap} (V)	*n*	R_{ap} (Ω)	φ_{ap} (V)	*n*	R_{ap} (Ω)
100	0.272	1.127	1.7×10^{-4}	0.271	1.128	4.6×10^{-6}
150	0.345	1.143	3.6×10^{-4}	0.343	1.04	4.7×10^{-6}
200	0.421	1.155	6.2×10^{-4}	0.405	1.041	4.1×10^{-6}
250	0.497	1.165	9.6×10^{-4}	0.465	1.040	3.8×10^{-6}
300	0.574	1.172	1.4×10^{-3}	0.522	1.040	3.6×10^{-6}

Table 2
Dependence of extracted apparent barrier height parameters of the Si Schottky diodes *I-V* curves calculated for the cases of the full current spreading and without the current spreading for various temperatures. The input values for *I-V* curve generation were $\bar{\varphi}$ = 0.7 V, σ = 0.08 V and the series resistance *R* = 1 Ω.

No spreading				Full spreading		
T (K)	φ_{ap} (V)	*n*	R_{ap} (Ω)	φ_{ap} (V)	*n*	R_{ap} (Ω)
100	0.362	2.319	1.12	0.340	1.000	1.00
150	0.459	1.815	1.12	0.452	1.000	1.00
200	0.518	1.682	1.06	0.514	1.000	1.00
250	0.557	1.765	0.99	0.551	1.000	1.00
300	0.587	2.107	0.81	0.576	1.000	1.00

is the highest for the lowest temperature, but from 150 to 300 K is practically constant and very close to unity.

The fact that the diode has different barrier height for different temperature leads to the intersecting behaviour of the curves which is at first glimpse not compatible with the fact that we expect higher current flowing for higher temperature [22].

In the first modification of usage of the thermionic emission theory the inhomogeneous diode consists of non-interacting set of small diode patches each of which has in series its own series resistance inversely appropriate to its area (Fig. 2). The value of the total series resistance 1 Ω was used as an input for the calculation. The *I–V* curves for this configuration were generated with expression (4). We received increasing effective barrier height with increasing temperature as in previous cases but the temperature dependence of the ideality factor was again not monotonous. The ideality factor for the lowest temperatures first decreases with increasing temperature and above 200 K starts to increase being again highest for the highest and lowest temperatures (Table 2).

For generation of *I–V* curves according to the expression (5) with the full current spreading in the semiconductor substrate the series resistance of 1 Ω was again used (Fig. 2). The fact that the diode has different barrier height for different temperature leads to the intersecting behavior of the curves what is again not compatible with the fact that we expect higher current flowing for higher temperature. This case can be solved also analytically [23]. We received increasing effective barrier height with increasing temperature as in previous cases. The extracted ideality factor of the whole diode was equal to unity for this configuration for every temperature (Table 2).

It is seen that for each way of *I–V* curve generation the effective barrier height of inhomogeneous diode increases with increasing temperature which is in accordance with experimental observations. The situation is not so unambiguous with ideality factor. The temperature dependence of the ideality factor for every kind of *I–V* curve generation is in Fig. 3. We obtained only relatively small dependence of the ideality factor on the temperature and these changes are not large enough to explain great ideality factor changes observed on experimental structures. The temperature dependence of the ideality factor is even not monotonous. It seems that other conduction mechanism could be responsible for strong temperature dependence of ideality factor. But for example even neither field emission nor thermionic field emission contribution to the current were obtained to be large enough for Cd/p-GaTe to increase ideality factor significantly. The contribution of these two current modes could increase ideality factor only to the value 1.05 [24].

Using the thermionic and drift-diffusion expressions for the current flowing through inhomogeneous diodes it is proved that for the temperature dependence of the barrier height the inhomogeneity of the barrier height may be responsible. But the response to the question whether the barrier height inhomogeneity is the reason for the experimentally observed ideality factor temperature dependence based on our simulation results is no. The same evidence for the temperature dependence of the ideality factor was not obtained and we may argue that the temperature dependence of the ideality factor is not the direct consequense of the barrier height inhomogeneity. It is

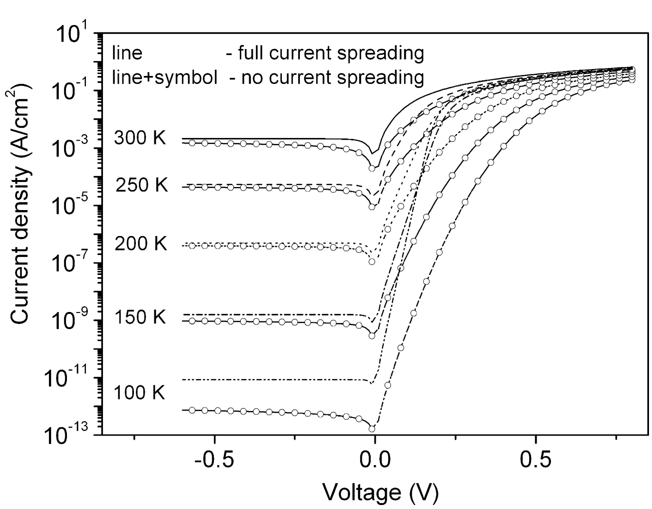

Fig. 2. Simulated *I–V–T* curves for Si Schottky diodes with no current and full current spreading in the semiconductor substrate. The mean barrier height is $\bar{\varphi}$ = 0.7 V, and the standard deviation of the barrier height distribution is σ = 0.08 V.

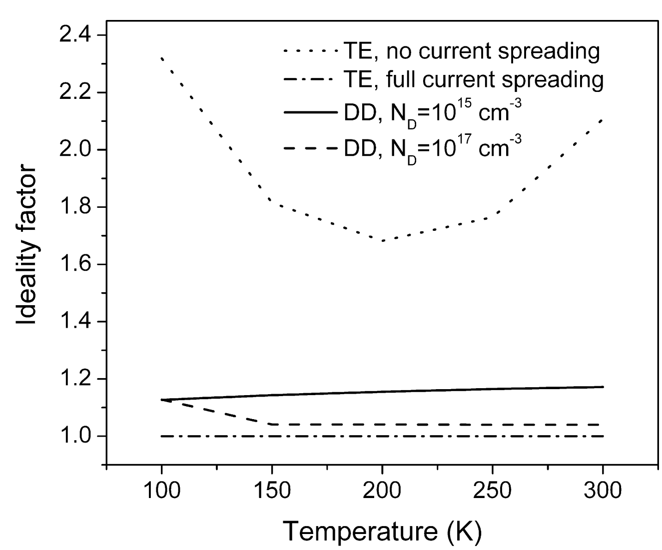

Fig. 3. The temperature dependence of the ideality factor of *I–V* curves generated by thermionic – TE and drift-diffusion – DD approaches.

necessary to realize that the ideality factor has not a clear physical basis. We may deduce from the simulations done that the ideality factor as it is defined is not temperature independent and we could treat it as a temperature dependent quantity $n = n(T)$. From this point of view the temperature dependence of the ideality factor is already not a result of the barrier height inhomogeneity but it is an intrinsic property also of homogemeous diodes.

The final conlusion of our considerations is that some other reason causes ideality factor increase in inhomogeneous diodes measured at lower temperatures. We may further conclude that also the experimentally observed temperature dependence of the barrier height is not caused by the barrier inhomogeneity since the temperature dependence of the ideality factor does not confirm the barrier inhomogeneity origin. The most probable reason is increasing influence of tunneling current because of lower number of electrons with energy high enough to pass over the barrier.

Acknowledgments

The author is thankful the financial support received during the development of this work from Slovak Grant Agency for Science under Contract No. 2/6097/26, and Agency for Science and Research No. APVV-51-040605 and APVV-0655-07. The financial support of the Centre of Excellence "CENG" SAS is also appreciated.

References

[1] K. Radermacher, A. Schüppen, S. Mantl, Solid-St. Electron. 37 (1994) 443–449.
[2] S. Chand, J. Kumar, Semicond. Sci. Technol. 10 (1995) 1680–1688.
[3] R.F. Schmitsdorf, W. Mönch, Eur. Phys. J. B 7 (1999) 457–466.
[4] T.P. Chen, T.C. Lee, C.C. Ling, S.D. Beling, S. Fung, Solid-St. Electron. 36 (1993) 949–954.
[5] S. Chand, J. Kumar, Appl. Phys. A 63 (1996) 171–178.
[6] J.H. Werner, H.H. Güttler, J. Appl. Phys. 73 (1993) 1315–1319.
[7] Ş. Karataş, Ş. Altındal, Solid-St. Electron. 49 (2005) 1052–1054.
[8] S. Chattopadhyay, L.K. Bera, S.K. Ray, K. Maiti, Appl. Phys. Lett. 71 (1997) 942–944.
[9] Y. Kribes, I. Harrison, B. Tuck, T.S. Chengm, C.T. Foxon, Semicond. Sci. Technol. 9 (1997).
[10] Ö.S. Aniltürk, R. Turan, Semicond. Sci. Technol. 14 (1999) 1060–1064.
[11] Ö.S. Aniltürk, R. Turan, Solid-St. Electron. 44 (2001) 41–48.
[12] M.K. Hudait, P. Venkatesvarlu, S.B. Krupanidhi, Solid-St. Electron. 45 (2001) 133–141.
[13] Ş. Karataş, Ş. Altındal, A. Türüt, A. Özmen, Appl. Surf. Sci. 217 (2003) 250–260.
[14] T. Sawada, Y. Ito, N. Kimura, K. Imai, K. Suzuki, S. Sakai, Appl. Surf. Sci. 190 (2002) 326–329.
[15] M. Nathan, Z. Shoshani, G. Askinazi, B. Meyler, O. Zolotarewski, Solid-St. Electron. 39 (1996) 1457–1462.
[16] A. Sefaoğlu, S. Duman, S. Doğan, B. Gürbulak, S. Tüzemen, A. Türüt, Microelectron. Eng. 85 (2008) 631635.
[17] N. Tuğluoğlu, S. Karadeniz, H. Şahin, H. Şafak, Semicond. Sci. Technol. 19 (2004) 1092–1097.
[18] J.S. Blakemore, Semiconductor Statistics, Pergamon Press, Oxford, 1962.
[19] L.A. Akers, W.M. Portnoy, Int. J. Num. Meth. Engn. 15 (1980) 1221.
[20] J. Osvald, J. Appl. Phys. 99 (2006) 033708.
[21] J. Osvald, E. Dobročka, Semicond. Sci. Technol. 11 (1996) 1198–1202.
[22] J. Osvald, Solid-St. Electron. 50 (2006) 228–231.
[23] J.H. Werner, H.H. Güttler, J. Appl. Phys. 69 (1991) 1522–1533.
[24] B. Abay, G. Çankaya, H. Efeoğlu, Y.K. Yoğurtçu, Semicond. Sci. Technol. 18 (2003) 75–81.