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A simple model for extraction of interface state density of a Schottky barrier diode using reverse bias C – V plots

SANTOSH PANDEY† and S. KAL‡

The reverse bias $1/C^2$ vs. V plots of Schottky barrier diodes are studied here. The expressions for the slope and voltage intercept of Schottky diodes, as given in the literature, are approximated to obtain a general expression relating the diffusion potential, slope and voltage intercept of $1/C^2$ vs. V plots. The expressions for the interface state density are derived. The simulated results are compared with those available in the literature. The validity of our model is established with reasonable accuracy. Based on the model, the characteristics of $1/C^2$ vs. V plots are studied with variations in the interface oxide thickness and temperature.

Nomenclature

C	diode capacitance (F cm^{-2})
C_{sc}	depletion capacitance (F cm^{-2})
C_{i}	oxide capacitance (F cm^{-2})
$D_{\text{Sa}}, D_{\text{Sb}}$	density of interface states ($\text{cm}^{-2} \text{eV}^{-1}$)
E_{g}	energy bandgap of semiconductor (J)
N_{D}	doping concentration (cm^{-3})
q	electronic charge (C)
Q_{sc}	space charge density (cm^{-2})
$Q_{\text{SSa}}, Q_{\text{SSb}}$	interface state charge density (C cm^{-2})
Q_{M}	charge density in metal (C cm^{-2})
T	temperature (K)
V	applied bias voltage (V)
V_{B}	band bending in the semiconductor at some bias (V)
V_{BO}	diffusion potential (V)
V_0	voltage intercept of $1/C^2$ vs. V plot (V)
$V_{\text{B}}, \psi_{\text{S}}$	surface potential (V)
ϕ_{B}	barrier height (V)
$\phi_{\text{oa}}, \phi_{\text{ob}}$	neutral levels (V)
ϕ_{m}	metal work function (V)
ϕ_{ms}	difference between metal and semiconductor work functions (V)
δ	oxide thickness (cm)

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Δ	potential drop across oxide layer (V)
χ	electron affinity of semiconductor (V)
ϵ_s	permittivity of semiconductor ($\text{CV}^{-1} \text{cm}^{-1}$)
ϵ_i	permittivity of oxide ($\text{CV}^{-1} \text{cm}^{-1}$)

1. Introduction

Schottky barrier diodes have been studied extensively in the past and numerous methods have been suggested for the extraction of their different parameters (Cowley 1966, Card and Rhoderick 1971, Sze 1981, Fonash 1983, Tseng and Wu 1987, Maeda *et al.* 1993, Pandey and Kal, 1998). The current–voltage (I – V) and capacitance–voltage (C – V) plots (both forward and reverse voltages) contain a lot of information about the device characteristics and by using suitable models, it is possible to estimate the values of doping concentration, oxide thickness, diffusion potential, interface state density, etc.

The interface states play an important role in deciding the nature of C – V characteristics and so it is necessary that we are able to quantify these states accurately. A number of models have been suggested to calculate the interface state density, either by using the I – V plot or C – V plot. The interface state density may be calculated using the ideality factor obtained from the current–voltage plots (Card and Rhoderick 1971). Two cases are discussed in Card and Rhoderick (1971), namely where the occupation of interface states is governed entirely by the metal Fermi level and where the occupation of interface states is governed entirely by the semiconductor Fermi level. But in reality, interface states of both the groups are present and so a model developed for interface state density calculations should consider the effect of both these groups of interface states. The multifrequency admittance method of Maedo *et al.* (1993) and the high frequency–low frequency capacitance method of Pandey and Kal (1998) determined the density of interface states using the forward biased C – V plots. The basic idea used in those methods is that at higher frequencies, the interface states are unable to follow the ac signal and so they do not contribute to the overall capacitance of the diode. In the proposed model presented here, which uses reverse bias C – V plots, interface states are assumed to be of two types: interface states of group A that are in equilibrium with the semiconductor Fermi level, and interface states of group B that are in equilibrium with the metal Fermi level. At higher frequencies, although interface states of group A cannot follow the ac signal, group B interface states can follow the ac signal and affect the C – V plots. This division of interface states into two groups gives a more realistic approach to the analysis of C – V plots.

In this paper, an attempt has been made to extend the work of Fonash (1983) to obtain an approximate expression for the diffusion potential of Schottky diodes. The interface state density expressions (for both groups A and B) are also derived in terms of the slope and voltage intercept of $1/C^2$ vs. V plot. The accuracy of the proposed model has been compared in § 3 with the available experimental results in the literature. The effect of temperature and oxide thickness on the C – V characteristics of Schottky diodes has been simulated using the proposed model and the results are discussed in § 3.

2. Theory

The energy band diagram of a MIS structure is shown under thermodynamic equilibrium (figure 1 (a)) and under reverse bias V (figure 1 (b)). Some of the equations of Fonash (1983) which are used in our modelling are reproduced for the convenience of the reader. It is assumed that the interface states of constant density D_{sa} ($\text{cm}^{-2} \text{eV}^{-1}$) follow the semiconductor Fermi level and interface states of constant density D_{sb} ($\text{cm}^{-2} \text{eV}^{-1}$) follow the metal Fermi level for quasistatic variations in the bias. Under no bias,

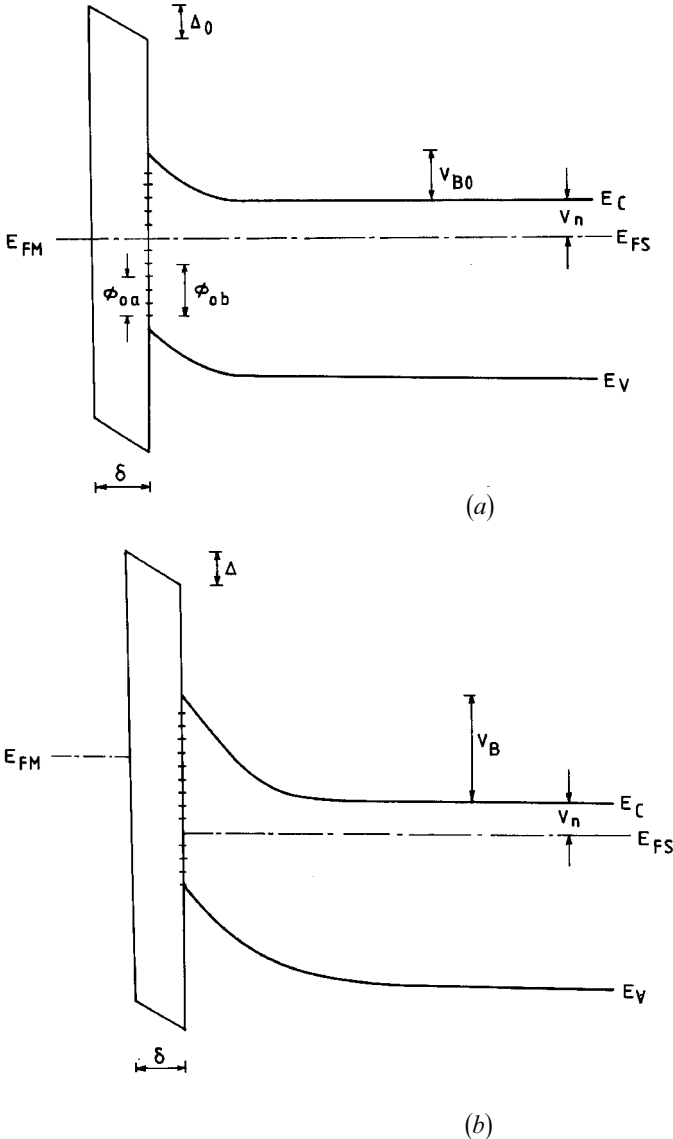


Figure 1. Energy band diagram of a Schottky diode. (a) Under thermodynamic equilibrium. (b) Under reverse bias V .

$$\left. \begin{aligned} Q_{SSa}(0) &= -qD_{sa}(E_g - V_n - V_{BO} - \phi_{oa}) \\ Q_{SSb}(0) &= -qD_{sb}(E_g - V_n - V_{BO} - \phi_{ob}) \\ Q_{Sc}(0) &= (2q\epsilon_s N_D)^{1/2} (V_{BO} - V_2)^{1/2} \end{aligned} \right\} \quad (1a)$$

where $V_2 = kT/q$.

Also, the following notations are used

$$\left. \begin{aligned} E_a &= E_g - V_n - V_{BO} - \phi_{oa} \\ E_b &= E_g - V_n - V_{BO} - \phi_{ob} \\ \phi_{MS} &= \phi_M - \phi_S \\ \phi_o &= \phi_{oa} - \phi_{ob} \end{aligned} \right\} \quad (1b)$$

Use of Gauss's law under thermodynamic equilibrium yields,

$$\phi_M - \phi_S = V_{BO} + \frac{\delta}{\epsilon_i} [Q_{Sc}(0) + Q_{SSa}(0) + Q_{SSb}(0)] \quad (2)$$

Fonash (1983) has discussed different cases into which the behaviour of any MIS diode can fall depending on whether the interface states (D_{sa} or D_{sb}) can follow or cannot follow ac signal. Out of these cases, some are true for MIS structures with thick oxides ($\delta > 30 \text{ \AA}$), some hold good for nearly ideal MS structures ($\delta < 5 \text{ \AA}$) while some depict the behaviour of Schottky diodes ($5 \text{ \AA} < \delta < 30 \text{ \AA}$).

The experimental results available on Schottky structures (Fonash 1983, Tseng and Wu 1987) indicate that the reverse $1/C^2$ vs. V plot (though nonlinear at lower voltages) is linear at higher voltages. An attempt has been made in this section to formulate a generalized expression of diffusion potential in terms of the slope and voltage intercept of $1/C^2$ vs. V plot so that it follows the experimental results.

Out of all the different cases mentioned in Fonash (1983), we have selected only those five which give a linear slope for $1/C^2$ vs. V plot at large reverse bias. These five cases which can be approximated to explain the nature of experimental results mentioned above are now discussed. The approximation used is that in a MIS Schottky diode with a typical doping ($N_D < 10^{16} \text{ cm}^{-3}$) and an oxide thickness $\delta < 40 \text{ \AA}$, the insulator capacitance C_i is much greater than the space charge capacitance C_{sc} , so that the total capacitance C can be approximated by C_{sc} only. For instance

$$\text{if } N_D < 10^{16} \text{ cm}^{-3} \quad \text{and} \quad \delta < 40 \text{ \AA} \quad \text{then} \quad C_i \gg C_{sc}$$

If $K_0 = -2/q\epsilon_s N_D$ is the slope equation for the ideal MS diode case, then the slope (K) and voltage intercept (V_0) of $1/C^2$ vs. V plots for five different cases as discussed in Fonash (1983) are derived as follows. Using $C_i = \epsilon_i/\delta$,

$$\alpha' = qD_{sa}/C_i, \quad \alpha'' = qD_{sb}/C_i \quad (3)$$

Case 1: $\alpha' \neq 0$, $\alpha'' = 0$, interface states cannot follow ac signal

Under the above approximation, equation (36) of Fonash (1983)

$$K = K_0 [C_{sc} + C_i] / [C_{sc} + (1 + \alpha') C_i]$$

reduces to

$$K = K_0 / (1 + \alpha')$$

Also, equation (38) of Fonash (1983)

$$V_0 = V_1^{0.5}(V_{BO} - V_2)^{0.5} + (1 + \alpha')(V_{BO} - V_2) + (1 - \alpha')V_1/4$$

reduces to

$$V_0 = (1 + \alpha')(V_{BO} - V_2)$$

because V_1 is defined as (Fonash 1983)

$$V_1 = 2e\epsilon_s N_D \delta^2 / \epsilon_1^2 = 2e\epsilon_s N_D / C_1^2$$

So the first and last terms in equation (38) of Fonash (1983) can be neglected using the approximation mentioned above. In other words

$$K = K_0 / (1 + \alpha'), \quad V_0 = (1 + \alpha')(V_{BO} - V_2) \quad (4)$$

Case 2: $\alpha' \neq 0$, $\alpha'' \neq 0$, interface states cannot follow ac signal

Proceeding in a similar manner, as done for Case 1, the rigorous expressions for slope and voltage intercept given in Fonash (1983) as equations (46) and (47) can be written as

$$K = K_0 \left(\frac{1 + \alpha''}{1 + \alpha' + \alpha''} \right), \quad V_0 = \left(\frac{1 + \alpha' + \alpha''}{1 + \alpha''} \right) (V_{BO} - V_2) \quad (5)$$

Case 3: $\alpha' = 0$, $\alpha'' \neq 0$, interface states cannot follow ac signal

Similarly, equations (62) and (64) of Fonash (1983) reduce to

$$K = K_0, \quad V_0 = (V_{BO} - V_2) \quad (6)$$

Case 4: $\alpha' = 0$, $\alpha'' \neq 0$, interface states can follow ac signal

The slope and voltage intercept expressions are the same as those of Case 3.

Case 5: $\alpha' \neq 0$, $\alpha'' \neq 0$, D_{sa} cannot follow ac signal. D_{sb} can follow ac signal.

The slope and voltage intercept expressions are the same as those of Case 2.

The above equations (4)–(6) can be generalized to give

$$V_{BO} = \frac{K}{K_0} V_0 + V_2 \quad (7)$$

Now, for the formulation of the generalized expression of diffusion potential, we considered only the expressions derived under Cases 2 and 5. This is because only in these cases, the effect of both the groups of interface states are taken into account, giving a more realistic approach to the problem.

So from equation (5) we get

$$\left(\frac{K_0}{K} - 1 \right) = \frac{\alpha'}{1 + \alpha''} \quad (8)$$

Then in equation (2), the expressions for $Q_{sc}(0)$, $Q_{ssa}(0)$ and $Q_{ssb}(0)$ are substituted. Using the expressions of α' , α'' , E_a and E_b , equation (2) is written in a compact form as equation (9)

$$\phi_{MS} = V_{BO} + \frac{Q_{SC}(0)}{C_i} - \alpha' E_a - \alpha'' E_b \quad (9)$$

Then α' is written in terms of α'' using equation (8) and is substituted in equation (9). The value of α'' is obtained and written as equation (10). The value of α' is then obtained from equations (8) and (10)

$$\alpha'' = \frac{V_{BO} + \frac{Q_{SC}(0)}{C_i} - \phi_{MS} - E_a \left(\frac{K_0}{K} - 1 \right)}{\phi_0 + \frac{K_0}{K} E_a} \quad (10)$$

$$\alpha' = \frac{\left\{ V_{BO} + \frac{Q_{SC}(0)}{C_i} - \phi_{MS} + E_b \right\} \left(\frac{K_0}{K} - 1 \right)}{\phi_0 + \frac{K_0}{K} E_a} \quad (11)$$

The interface state density can be calculated as

$$D_{Sa} = \frac{C_i}{q} \alpha' \quad D_{Sb} = \frac{C_i}{q} \alpha'' \quad (12)$$

3. Results and discussion

Our main objective in this section is to validate the model for the calculation of interface state density. First of all, we check how accurate equation (7) is, because our interface state density calculations are based on this equation. To check the accuracy of equation (7), the experimental plots of variation of V_{BO} and V_0 with oxide thickness (given in Cowley (1966)) have been used and the same is reproduced in figure 2. The parameter values chosen are $\phi_m = 4.7 \text{ eV}$, $\chi_s = 4.0 \text{ eV}$,

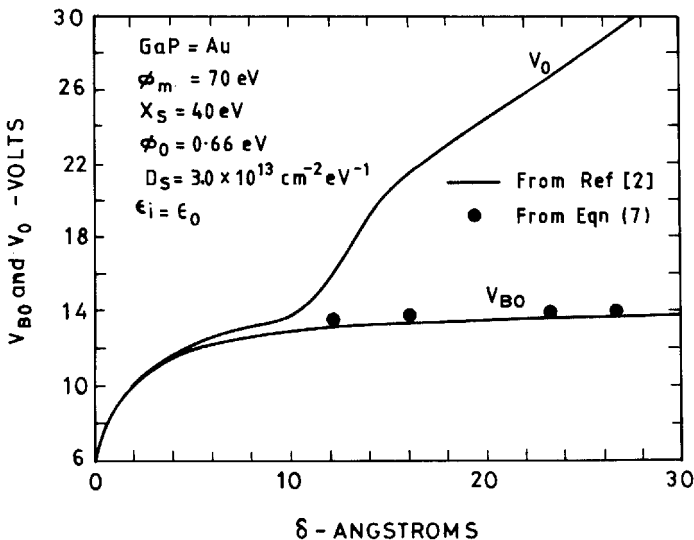


Figure 2. Plots of diffusion potential (V_{BO}) and voltage intercept (V_0) of $1/C^2$ vs. V plots for GaP-Au diode.

$\phi_{oa} = \phi_{ob} = 0.66 \text{ eV}$, $\varepsilon_i = \varepsilon_o$ and $D_{Sa} + D_{Sb} = 3 \times 10^{13} \text{ cm}^{-2} \text{ eV}^{-1}$. D_{Sa} and D_{Sb} are chosen such that as the oxide thickness varies from 0 to 30 Å, D_{Sa} increases (D_{Sb} decreases) from 0 to $3 \times 10^{13} \text{ cm}^{-2} \text{ eV}^{-1}$. The values of α' , α'' and K_0 are calculated using the chosen parameter values. The slope (K) of $1/C^2$ vs. V plot is calculated using equation (5). Using the experimental values of V_0 from figure 2, diffusion potential (V_{BO}) values are computed using equation (7) and are shown in figure 2. The close agreement of V_{BO} values obtained from simulation using equation (7) and experimental values (Cowley 1966) suggests that equation (7) can be used in the modelling of interface state densities of Schottky barrier diodes.

Now we proceed to check the accuracy of interface state density expressions given by equations (10) and (11). For this we use the $1/C^2$ vs. V plots given in Card and Rhoderick (1971). The values of slope (K) and voltage intercept (V_0) of the linear $1/C^2$ vs. V plots are obtained from the experimental results of Card and Rhoderick (1971) and from there the values of V_{BO} are obtained using equation (7). The V_{BO} values are listed in table 1. Then using the other parameter values (Card and Rhoderick 1971), the interface state density values contributed from both group A and B are computed using equation (12) and the results are compared in table 1 with the available values in the literature (Card and Rhoderick 1971). In table 1 the calculations are done using the parameter values of Card and Rhoderick (1971) and the density of interface states (as defined by Card and Rhoderick (1971)) $D'_{Sb} = D_{Sb}/[1 + (\delta/\varepsilon_i)qD_{Sa}]$ is listed in table 1.

A comparison of the two sets of results of interface state density (shown in table 1) suggests that the model proposed in this work can be used with reasonable accuracy. However, the present model is simpler and one can easily calculate the interface state densities contributed from groups in equilibrium with the metal and semiconductor Fermi level.

It would be useful to find the reverse bias $1/C^2$ vs. V characteristics as the oxide thickness and temperature changes. The model presented here provides a very simplistic approach to this problem. Figure 3 shows the simulated $1/C^2$ vs. V plots (at 1 MHz and 300 K) as the oxide thickness δ is varied assuming $N_D = 7 \times 10^{15} \text{ cm}^{-3}$, $D_{Sa} + D_{Sb} = 7 \times 10^{12} \text{ cm}^{-2} \text{ eV}^{-1}$. D_{sa} and D_{sb} are chosen such that the contribution from D_{sa} increases (D_{sb} decreases) as the oxide thickness increases. From figure 3, it is seen that as the oxide thickness increases, the slope decreases and the voltage intercept increases. In the ideal case, when no interface states are present or when only D_{sb} is present (which can follow the metal Fermi level), the slope is given by equation (6). But when interface states of density D_{Sa} are also present in addition to

Device	V_{BO}	δ (Å)	$D_{sb} \times 10^{12} \text{ (cm}^{-2} \text{ eV}^{-1}\text{)}$ (Card and Rhoderick 1971)	$D_{sb} \times 10^{12} \text{ (cm}^{-2} \text{ eV}^{-1}\text{)}$ equation (12)
1(A)	0.53	8	3	1.4
2(A)	0.53	12	3.6	1.8
3(A)	0.35	15	4.8	2.6
4(A)	0.20	22	5.5	3.6
5(B)	0.55	10	< 1	0.5
6(B)	0.45	15	1.6	0.9
7(B)	0.35	19	2.3	1.5
8(B)	0.30	26	3.1	2.3

Table 1. Comparison of the interface state density values as obtained from equation (13) and those of Card and Rhoderick (1971).

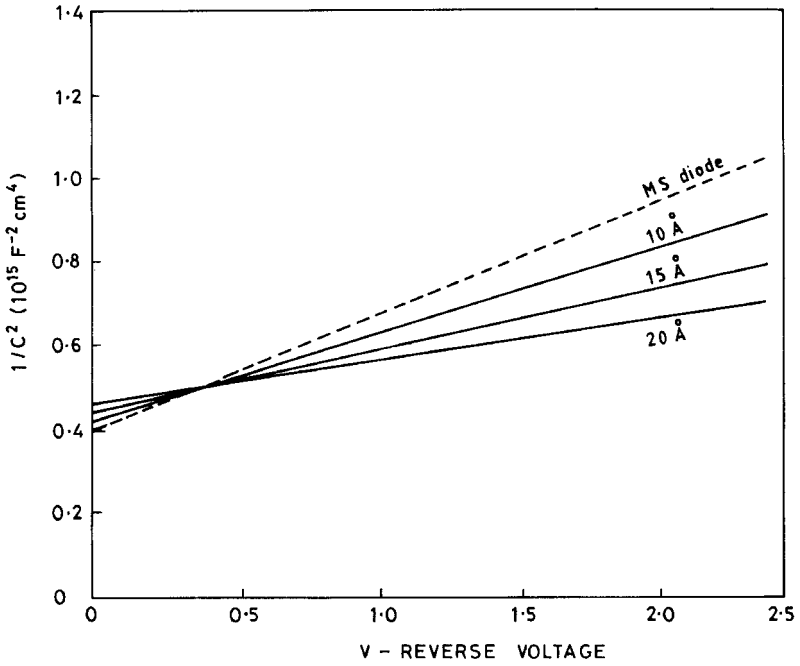


Figure 3. Reverse bias $1/C^2$ vs. V plots with varying oxide thickness.

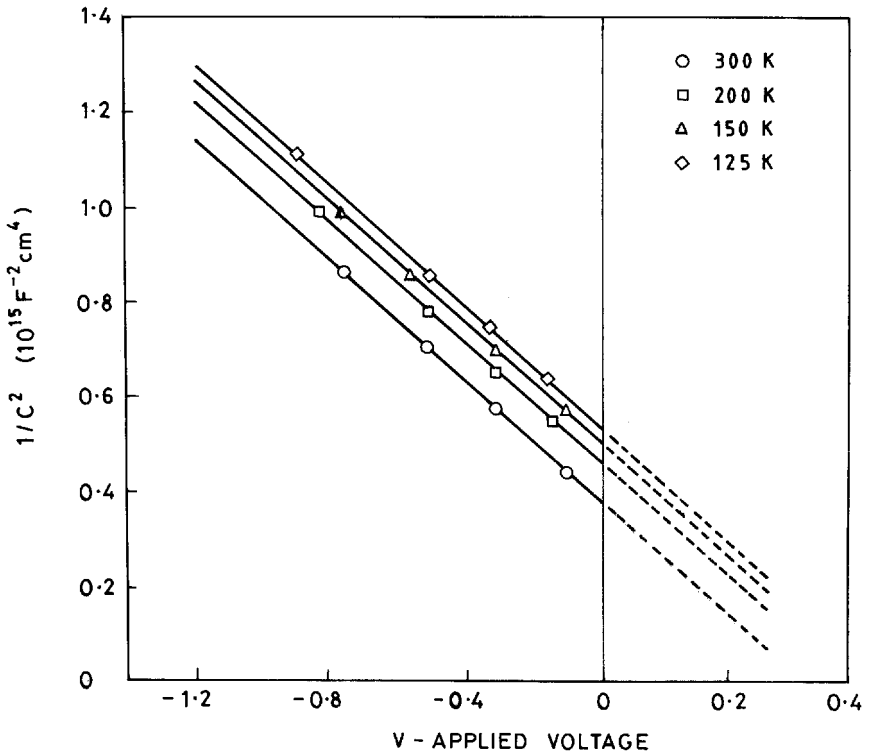


Figure 4. Reverse bias $1/C^2$ vs. V plots with varying temperature.

the above states, the $1/C^2$ vs. V characteristics deviate from the ideal case and its slope is smaller than the ideal case.

Figure 4 shows the effect of temperature on the $1/C^2$ vs. V plot using the same parameter values of figure 3. It is found that the slope is independent of temperature variation, though the voltage intercept decreases with increasing temperature. This observation is consistent with the theoretical expressions as shown in equations (5) and (7). In the slope expression $K = K_0(1 + \alpha''/(1 + \alpha' + \alpha''))$, we see that none of the terms are temperature dependent, so the slope is independent of temperature variation. In the voltage intercept expression $V_0 = ((1 + \alpha' + \alpha'')/1 + \alpha'')(V_{BO} - V_2)$, so as the temperature increases, V_0 value decreases.

4. Conclusion

A simple and novel technique is presented in this paper to extract the diffusion potential and interface state densities from the reverse bias $1/C^2$ vs. V plot of Schottky barrier diodes. Though this is an approximate model, its accuracy can be compared to the other models available in the literature. On the other hand, the use of a very accurate model would involve lengthy expressions and the knowledge of numerous parameter values, thus making the whole simulation process very complex. This model, being simple and straightforward, helps one to calculate the interface state densities of Schottky barrier diodes very easily using the reverse biased capacitance–voltage plots.

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