



Physical origins of the ideality factor of the current equation in Schottky junctions

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Abstract. After the carrier drift velocity at the semiconductor/metal interface is considered, current transport in Schottky diodes under a forward electric field is physically modelled. This model reveals that the ideality factor can be physically originated from the drift velocity and the drift velocity can also reduce the effective Schottky barrier height. This proposed model predicts that both the ideality factor and the Schottky barrier height depend on temperature, voltage and doping density, which agree well with the experimental results reported in the literature. The proposed diode current model also predicts a linear dependent relation between the reciprocal of the ideality factor and the effective Schottky barrier height, which is validated by experimental results. Such a model is useful to better understand the thermionic emission current physically in semiconductor/metal contact. It is also useful to characterise the material properties by using the ideality factor.

Keywords. Schottky junction; Schottky barrier diode; semiconductor; thermal emission.

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1. Introduction

Diodes are one of the basic building blocks of electronic circuits, which are widely used in electronic equipments of all kinds [1–20]. A Schottky junction is an interface between a semiconductor material and a metal. Schottky junctions are elementary ‘building blocks’ of electronic devices such as diodes and transistors. Thus, it is very important to accurately and physically model the current transport in Schottky junctions for applications in devices [1–17]. The Schottky diodes are also known as Schottky barrier diodes or hot-carrier diodes, which are semiconductor diodes formed by the junction of a semiconductor with a metal [1–17]. If the space charge region in a Schottky junction is large enough, the tunnelling probability should be very small. Thermionic emission current in diodes or thermally induced flow of carriers over a potential energy barrier should give a larger contribution to the total diode current compared to that due to the tunnelling. This is the reason why the Schottky diodes are also named as hot-carrier diodes.

The Shockley diode current equation gives the current–voltage characteristic of an ‘idealised’ diode, which is widely used [1–17]. Diodes that are not

‘idealised’ diodes are believed to come from where there are second-order effects. In this viewpoint, the second-order effects are the reason why the diodes do not follow an ‘idealised’ diode [1–17]. An ideality factor has been introduced to measure how closely a diode current follows the ideal diode current equation. With the help of an ideality factor introduced into this ‘idealised’ diode current equation, the experimental current data can be described. However, the physical understanding of an ideality factor is not clear.

A very large carrier drift velocity in electronic devices can be caused by ballistic transport or very high carrier mobility. A very large electron drift velocity in the channel can result in a decrease in channel electron density of GaN-based devices [21]. A very large electron drift velocity can give a large contribution to the tunnelling current in graphene transistors [22]. It can change the effective activation energy in organic transistors [23]. It can change the short channel effects in nanoscale silicon transistors [24]. It can shift the spectra of Raman photo- and electroluminescence and affect the diode current of graphene-based devices [25,26]. The effective Schottky barrier height is defined as the lowest incident electron energy to overcome the barrier. And it can be determined by the current–voltage curves based on the

thermic emission theory [26]. Lastly, a very large carrier drift velocity can reduce effective barrier height at the semiconductor/metal (semiconductor/oxide) interface via the quantum coupling [27–34].

Note that the effects of drift velocities at the semiconductor/metal interface before carriers overcome the Schottky barrier on the thermionic emission had not been included in the Shockley diode current equation [17]. Neglecting carriers having large drift velocities at the semiconductor/metal interfaces of Schottky diodes before carriers overcome the Schottky barrier will underestimate the thermionic emission current. Because such a Schottky contact is one of the most important component of semiconductor devices, it is necessary to accurately and physically model the effects of drift velocities on the thermionic emission current to explore them better. In other words, the effects of drift velocities on the thermionic emission current should be considered in the modelling and designation of Schottky diodes. The purpose of this paper is to develop a current equation that includes the effects of drift velocities at the interface of a semiconductor junction on the thermionic emission current. It can shed some light on how to physically understand the ideality factor of the Shockley diode equation in Schottky junctions based on the thermionic emission theory. In particular, an analytical physical model including the effects of carrier drift velocity on the thermionic emission is proposed. It can explain the experimental relation of the diode current dependent on the temperature, doping concentration, and applied voltage. The proposed model can clearly demonstrate the possible physical origin of the ideality factor of diode current equation through its simplicity and analytic nature.

2. Theory

According to the thermionic emission theory, the thermionic emission current density from a semiconductor to metal is [17,23]

$$J_{s \rightarrow m} = \int_{q\phi_B}^{\infty} q v_i dn, \quad (1)$$

where $q\phi_B$ is the minimum energy required for thermionic emission into the metal (effective Schottky barrier height), q is the electron charge and v_i is the carrier velocity along the transport direction in Schottky junctions before carriers overcome the Schottky barrier.

Because the process of the theoretical deduction for a p-type semiconductor/metal junction or other junctions is similar to that for an n-type semiconductor/metal junction, an n-type semiconductor/metal junction is used as an example in the following. An n-type semiconductor is formed by adding donor atoms in a

semiconductor, and a p-type semiconductor is formed by adding acceptor atoms in a semiconductor [17]. For an n-type semiconductor/metal junction at balance conditions, there is a depletion region with the built-in potential $q\psi_{bi} = q(\phi_m - \chi) - q\phi_n$ [17]. For a p-type semiconductor/metal junction at balance conditions, the built-in potential is $E_g - q(\phi_m - \chi) - q\phi_p$ [17]. ϕ_n is the Fermi potential from the conduction-band edge in the n-type semiconductor ($q\phi_n = E_C - E_F = -k_B T_L \log(N_D/N_C)$). ϕ_p is the Fermi potential from the conduction-band edge in p-type semiconductor ($q\phi_p = E_F - E_V = -k_B T_L \log(N_A/N_V)$). E_F is the Fermi level, N_D is the donor concentration, N_A is the acceptor concentration, N_C is the effective density of states in the conduction band, N_V is the effective density of states in the valence band, E_g is the band gap, k_B is the Boltzmann constant, T_L is the temperature, E_C is the energy at the bottom of the valence band and E_V is the energy at the top of the valence band [17]. The built-in electric field in the depletion region of the n-type semiconductor in a Schottky diode is $-(qN_D/\epsilon_S)(W_D(V) - x)$ [17]. Thus,

$$W_D(V) = \sqrt{\frac{2\epsilon_S}{qN_D} \left(\psi_{bi} - V - \frac{2k_B T_L}{q} \right)},$$

which is the width of the depletion region under an applied voltage [17]. Here, ϵ_S is the dielectric constant of the semiconductor and V is the applied voltage across the depletion region. A negative sign indicate that its direction is along the transport direction.

In the following, the effect of an applied forward electric field on the carrier velocity in Schottky diodes will be discussed. Note the formation of Schottky junction when an n-type semiconductor or a p-type semiconductor is fused to a metal [17]. In other words, excess electrons in the n-type semiconductor diffuse to the metal or excess holes in the p-type semiconductor diffuse to the metal. The diffusion of carriers in Schottky diodes under an applied forward electric field needs time before a balance is reached. More importantly, the time to apply an electric field to the Schottky junction is much faster than the diffusion time of the carriers. It means there will be a forward electric field F_{App} applied to the total depletion region. In other words, the forward voltage across the depletion region $V = F_{App} W_D(0)$. Thus, the forward applied electric field is $V/W_D(0)$. It means that the former depletion region in the n-type semiconductor of the Schottky diodes will be divided into a depletion region and an accumulation region due to the forward applied electric field. This implies that carriers in Schottky diodes under an applied forward electric field will be accelerated in the accumulation region, which is from

$$\sqrt{\frac{2\epsilon_S}{qN_D} \left(\psi_{BI} - V - \frac{2k_B T_L}{q} \right)}$$

to

$$\sqrt{\frac{2\epsilon_S}{qN_D} \left(\psi_{BI} - \frac{2k_B T_L}{q} \right)}$$

from the semiconductor/metal interface. Thus, the average net electric field across such an accumulation region is

$$\lambda = \frac{v_{0i}}{v_{0x}} = \begin{cases} \exp\left(\frac{qV}{2m^*} \left(1 - \sqrt{1 - \frac{V}{\psi_{BI} - \frac{2k_B T_L}{q}}}\right)\right) & \text{(ballistic transport)} \\ 1 + \mu \frac{V}{2v_{0x} \left(\frac{2\epsilon_S}{q^2 N_D}\right)^{1/2} (q\psi_{BI} - 2k_B T_L)^{-1/2}} & \text{(constant mobility)} \end{cases} \quad (4)$$

$$\frac{V}{2\sqrt{\frac{2\epsilon_S}{qN_D} \left(\psi_{BI} - \frac{2k_B T_L}{q} \right)}}$$

Such a net electric field will accelerate the carriers. And carriers will get a drift velocity before entering the depletion region or the potential barrier region. If ballistic transport of carriers (ballistic transport means no scattering) occurs in Schottky diodes and

$$m^* \frac{1}{v} \frac{dv}{dx} = -qF_{App}(x),$$

where m^* is the effective mass of carrier and v is the carrier velocity, is considered, the carrier velocity before carriers overcome the depletion region or the potential barrier region is

$$v_i = v_x \exp\left(\frac{qV}{2m^*} \left(1 - \sqrt{1 - \frac{V}{\psi_{BI} - \frac{2k_B T_L}{q}}}\right)\right), \quad (2)$$

where v_x is the carrier velocity along the transport direction before entering into the space charge region. On the other hand, if the scattering occurs in the accumulation region, carriers can get a drift velocity of

$$\frac{\mu V}{2\sqrt{\frac{2\epsilon_S}{qN_D} \left(\psi_{BI} - \frac{2k_B T_L}{q} \right)}}$$

$$\sqrt{n} = \lambda = \begin{cases} \exp\left(\frac{qV}{2m^*} \left(1 - \sqrt{1 - \frac{V}{\psi_{BI} - \frac{2k_B T_L}{q}}}\right)\right) & \text{(ballistic transport)} \\ 1 + \mu \frac{V}{2v_{0x} \left(\frac{2\epsilon_S}{q^2 N_D}\right)^{1/2} (q\psi_{BI} - 2k_B T_L)^{-1/2}} & \text{(constant mobility)} \end{cases} \quad (6)$$

which is along the transport direction (μ is the carrier mobility). The carrier velocity along the transport direction before carriers overcome the depletion region or the potential barrier region is

$$v_i = v_x + \mu \frac{V}{2\left(\frac{2\epsilon_S}{q^2 N_D}\right)^{1/2} (q\psi_{BI} - 2k_B T_L)^{-1/2}}. \quad (3)$$

Let

The minimum velocity required in the transport direction to surmount the Schottky barrier (before carriers enter the charge depletion region) is

$$\frac{1}{2} m^* v_{0i}^2 = \frac{1}{2} m^* \lambda^2 v_{0x}^2 = q(\psi_{bi} - V).$$

v_{0x} is the minimum electron velocity along the transport direction before it enters the charge accumulation region. It means that $v_{0x} = \lambda v_{0x}$. When the carriers reach a velocity higher than v_{0x} , they can contribute to the thermionic emission current. The corresponding carrier density can be written as

$$dn = N(E)F(E)dE \approx \frac{(m^*)^3}{4\pi^3 \hbar^3} e^{-\frac{q\phi_n}{k_B T_L}} e^{-\frac{m^* v^2}{2k_B T_L}} \times 4\pi v^2 dv.$$

Here, \hbar is the reduced Planck's constant, N is the density of states, F is the Fermi distribution function and E is the energy. The thermionic emission current through the Schottky junction is

$$J_{s \rightarrow m} = \lambda \frac{m^* (k_B T_L)^2}{2\pi^2 \hbar^3} e^{-\frac{q\phi_n}{k_B T_L}} e^{-\frac{(\psi_{bi} - V)}{\lambda^2 k_B T_L}} = \lambda \frac{m^* (k_B T_L)^2}{2\pi^2 \hbar^3} e^{-\frac{(q\phi_n + \frac{q\psi_{bi}}{\lambda^2})}{k_B T_L}} e^{\frac{qV}{\lambda^2 k_B T_L}}. \quad (5)$$

Obviously,

The above equation says that the ideal factor $n = \lambda^2$. The effective barrier height determined by the diode current equation (eq. (5)) in Schottky diodes is

$$q\phi_{BE} = q\phi_n + \frac{q\psi_{bi}}{\lambda^2} = q\phi_n + \frac{q\psi_{bi}}{n} \quad (7)$$

One can note that ballistic transport in Schottky diodes is relatively rare. Therefore, only the carrier drift velocities with the constant mobility assumption for Schottky diodes are discussed in the following. Theoretical calculations show that the carrier mobility in a non-polar semiconductor is dominated by the acoustic phonon interaction and the carrier mobility is proportional to $(T_L)^{-3/2}$ [15]. Using $\mu = A(T_L)^{-3/2}$ (A is the fit parameter) when

$$k_B T_L \left(2 - \ln \left(\frac{N_D}{N_C} \right) \right) < q(\phi_m - \chi),$$

the ideality factor under one order Taylor expansion is

$$\sqrt{n} = \lambda = D + E T_L^{-3/2} \left(1 + \frac{1}{2} F T_L \right), \quad (8)$$

where

$$D = 1, \quad E = \frac{AV}{2v_{0x} \sqrt{\frac{2\varepsilon_S q(\phi_m - \chi)}{q^2 N_D}}}$$

and

$$F = \frac{k_B \left(\ln \frac{N_D}{N_C} - 2 \right)}{q(\phi_m - \chi)}.$$

$$\sqrt{n} - 1 = \frac{V(\mu_{\max} - \mu_{\min})}{2v_{0x}(N_R)^\beta \left[\frac{2\varepsilon_S}{q^2} \left(k_B T_L \left(\ln \left(\frac{N_D}{N_C} \right) - 1 \right) - q + q(\phi_m - \chi) \right) \right]^{1/2}} (N_D)^{-\beta+0.5}. \quad (12)$$

When the carrier mobility is not proportional to $(T_L)^{-3/2}$ and it is proportional to $(T_L)^{-\gamma}$, eq. (8) will be in the form of

$$\sqrt{n} = E T_L^{-\gamma} \left(1 + \frac{1}{2} F T_L \right).$$

γ is a parameter. If $E(T_L)^{-1} \gg F(T_L)^{-2}$, eq. (8) can be further simplified as

$$\sqrt{n} = \lambda = D + E(T_L)^{-3/2}. \quad (9)$$

Equations (8) and (9) demonstrate that

$$\sqrt{n} \propto T_L^{-3/2} \quad \text{or} \quad \sqrt{n} \propto E T_L^{-1/2} + \frac{EF}{2} T_L^{-3/2}.$$

When the mobility is proportional to $(T_L)^{-\gamma}$, eq. (9) will be in the form of $\sqrt{n} = E T_L^{-\gamma}$. According to eqs (7) and (8), the effective barrier height under one-order Taylor expansion is

$$\begin{aligned} q\phi_{BE} &= (q\phi_n + q(\phi_m - \chi)) + k_B \ln \left(\frac{N_D}{N_C} \right) T_L \\ &\quad - \frac{EFk_B}{2} \ln \frac{N_D}{N_C} T_L^{1/2} \\ &\quad - \left[\frac{q(\phi_m - \chi)EF}{2} + 2Ek_B \ln \left(\frac{N_D}{N_C} \right) \right] (T_L)^{-1/2} \\ &\quad - 2Eq(\phi_m - \chi)(T_L)^{-3/2} \end{aligned} \quad (10)$$

According to eqs (6) and (10), the dependent relationship between temperature and the Schottky barrier height of the Schottky diode can be conveyed by the equation

$$q\phi_{BE} \propto T^\alpha, \quad (11)$$

where α is a parameter and $\alpha < 1$.

$$\mu = \mu_{\min} + \frac{\mu_{\max} - \mu_{\min}}{1 + \left(\frac{N_D}{N_R} \right)^\beta}$$

is the relation between mobility and the doping concentration [15]. Here μ_{\min} , μ_{\max} , β and N_R are fit parameters. When $(\mu_{\max} - \mu_{\min}) \gg \mu_{\min}$ and $N_D/N_R \gg 1$,

$$\mu \approx (\mu_{\max} - \mu_{\min}) \left(\frac{N_D}{N_R} \right)^{-\beta}.$$

According to eq. (4), the ideality factor can be rewritten as

3. Results and discussion

Although it is more common to plot n vs. barrier height, there is no linear relation between n and the barrier height according to eq. (7) ($q\phi_{BE} = q\phi_n + \frac{q\psi_{bi}}{n}$). In order to prove the validity of eq. (7), it is necessary to plot $1/n$ vs. barrier height. Figure 1 depicts how the effective barrier height ϕ_{BE} changes with the reciprocal of the ideality factor $1/n$. The experimental ϕ_{BE} vs. $1/n$ plots have good linear relations. It implies that the proposed model can describe these experimental data very well. The data of figure 1a come from Au/n-Si Schottky diodes [1]. The data of figure 1b come from Au/n-type Si Schottky diodes with

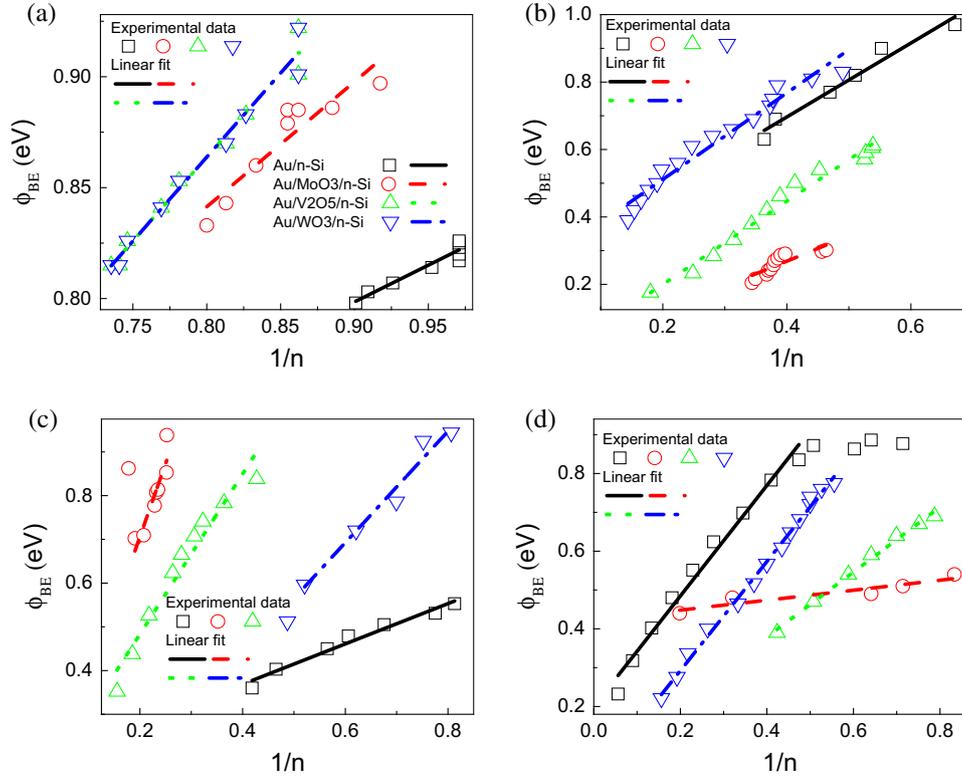


Figure 1. The comparison of the effective Schottky barrier height ϕ_{BE} vs. the reciprocal of the ideality factor $1/n$. **(a)** The experimental data from [1], **(b)** the experimental data of open squares from [2], open circles [3], up triangles [4], down triangles [5], **(c)** the experimental data of open squares from [6], open circles [7], up triangles [8], down triangles [9] and **(d)** the experimental data of open squares from [10], open circles [11], up triangles [12], down triangles [13].

interlayer, PtSi/p-Si Schottky barrier diodes, Re/n-Si Schottky contacts and Au/V₂O₅/n-Si Schottky diode [2–5]. The data of figure 1c come from Au/n-Ge Schottky diodes with Rubrene interlayer, Pd/ZnO/n-Si Schottky diodes, Au/C₂₀H₁₂/n-Si Schottky diodes, and polycrystalline silicon Schottky diodes [6–9]. The data of figure 1d come from Te/NaF:CdS/SnO₂ structure, F-doped SnO₂/TiO₂ structure, Ni/V/n-InP Schottky diodes and Au/n-type 6H-SiC Schottky diodes [10–13]. It also implies that the proposed model is valid for semiconductor Schottky diodes with different materials and structures.

The square root of the ideality factor on the temperature can be described by eq. (8). Equations (8) and (9) show that

$$\sqrt{n} \propto T_L^{-3/2} \quad \text{or} \quad \sqrt{n} \propto ET_L^{-1/2} + \frac{EF}{2}T_L^{-3/2}.$$

Figure 2 clearly demonstrates that the proposed model can describe these experimental results very well. The proposed model (eq. (8)) and a more rigorous equation (eq. (9)) ($\sqrt{n} \propto T_L^{-3/2}$), shows that \sqrt{n} is roughly linearly dependent on $1/T$, which is also shown in

figure 2. It seems that both equations can describe the dependent relation between \sqrt{n} and $1/T$. Additionally,

$$\sqrt{n} \propto ET_L^{-1/2} + \frac{EF}{2}T_L^{-3/2}$$

is the general expression for describing the correlation between the ideality factor and the temperature. One can note that figure 1 only shows a special case

$$\sqrt{n} \propto T_L^{-3/2} \quad \text{or} \quad \sqrt{n} \propto ET_L^{-1/2} + \frac{EF}{2}T_L^{-3/2}$$

(for example, for silicon Schottky diodes), whereas for other cases, using

$$\sqrt{n} \propto T_L^{-\gamma} \quad \text{or} \quad \sqrt{n} \propto ET_L^{-\gamma+1} + \frac{EF}{2}T_L^{-\gamma}$$

could be more suitable.

According to eq. (11), $\phi_{BE} \propto T^\alpha$ with $-3 < \alpha < 1$. Figure 3 clearly demonstrates that the experimental

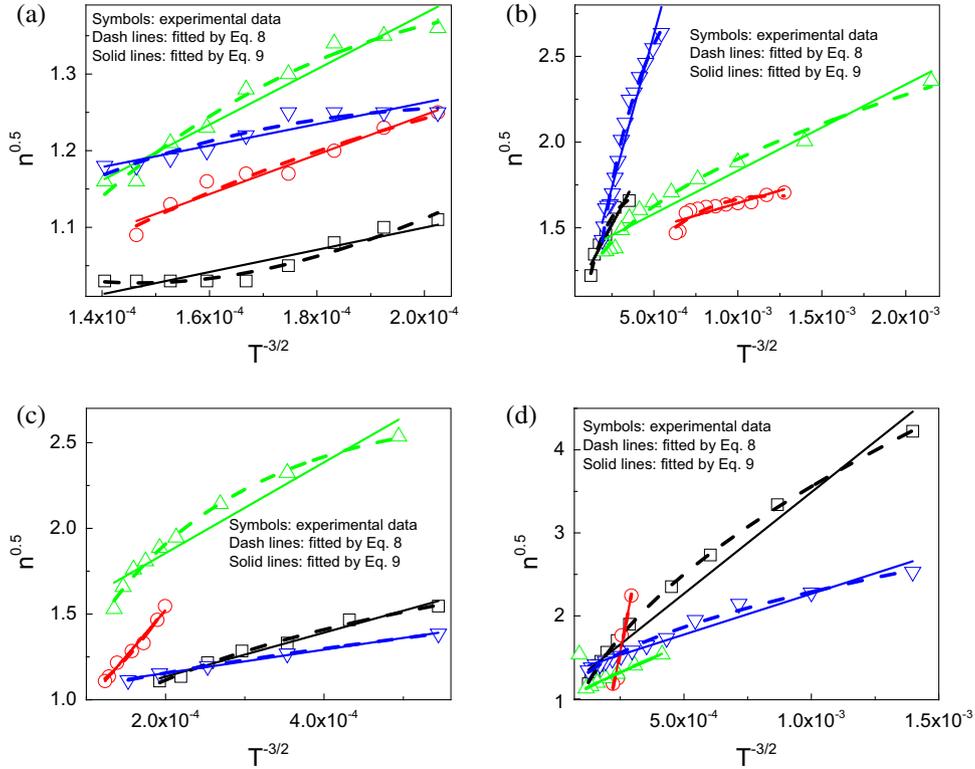


Figure 2. The comparison of the square root of the ideality factor $1/n$ vs. T^{-2} . (a) the experimental data from [1], (b) the experimental data of open squares from [2], open circles [3], up triangles [4], down triangles [5], (c) the experimental data of open squares from [6], open circles [7], up triangles [8], down triangles [9] and (d) the experimental data of open squares from [10], open circles [11], up triangles [12], down triangles [13].

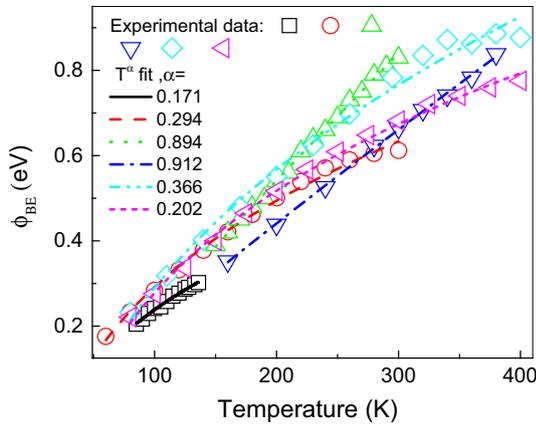


Figure 3. The comparison of the plot of the effective Schottky barrier height ϕ_{BE} vs. T^α . The experimental data of open squares from [3], open circles [4], up triangles [5], down triangles [8], diamonds [10], left triangles [13].

results reported in the literature have a very good fitting between ϕ_{BE} and T^α with α varying from 0.1 to 1. It implies that the proposed diode current model can explain the temperature-dependent Schottky barrier height observed in experiments.

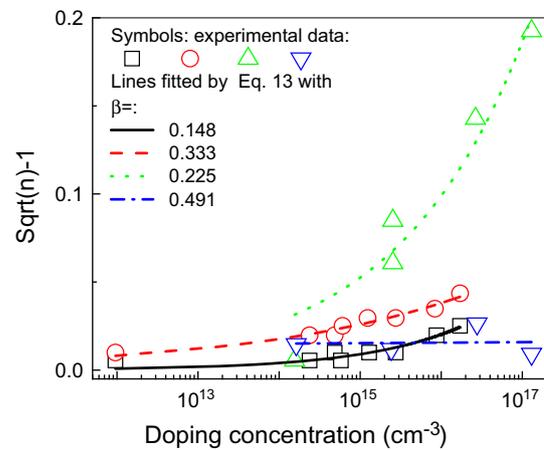


Figure 4. The comparison of the plot of $(n^{0.5} - 1)$ vs. the doping concentration. The experimental data are from [14], open squares and circles represent 450 and 1000°C in BF_2^+ implanted junctions, respectively. Up triangles and down triangles represent 450 and 1000°C in As^+ implanted junctions, respectively.

Considering that the sensitivity of the natural logarithm function of a variable is much less than that of the power function, eq. (12) can be rewritten as

$$\sqrt{n} - 1 = G(N_D)^{-\beta+0.5}, \tag{13}$$

where

$$G = \frac{V(\mu_{\max} - \mu_{\min})}{2v_{0x}(N_R)^\beta} \left[\frac{2\varepsilon_S}{q^2} \left(k_B T_L \left(\ln \left(\frac{N_D}{N_C} \right) - 3 \right) + q(\phi_m - \chi) \right) \right]^{-1/2}.$$

This represents that the ideality should be proportional to $(N_D)^{-\beta+0.5}$. Figure 4 clearly demonstrated such a doping concentration-dependent ideality factor with β varying from 0.1 to 0.5. Experimental data come from ref. [14]. It can be clearly seen from this figure that the proposed model can agree very well with the experimental results.

4. Conclusions

The effects of drift velocities before the carriers overcome the Schottky barrier on the thermionic emission current are considered. Thus, an analytical and physical diode current equation has been developed. According to the proposed model, the ideality factor physically originates from an additional drift velocity in Schottky diodes before carriers overcome the Schottky barrier. The results demonstrate that a larger drift velocity can reduce the effective Schottky barrier height determined by the current–voltage measurements. The effective barrier height ϕ_{BE} obtained in experiments and the reciprocal of the ideality factor $1/n$ have a very good linear fit. Such a linear relationship has been predicted by the proposed model. A dependent relation in the form of exponential function can be used to fit the ideality factor and temperature obtained in experiments. Exponential relation such as $\sqrt{n} \propto T_L^{-3/2}$ or $\sqrt{n} \propto ET_L^{-1/2} + (EF/2)T_L^{-3/2}$ has been predicted by the proposed model. The effective Schottky barrier height and temperature obtained in the experiments can be fitted very well with an exponential relation. Such an exponential relationship ($\phi_{BE} \propto T^\alpha$ with $-3 < \alpha < 1$) is predicted by the proposed model, and it is validated by a very good fit with α being found to vary from 0.1 to 1 in experiments. The power exponent of the doping concentration-dependent ideality factor obtained in experiments have been found that can be well fitted by using an exponential function. Such an exponential function ($n \propto (N_D)^{-\beta+0.5}$) is valid to describe the results of the experiments reported in the literature with β varying from 0.1 to 0.5. The ideality factor proposed in this paper provides a way for describing the effect of drift velocity on the diode current in Schottky diodes. The proposed diode current model predicts that

the ideality factor can be very much large when ballistic transport occurs. The Schottky barrier height can be measured with the ideality factor of 1. The validity of the proposed diode current model has been checked by comparing the predicted results with the experimental data reported in refs [1–14]. The results clearly demonstrate that the proposed model is good to describe the experimental results. How both the ideality factor and the effective Schottky barrier height depend on the applied forward voltage, temperature and the doping concentration is intuitively expressed in the proposed diode current equation. Accurate and physical model of the thermal emission current in semiconductor Schottky contacts can help us to understand and improve the performance of semiconductor materials and devices.

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