Thermal activation of current in an inhomogeneous Schottky diode with a Gaussian distribution of barrier height*

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This paper investigates the thermal activation behaviour of current in an inhomogeneous Schottky diode with a Gaussian distribution of barrier height by numerical simulation. The analytical Gaussian distribution model predicted that the I–V–T curves may intersect with the possibility of the negative thermal activation of current, but may be contradictory to the thermionic emission mechanism in a Schottky diode. It shows that the cause of the unphysical phenomenon is related to the incorrect calculation of current across very low barriers. It proposes that junction voltage $V_{\rm j}$, excluding the voltage drop across series resistance from the external bias, is a crucial parameter for correct calculation of the current across very low barriers. For correctly employing the thermionic emission model, $V_{\rm j}$ needs to be smaller than the barrier height ϕ. With proper scheme of series resistance connection where the condition of $V_{\rm j} > \phi$ is guaranteed, I–V–T curves of an inhomogeneous Schottky diode with a Gaussian distribution of barrier height have been simulated, which demonstrate normal thermal activation. Although the calculated results exclude the intersecting possibility of I–V–T curves with an assumption of temperature-independent series resistance, it shows that the intersecting is possible when the series resistance has a positive temperature coefficient. Finally, the comparison of our numerical and analytical results indicates that the analytical Gaussian distribution model is valid and accurate in analysing I–V–T curves only for small barrier height inhomogeneity.

Keywords: Schottky diode, barrier height inhomogeneity, I–V–T, thermal activation
PACC: 7330, 7340N, 7340E

1. Introduction

Current transport mechanism in a Schottky diode has been a subject for a long history. Traditionally Schottky barrier height (SBH) was considered to be uniform across the entire interface and thermionic emission (TE) theory was applied to a large variety of Schottky diodes with great success.[1] However it was recently recognized that barrier height inhomogeneity is very common for a real metal–semiconductor (M–S) contact. In the early days, a parallel conduction model was proposed for the current transport in an inhomogeneous Schottky diode.[2] Based on this concept, recently many kinds of SBH distributions as well as different transport models were proposed.[3−7] Among them, the Gaussian distribution model (GDM) is one of the most frequently used ones, due to its clear physical meaning and convenient applicability.[3,4,8−15] In addition Palm *et al.* have even shown direct images of SBH fluctuations in Au/Si contacts by using ballistic electron emission microscopy techniques and have represented them with a Gaussian distribution function,[16] supporting the GDM with experimental results instead of pure theoretical assumption.

Though a lot of examples have shown the success of the GDM, little attention has been paid to its application range or limits. By simple simulation, some people suggested that under certain conditions (at low temperature and/or with large inhomogeneity), current–voltage curves at different temperature (I–V–T) may intersect each other, indicating that the current at low temperature may be higher than that at high temperature in certain voltage range.[17−21] But this is unphysical and contradictory to the thermal activation mechanism of current transport in a Schottky diode. In this paper, the GDM is examined by numerical calculation and the cause of unphysical intersection of the I–V–T curves is revealed. The numerical calculation results are also compared with the analytical equations to give a hint to the application range of the analytical GDM. Finally possible reason for experimentally observed intersection of I–

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V–T curves is also demonstrated through numerical simulation.

2. Physical models and numerical method

The numerical calculation of current in a Schottky diode is based on the TE theory, which states[1]

$$I = aA^{**}T^2 \exp\left(-\frac{q\phi}{k_{\rm B}T}\right) \exp\left[\frac{q(V-IR_{\rm S})}{nk_{\rm B}T}\right] \times \left\{1-\exp\left[-\frac{q(V-IR_{\rm S})}{k_{\rm B}T}\right]\right\}, \quad (1)$$

where a is the diode area, A^{**} is the effective Richardson constant, q is electronic charge, $q\phi$ is the SBH, $k_{\rm B}$ is Boltzmann constant, T is the temperature in Kelvin, n is the ideality factor, V is the external bias, and $R_{\rm S}$ is the series resistance. The V–$IR_{\rm S}$ is the effective voltage drop across the M–S junction, which can be denoted as $V_{\rm j}$ (junction voltage).

For a homogeneous Schottky diode with a specific barrier height, the I–V–T curves can be then calculated by solving Eq. (1). Simple half interval method was used, where the loop is stopped when the relative deviation of high and low $V_{\rm j}$'s, i.e., $(V_{\rm jH}-V_{\rm jL})/(V_{\rm jH}+V_{\rm jL})$ is less than certain critical error, for example, 10^{-8} in this work.

For an inhomogeneous Schottky diode with a specific barrier height distribution, for example, Gaussian distribution, the I–V–T curves can be calculated by summing all the current across individual diodes with different SBH. In order to include $R_{\rm S}$ effect, the connection of intrinsic diodes with $R_{\rm S}$ can be classified into three schemes.[22] In Fig. 1(a), all the diodes are assumed to be connected in parallel, and connected in series with a common $R_{\rm S}$, this is a case so-called fully spreading of current. In Fig. 1(b), individual diodes are assumed to be connected with their own $R_{\rm S}$, this is a case so-called non-spreading of current. In Fig. 1(c), which is the most realistic case (partially spreading of current), individual diodes are first connected with their own $R_{\rm S}$, and then connected in series with a common $R'_{\rm S}$. Numerical calculation process for an individual diode is similar to that for a homogeneous Schottky diode. $V_{\rm j}$ is first calculated for the diode at a given external bias, and current is then calculated by Eq. (1).

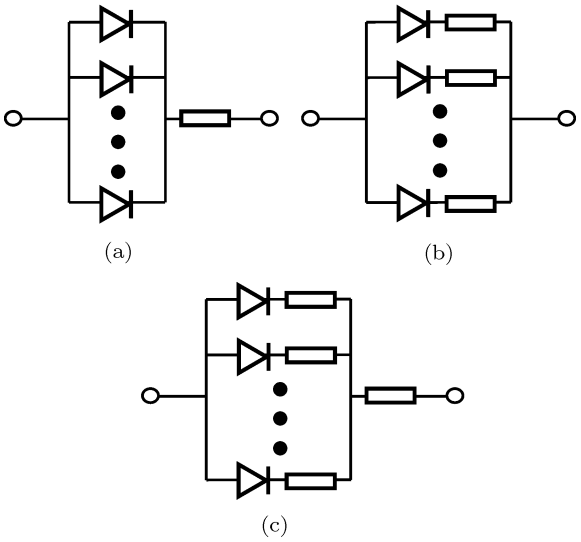


Fig. 1. Series resistance connection scheme of an inhomogeneous Schottky diode with current: (a) fully spreading; (b) non-spreading; (c) partially spreading.

3. Results and discussion

3.1. The TE model

For a homogeneous n-Si Schottky diode with an SBH of 0.8 eV, its I–V–T curves can be calculated by solving Eq. (1), by assuming $n = 1$, $R_{\rm S} = 10\ \Omega$, and $a = 0.01\ {\rm cm}^2$, for example. Figures 2(a) and 2(b) show the current under forward bias from 0.01 to 1.00 V and at temperature from 50 to 300 K. Figure 2(a) resembles experimental I–V–T curves very much. Under low bias, current increases linearly with voltage in the semi-logarithmic plot while the curves bend in high bias region where the voltage drop across $R_{\rm S}$ is not negligible. It can also be seen that all the I–V–T curves line up in good order, no intersection is observed, which is in good agreement with the thermal activation mechanism of a Schottky diode. To more clearly illustrate such mechanism, I–T curves at ten biases (0.1–1.0 V) were plotted in Fig. 2(b). The current at a fixed bias increases monotonically with temperature. Under low bias, the thermal activation transport mechanism is very pronounced. Under high bias, the mechanism is screened by the $R_{\rm S}$ effect, but negative thermal activation is not observed.

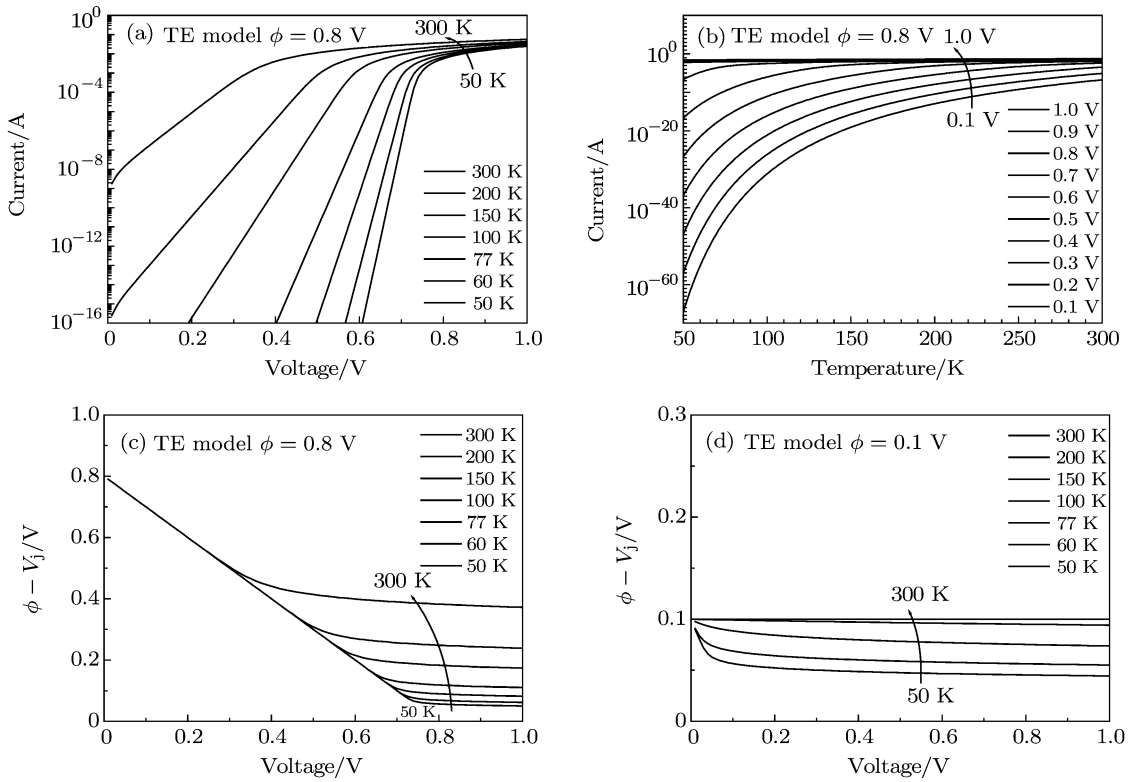


Fig. 2. Simulated characteristics of a homogeneous Schottky diode in TE model: (a) I–V–T with $\phi = 0.8$ V; (b) I–T with $\phi = 0.8$ V; (c) $(\phi - V_j) - V$ with $\phi = 0.8$ V; (d) $(\phi - V_j) - V$ with $\phi = 0.1$ V.

By examining Eq. (1), one can easily find that the sign of $\phi - V_j$ determines the thermal activation process in a Schottky diode. When $\phi - V_j > 0$, normal thermal activation occurs. Only when $\phi - V_j < 0$, negative thermal activation may be possible. Figure 2(c) shows $\phi - V_j$ as a function of voltage at different temperatures. It can be seen that $\phi - V_j > 0$ holds for all the bias and temperature. Generally the external bias across a Schottky diode can be sum of the voltage drop across the junction V_j and the voltage drop across the series resistance IR_S. Under low bias, the current is so small that the voltage drop across R_S is negligible, therefore V_j almost equals V, $\phi - V_j$ decreases linearly with V, and does not depend on temperature. Under high bias, voltage drop across R_S becomes more and more important. To some extent, the current is solely limited by R_S so that V_j will almost saturate. Since the current almost saturates at a constant ($\sim V/R_S$), V_j needed to drive a constant current at higher temperature should be lower, therefore $\phi - V_j$ at higher temperature saturates at higher value. The trend of V_j variation can also be understood from the viewpoint of resistance. A real Schottky diode can be modeled as series connection of two resistances. One is the series resistance R_S mentioned before, the other is the ideal diode resistance R_d (or junction resistance), which is a variable resistance, depending on V_j or equivalently on I (reciprocal to $\exp(qV_j/k_BT)$). For series connection, the voltage drop across either resistance will be larger than zero but smaller than the external voltage. The higher the resistance, the higher percentage the voltage drop. For low bias, R_d is so large that the external bias V almost completely drops across the junction, in other words, the voltage drop across R_S is negligible, then the current is determined by R_d itself, like that in the ideal Schottky diode case. For high bias, I becomes larger and larger, then R_d becomes so small that most of the external biases V drop across the R_S. In that case, the current is limited by R_S, and the Schottky diode is more or less like a resistor.

In order to investigate inhomogeneous Schottky diode in following subsections, similar calculation on a Schottky diode with a very low SBH, for example 0.1 eV, was also performed. Figure 2(d) shows $\phi - V_j$ as a function of voltage at different temperatures. It again can be seen that $\phi - V_j > 0$ still holds for all the biases and temperatures, though linear reduction part almost disappears. It is reasonable that for a diode with very low SBH, its I–V characteristic is almost

Ohmic with a very low $R_{\rm d}$ because $R_{\rm d}$ is also proportional to $\exp(q\phi/k_{\rm B}T)$. The current is limited by $R_{\rm S}$, and most of the external biases V drop across the $R_{\rm S}$. Although it is small, $V_{\rm j}$ is always larger than zero. And $V_{\rm j} < \phi$ assures the normal thermal activation of current transport across a Schottky diode.

3.2. Analytical GDM

In the GDM, SBH fluctuation of an inhomogeneous Schottky contact is assumed to be a Gaussian distribution function as follows:

$$\rho(\phi) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(\phi-\phi_0)^2}{2\sigma^2}\right], \tag{2}$$

where ϕ_0 and σ are the mean and standard deviation of the distribution, respectively. The current across the inhomogeneous Schottky diode is then calculated by integrating all the different-height barrier contribution, by using TE theory for an individual diode.

$$I = \int_{-\infty}^{+\infty} I(V,\phi)\rho(\phi)\mathrm{d}\phi, \tag{3}$$

where $I(V, \phi)$ is the expression of Eq. (1). But here it should be noted that it is only for the fully spreading case (Fig. 1(a)) that an analytical expression of the total current is possible. By performing integration of ϕ from $-\infty$ to $+\infty$, the total current can be obtained as follows:[3,4,12]

$$I = aA^{**}T^2 \exp\left(-\frac{q\phi_{\rm ap}}{k_{\rm B}T}\right) \exp\left[\frac{q(V-IR_{\rm S})}{nk_{\rm B}T}\right] \times \left\{1-\exp\left[-\frac{q(V-IR_{\rm S})}{k_{\rm B}T}\right]\right\}, \tag{4}$$

which is similar to the standard TE model, except that the barrier height should be replaced by a temperature-dependent apparent one

$$\phi_{\rm ap} = \phi_0 - \frac{q\sigma^2}{2k_{\rm B}T}. \tag{5}$$

Equation (5) is one of the main results of the analytical GDM, which shows that $\phi_{\rm ap}$ has a linear relationship with $1/T$. The slope of $\phi_{\rm ap} - 1/T$ is proportional to the square of SBH inhomogeneity σ. The equation was frequently used to extract the mean barrier height ϕ_0 and standard deviation σ from I–V–T measurements, and it showed some success.[3,4,8–15] However, one must remember that to reach Eqs. (4) and (5), an assumption of small σ has to be made.[3] If σ is not small enough, Eqs. (4) and (5) may give incorrect predictions in some cases.

Here we give some examples. According to Eqs. (4) and (5), I–V–T curves can be calculated if one knows ϕ_0 and σ. We adopt $\phi_0 = 0.8$ V, $\sigma = 0.07$ V, and $R_{\rm S} = 10\ \Omega$ as a typical case for the calculation. Figures 3(a) and 3(b) show the I–V–T and I–T characteristics of such a diode. From Fig. 3(a), one can see that the I–V–T curves intersect each other, this phenomenon means that at certain voltages, the current at low temperature may be larger than that at high temperature. This is opposed to thermal activation transport mechanism of a Schottky diode. Figure 3(b) illustrates such a negative thermal activation phenomenon more clearly. At low temperature, the current decreases with the increase of temperature (negative thermal activation). Above certain temperatures, the current increases with the increase of temperature (normal thermal activation). Chand and Osvald initially believed that the cause of such an abnormal phenomenon is related to the inclusion of negative SBH in the integration of Eq. (3).[17,18] But both of them accepted the possibility of the intersection though disagreement exists on the role of $R_{\rm S}$ in the abnormal phenomenon.[19,20]

In this work, we believe that the negative thermal activation is unphysical and it is the incorrect $V_{\rm j}$ which leads to this phenomenon. Figure 3(c) shows $V_{\rm j}$ as a function of voltage at different temperatures. The trend of $V_{\rm j}$ variation seems similar to that of the homogeneous Schottky diode. The $V_{\rm j}$ almost equals V under low bias while it saturates under high bias. Although $V_{\rm j}$ is still larger than zero for all the bias and temperature, $\phi - V_{\rm j}$ may be either larger or smaller than zero, which means that either normal or negative thermal activation may occur. Since $\phi - V_{\rm j}$ can be smaller than zero only for low SBH, and relative contribution of low barrier diode is high at low temperature, negative thermal activation occurs at low temperature, as shown in Fig. 3(b).

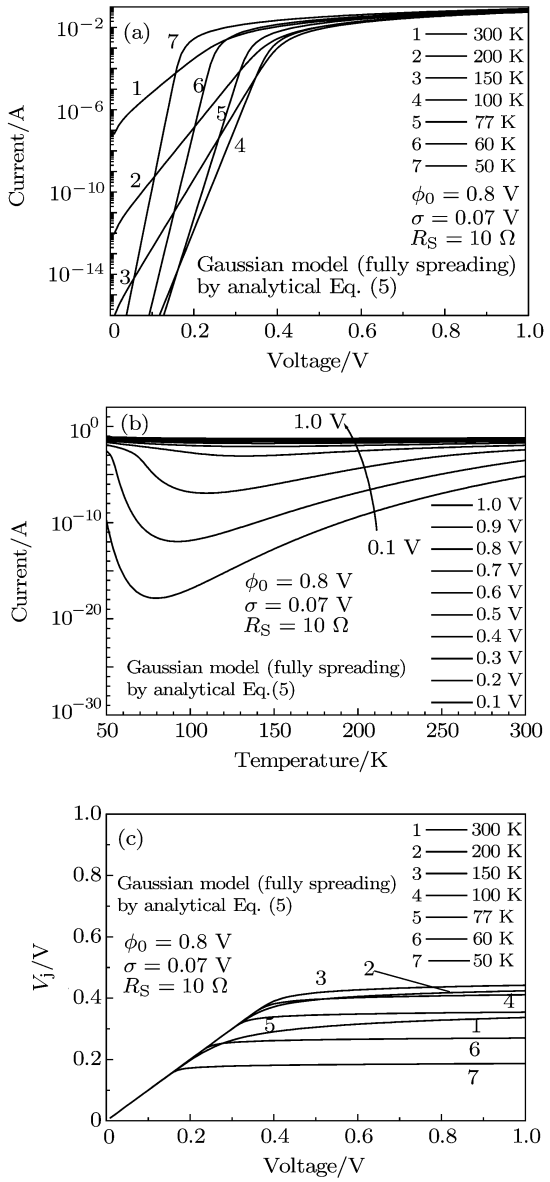


Fig. 3. Simulated characteristics of an inhomogeneous Schottky diode in analytical GDM (fully spreading) with $\phi_0 = 0.8$ V, $\sigma = 0.07$ V, and $R_S = 10\ \Omega$: (a) I–V–T; (b) I–T; (c) $V_j - V$.

Although such negative thermal activation may be possible from mathematic point of view, it is physically contradictory to the TE mechanism. If one accepts that TE mechanism holds for all the individual diodes, the sum of them should not violate the thermal activation law. The cause of such an unphysical phenomenon comes from the improper model of R_S connection and incorrect calculation for $V_j > \phi$. In Fig. 1(a), all the diodes are connected to a common R_S. All the diodes have a same V_j, which means that V_j may be larger than ϕ for some low barrier diodes. But in reality, when $V_j > \phi$, the conduction band of the semiconductor already bends down instead of bending up. Therefore the highest potential barrier is not located at the M–S interface like that in the usual case, indicating the invalidity of the TE model in this case. Unfortunately this was ignored in all the previous discussion of the analytical GDM.[17–21] In addition, it is not appropriate to assume a common R_S for different-size diodes. For low SBH, the diode area is small, therefore the diode should be connected with a large R_S, from either bulk or spreading resistance point of view. So the R_S connection schemes in Figs. 1(b) and 1(c) are more realistic, where individual diodes are connected with their own R_S. Then in either case, all the diodes will not share a common V_j. For a very low SBH, the diode has a very low R_d, and meanwhile the R_S is very large due to its small dimension. Therefore V_j across a diode with a very low SBH should be very low, in other words, most of external voltages should drop across R_S. So $\phi - V_j > 0$ may still hold for those very small SBH, and the TE model will be still valid for the calculation of the current in any individual diode.

3.3. Numerical GDM

To investigate I–V characteristics of R_S connection schemes in Figs. 1(b) and 1(c), numerical calculation has to be employed. Generally the R_S connection scheme in Fig. 1(c) should be the most realistic one. But as shown in Ref. [22], R_S connection scheme in Fig. 1(b) essentially gives very close results to those of Fig. 1(c). For simplicity, in this work, we adopt the scheme in Fig. 1(b) for numerical calculation.

For a Schottky diode with a Gaussian distribution of SBH as Eq. (2), the summation range of ϕ is chosen to be $(0, 2\phi_0)$. The step of ϕ is 0.005 V. For the diode corresponding to a barrier height of $q\phi$, the area is then $a\rho(\phi)\Delta\phi$. The series resistance is assumed to be reciprocal to the area of individual diode so that the calculation results will not be dependent on $\Delta\phi$. Then the series resistance is $\rho_S/a\rho(\phi)\Delta\phi$, where ρ_S is area resistivity with a unit of $\Omega{\cdot}\mathrm{cm}^2$.

Figures 4(a) and 4(b) show the simulated characteristics of an inhomogeneous Schottky diode with $\phi_0 = 0.8$ V, $\sigma = 0.07$ V, and $\rho_S = 0.1\ \Omega{\cdot}\mathrm{cm}^2$. In contrast to the analytical GDM, all the I–V–T curves line up in good order without any intersection. From Fig. 4(b), it can be more clearly seen that the current increases monotonically with the increase of temperature at a fixed voltage, which is consistent with the thermal activation mechanism of a Schottky diode.

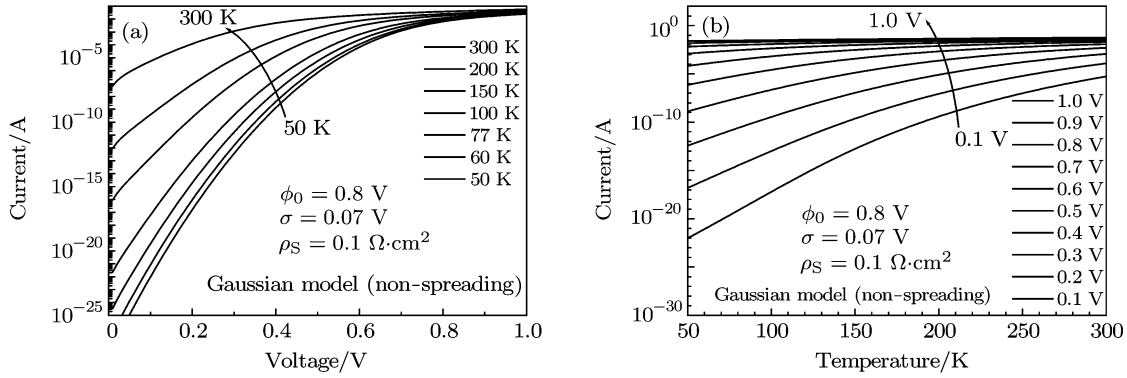


Fig. 4. Simulated characteristics of an inhomogeneous Schottky diode in numerical GDM (non-spreading) with $\phi_0 = 0.8$ V, $\sigma = 0.07$ V, and $\rho_S = 0.1\ \Omega\cdot cm^2$: (a) I–V–T; (b) I–T.

To reveal the thermal activation mechanism more clearly, V_j and $\phi - V_j$ for individual diode were plotted in Fig. 5. Figures 5(a) and 5(b) show V_j and $\phi - V_j$ for individual diode at an external bias of 0.1 V. One can see that for any diode, V_j is located between 0 and 0.1 V. It can be seen that V_j is different for each diode. For a diode with a high SBH, V_j almost equals the external bias because the current is so small that the voltage drop across its R_S is negligible or its R_d is too big in comparison to its R_S. For a diode with a low SBH, V_j almost equals zero because its R_d is too small in comparison with its R_S so that the external bias almost drops across its R_S. For a diode with an intermediate SBH, V_j ranges from zero to external bias. No matter how V_j varies, $\phi - V_j > 0$ holds for all the diodes as shown in Fig. 5(b). Similar conclusion can also be drawn for other external bias, for example, 1.0 V, as shown in Figs. 5(c) and 5(d). From these results, one can find it quite reasonable to observe normal thermal activation of current transport in this case.

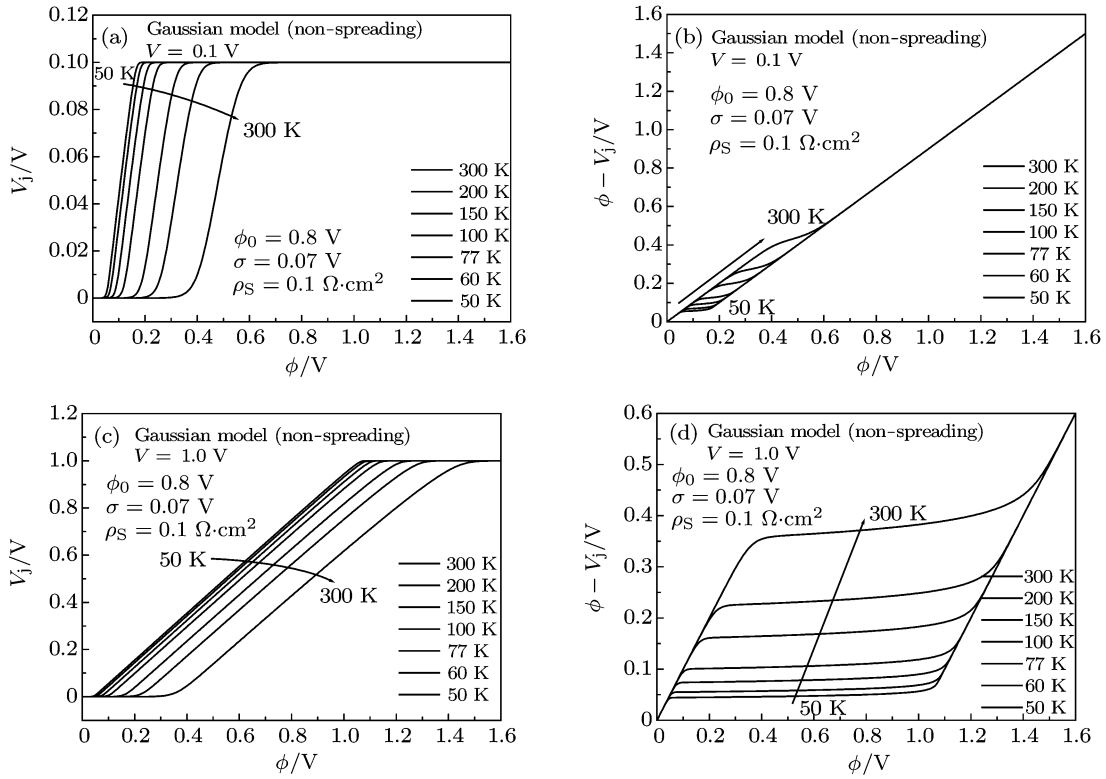


Fig. 5. The V_j and $\phi - V_j$ as functions of ϕ for an inhomogeneous Schottky diode in numerical GDM (non-spreading) with $\phi_0 = 0.8$ V, $\sigma = 0.07$ V, and $\rho_S = 0.1\ \Omega\cdot cm^2$: (a) $V_j - \phi$ at $V = 0.1$ V; (b) $(\phi - V_j) - \phi$ at $V = 0.1V$; (c) $V_j - \phi$ at $V = 1.0$ V; (d) $(\phi - V_j) - \phi$ at $V = 1.0$ V.

3.4. Comparison of numerical GDM with analytical GDM

For the unphysical negative thermal activation, some people thought it is related to the improper inclusion of negative SBH in the integration of Eq. (3).[17,18] However, after changing the integration limits to 0 and $2\phi_0$, intersection of I–V–T curves still takes place.[17,18,21] Figure 6 shows our numerical simulation results of an inhomogeneous Schottky diode with R_S connection as shown in Fig. 1(a). The diode has the same parameters as those in the analytical GDM, $\phi_0 = 0.8$ V, $\sigma = 0.07$ V, $R_S = 10\ \Omega$, but the integration limits are changed to 0 and $2\phi_0$. Figure 6(a) clearly shows that the I–V–T curves intersect again. Figure 6(b) shows similar I–T curves as those in Fig. 3(b), except that the current at low temperature (~ 50 K) is appreciably lower than that in Fig. 3(b). But the negative thermal activation still appears. So the results suggest that the integration limit is not the cause for the unphysical negative thermal activation, instead the R_S connection scheme is. Of course if one could correctly calculate the I–V curve for a diode with $V_j < \phi$, normal thermal activation should still be expected, even for the R_S connection scheme in Fig. 1(a).

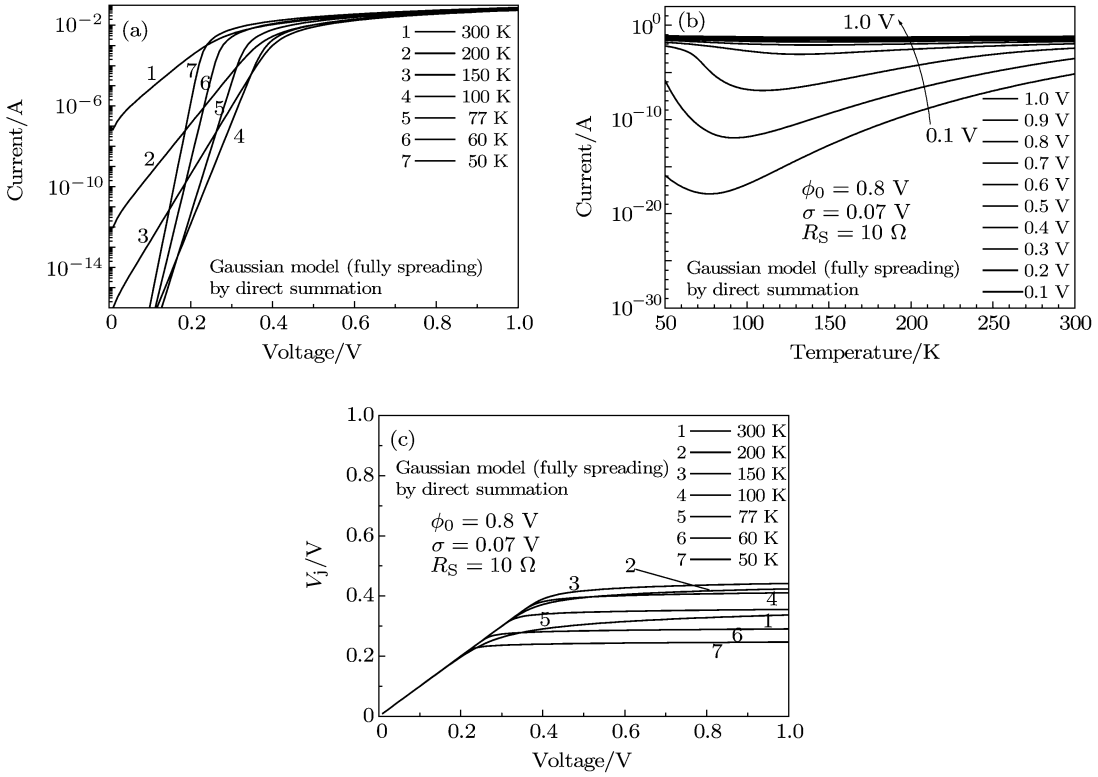


Fig. 6. Simulated characteristics of an inhomogeneous Schottky diode in numerical GDM (fully spreading) with $\phi_0 = 0.8$ V, $\sigma = 0.07$ V, and $R_S = 10\ \Omega$: (a) I–V–T; (b) I–T; (c) $V_j - V$.

Although the application of the analytical GDM has some limits, it still shows some success in explaining experimental I–V–T curves. To know the application range and the accuracy of the analytical GDM, different sets of Schottky barrier parameters, ϕ_0, σ, ρ_S, were chosen for numerical simulation of I–V–T curves. Apparent SBH ϕ_{ap} and apparent ideality factor n_{ap} can be extracted from those curves. Then ϕ_{ap}, n_{ap} versus $1/T$ can be plotted. Figure 7 shows $\phi_{ap} - 1/T$ and $n_{ap} - 1/T$ relations for seven inhomogeneous Schottky diodes with parameters as shown in Table 1. Finally ϕ_0 and σ for the analytical GDM can be obtained by fitting with Eq. (5), as listed in Table 1.

From Fig. 7(a) and Table 1, it can be seen that to the first order of approximation, all the ϕ_{ap} vary linearly with $1/T$, and the extracted ϕ_0 and σ are close to the initial values to generate those I–V–T curves, indicating the validity of analytical GDM. However, there is some deviation of the numerical $\phi_{ap} - 1/T$ relation from the exact straight line except for the smallest σ. For $\sigma = 0.07$ and 0.10 V, the deviation is appreciable, and the larger the σ, the larger the deviation. The results indicate that the analytical GDM is valid and accurate in analysing I–V–T curves only for small SBH inhomogeneity.

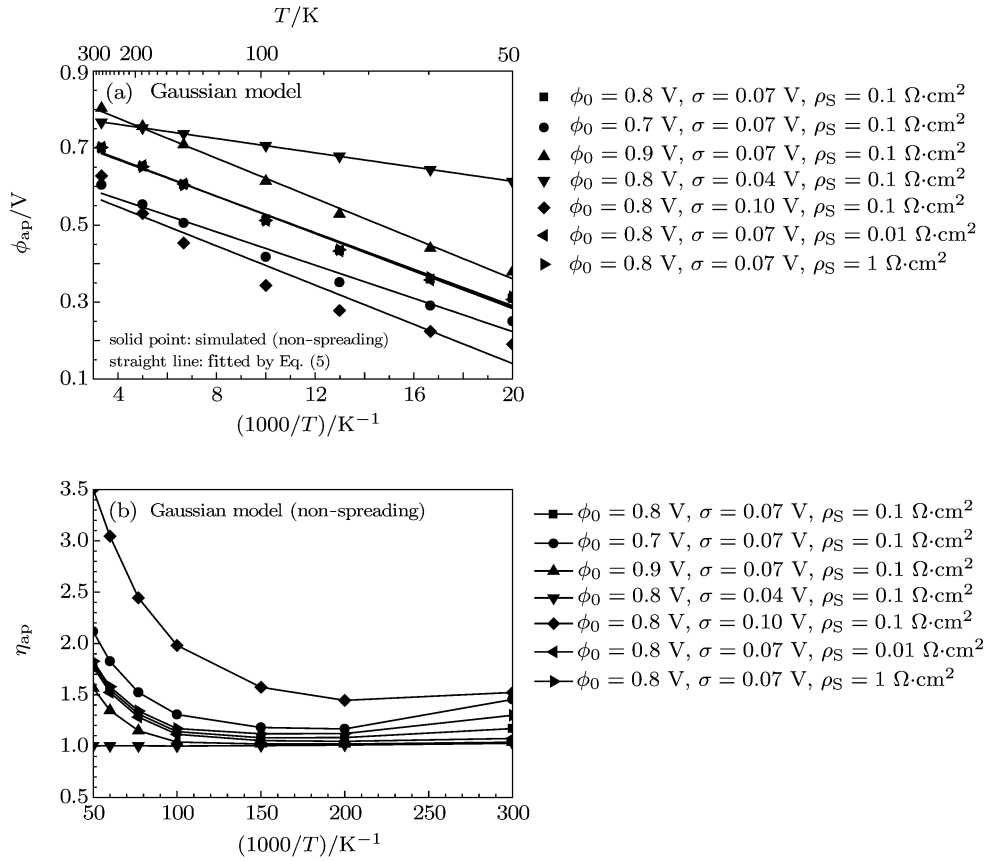


Fig. 7. The (a) $\phi_{ap} - 1/T$ and (b) $n_{ap} - 1/T$ relations for seven inhomogeneous Schottky diodes by numerical simulation (non-spreading) and analytical fitting (fully spreading).

Table 1. Barrier parameters for numerical simulation of I–V–T curves and their fitting results by Eq. (5).

parameters for numerical simulation			fitting results by Eq. (5)	
ϕ_0/V	σ/V	ρ_S/Ω·cm^2	ϕ_0/V	σ/V
0.8	0.07	0.1	0.766	0.064
0.7	0.07	0.1	0.654	0.061
0.9	0.07	0.1	0.882	0.067
0.8	0.04	0.1	0.799	0.040
0.8	0.10	0.1	0.649	0.066
0.8	0.07	0.01	0.770	0.065
0.8	0.07	1	0.764	0.064

From Fig. 7(b), one can see that n_{ap} is larger than unity for all the diodes at any temperature. Generally, the lower the temperature, the higher the n_{ap}. And the larger the inhomogeneity, the higher the n_{ap}. It should be emphasized that in numerical calculation for individual diode, the n is assumed to be unity ($n_{ind} = 1$). So our results confirm the conclusion that R_S influences n_{ap} for inhomogeneous Schottky diodes,[22,23] as opposed to the conclusion of Chand and Kumar.[24] Since V_j's of individual diodes are not the same for the R_S connection scheme in Fig. 1(b) even for low bias (Fig. 5(a)), the current for individual diode does not contribute proportionally, therefore an n_{ap} different from the n_{ind} is expected. By comparing the V_j under low and high biases as shown in Figs. 5(a) and 5(c), we can see that the relative contribution of low SBH to the total current is higher under low bias than that under high bias, so we can conclude that the n_{ap} should be larger than the n_{ind}. Furthermore the relative contribution of low SBH to the total current is high at low temperature, so larger deviation from n_{ind} at lower temperature is expected.

Although our numerical calculation results and analysis of V_j are opposed to the negative thermal activation of current transport in a Schottky diode, experimental observation of I–V–T curve intersection was occasionally reported.[25−31] But it should be noted that in our numerical calculation the R_S is assumed to be temperature independent, which may be an inappropriate assumption in some real cases. If we assume that the temperature dependence of R_S is exactly the same as that of the bulk resistivity of a semiconductor, I–V–T curves of a Schottky diode with an R_S connection scheme as shown in Fig. 1(b) can be recalculated. The temperature-dependent bulk resistivity is inversely proportional to the product of free carrier concentration and mobility. To calculate temperature-dependent free carrier concentration, the ionization energy of donors is assumed to be 50 meV. And the carrier mobility is assumed to follow Arora's formula.[32] Since the donors are almost fully ionized in the whole temperature range while the mobility decreases with temperature, the resultant resistivity has a positive temperature coefficient (TC). Figure 8 shows the calculated I–V–T and I–T characteristics of an inhomogeneous Schottky diode with following parameters, $\phi_0 = 0.8$ V, $\sigma = 0.07$ V, and ρ_S (300 K)=0.1 Ω·cm^2 but temperature-dependent. Interestingly it can be seen that the intersection of I–V–T curves is presented again. From Fig. 8(b) it can be also seen that the current under high bias may decrease with the increase of temperature. Considering the chosen temperature-dependent resistivity model, we find that the above results are quite reasonable because the calculated resistivity is found to decrease monotonically as the temperature decreases in the whole temperature range of our investigation. When the current of a Schottky diode is mainly controlled by the diode resistance R_d (usually under low bias), the current still shows normal thermal activation. But when the current is mainly controlled by the R_S (usually under high bias), it shows negative thermal activation instead. In fact, most cases of the experimental I–V–T curve intersection are accompanied by an R_S with a positive TC.[26−29,31]

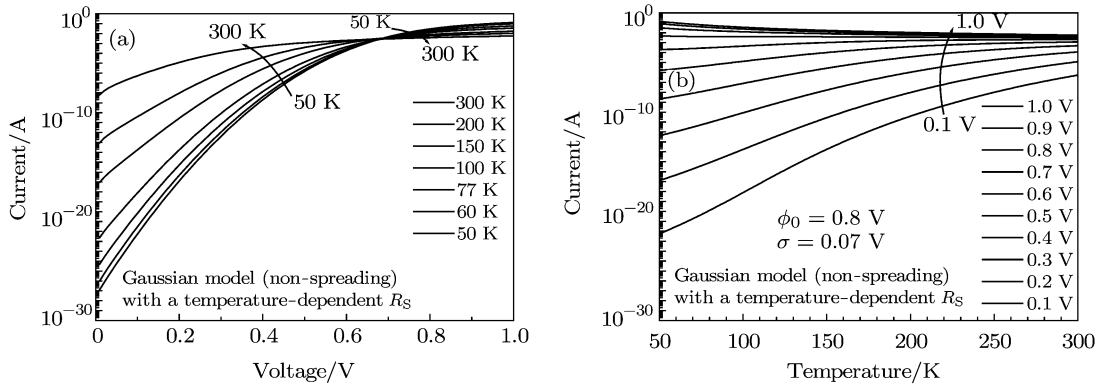


Fig. 8. Simulated characteristics of an inhomogeneous Schottky diode in numerical GDM (non-spreading) with $\phi_0 = 0.8$ V, $\sigma = 0.07$ V, and temperature-dependent ρ_S: (a) I–V–T; (b) I–T.

3.5. Comparison with experimental results

To verify the validity of the analytical and numerical GDMs, we have a summary for the available experimental data which were obtained from various inhomogeneous Schottky diodes with a Gaussian distribution of SBH. From Eq. (5), it is easy to see that when the temperature goes down, the apparent barrier height ϕ_{ap} is reduced. To some extent, it will become negative. In fact, before the ϕ_{ap} gets negative, when it is smaller than V_j, negative thermal activation already occurs. From this point of view, large inhomogeneity, low measurement temperature and high junction voltage in experiments will all be favourable for the observation of the negative thermal activation behaviour. Here we may have a rough estimate for the critical temperature T_C below which the negative thermal activation behaviour will occur according to the analytical GDM as follows:

$$T_C = \frac{q\sigma^2}{2k_B(\phi_0 - V_j)}. \tag{6}$$

Table 2 lists the experimental data dealt with GDM from various material systems and from different groups. The ϕ_0 is the mean SBH, σ is the standard deviation of a Gaussian distribution, V_j is the highest junction voltage or the junction voltage at the intersecting point in I–V–T curves, T_C is the critical temperature predicted by the analytical GDM, and $T_{measure}$ is the lowest measurement temperature in the experiments. If $T_{measure} < T_C$, negative thermal activation or intersection of I–V–T curves is observable. Otherwise such behaviour cannot be observed in the experiments. It can be seen that Ref. [4], [9], [12], [15], [27]–[29], [31] should all report the observation of the intersection of I–V–T curves, but in fact, Refs. [4], [9], [12], [15] did not. And all the experimental observed intersection of I–V–T curves are accompanied by the R_S with a positive TC as mentioned above.[26−29,31] These results show that the analytical GDM will lead to incorrect predictions if one uses it without checking the condition for its validity while the numerical GDM shows good agreement with the experimental results.

Table 2. Comparison of theoretical and experimental results for inhomogeneous Schottky diodes with a Gaussian distribution reported in literatures.

sample	ϕ_0/V	σ/V	V_j//V	T_C/K	$T_{measure}$/K	analytical GDM predicted crossing (Y/N)	experimentally observed crossing (Y/N)	TC of R_S	Ref.
Al/p-InP	1	0.08	0.5	74	289	N	N		[3]
PtSi/n-Si	0.837	0.0693	0.7	203	76	Y	N		[4]
PtSi/p-Si	0.242	0.011	0.08	4	77	N	N		[8]
TiN_x/n-Si	0.606	0.0784	0.4	173	77	Y	N		[9]
$CoSi_2$/n-Si (SSR epi)	0.64	0.11	0.2	160	173	N	N		[10]
PtSi/p-Si	0.223	0.0125	0.1	7	60	N	N		[11]
Pd_2Si/n-Si	0.8	0.05	0.7	145	52	Y	N		[12]
Pd_2Si/p-Si	0.38	0.03	0.3	65	60	Y	N		[12]
$CoSi_2$/n-Si (100)	0.65	0.053	0.4	65	89	N	N		[14]
$CoSi_2$/n-Si (111)	0.64	0.056	0.4	76	90	N	N		[14]
Au/n-GaAs (2.5×10^{15})	1.012	0.053	0.9	145	77	Y	N		[15]
Au/n-GaAs (1×10^{17})	0.9	0.05	0.75	97	83	Y	N		[15]
Au/n-GaAs (1×10^{18})	0.88	0.085	0.75	322	78	Y	N		[15]
Al/SiO_2/p-Si	1.136	0.159	4	∞	200	Y	Y	+	[27]
Al/TiO_2/p-Si	0.649	0.077	1.2	∞	100	Y	Y	+	[28]
Al/TiO_2/p-Si	1.108	0.137	1.2	∞	100	Y	Y	+	[28]
(Ni/Au)/$Al_{0.3}Ga_{0.7}N$/AlN/GaN	1.63	0.217	0.73	303	295	Y	Y	+	[29]
Au/Pd/n-GaN	1.03	0.118	0.8	351	90	Y	Y	+[a)]	[31]

[a)] Reference [31] gives a negative temperature coefficient of R_S by error. Correct non-linear fitting of the experimental I–V data gives R_S of about 200 Ω at 90 K and 1600 Ω at 410 K, i.e., a positive temperature coefficient.

Finally it should be noted that although a unity ideality factor was used for the calculation of all the individual diodes, the employment of non-unity ideality factor is straightforward. The simulated results, not shown here, do not change the obtained conclusion. And it also should be noted that our discussion was solely based on TE mechanism. In reality, the current across a Schottky diodi may be contributed from other mechanisms, for example, field emission or tunneling. But due to their insensitivity to temperature, the inclusion of their contribution should not change the trend of thermal activation obtained above.

4. Conclusion

The GDM for an inhomogeneous Schottky diode is examined by numerical simulation. The results show that the analytical formula based on the assumption of fully current spreading has some improper assumptions and has some limits in application. The most improper basis is that it employs the TE model for all the individual

diodes no matter whether V_j is smaller than ϕ or not. Therefore unphysical intersection of I–V–T curves or negative thermal activation of current in a Schottky diode is wrongly expected. Our numerical simulation shows that the inclusion of negative SBH in the integration is not the key cause of the unphysical phenomenon. With proper R_S connection scheme, the intersection of I–V–T curves is excluded in an assumption of temperature-independent R_S, this is in consistent with TE mechanism in a Schottky diode. Our numerical simulation also demonstrates that the intersection of I–V–T curves is possible when R_S has a positive TC. In general, it can be concluded that the analytical GDM is valid and accurate in analysing I–V–T curves only for small SBH inhomogeneity.

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