Study and modeling of the transport mechanism in a Schottky diode on the basis of a GaAs semiinsulator

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Abstract: The current through a metal–semiconductor junction is mainly due to the majority carriers. Three distinctly different mechanisms exist in a Schottky diode: diffusion of the semiconductor carriers in metal, thermionic emission-diffusion (TED) of carriers through a Schottky gate, and a mechanical quantum that pierces a tunnel through the gate. The system was solved by using a coupled Poisson–Boltzmann algorithm. Schottky BH is defined as the difference in energy between the Fermi level and the metal band carrier majority of the metal–semiconductor junction to the semiconductor contacts. The insulating layer converts the MS device in an MIS device and has a strong influence on its current–voltage (I–V) and the parameters of a Schottky barrier from 3.7 to 15 eV. There are several possible reasons for the error that causes a deviation of the ideal behaviour of Schottky diodes with and without an interfacial insulator layer. These include the particular distribution of interface states, the series resistance, bias voltage and temperature. The GaAs and its large concentration values of trap centers will participate in an increase in the process of thermionic electrons and holes, which will in turn act on the I–V characteristic of the diode, and an overflow maximum value [NT $= 3 \times 10^{20}$] is obtained. The I–V characteristics of Schottky diodes are in the hypothesis of a parabolic summit.

Key words: electrostatic potential and density of carriers; current thermionic emission-diffusion and tunnel current through the gate; current–voltage characteristics of Schottky diodes; temperature

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1. Introduction

The operation of semiconductor components at high temperature and high frequency, such as Schottky diodes and PN, is usually described by a set of features for the implementation of voltage, whose analysis provides some information about electricity from the transport mechanism.

The determination of the model parameters that are fundamental to the Schottky diode enables us to know the height of the gate, the ideality factor, and the resistance set, which plays an important role in the conception and the manufacture of semiconductor devices such as photopiles.

The goal of this thesis is to contribute to the mathematical modeling and the simulation of greatly inhomogeneous semiconductor devices.

Study of the physical origin of currents with low temperature of diode Schottky is on the basis of a GaAs. One finds that these excess currents are due to the generation of network shortcomings close to the metal–semiconductor interface at the time of irradiation, to heat or to an external distortion. These shortcomings produce levels of trap in some parts of the space load region.

This paper investigates the diffusive limit of the Boltzmann equations, to get a second order approximation of the concentration of the carriers. The drift–diffusion equations are unchanged, but a correction of the boundaries of layers, which is proportional to current flow, appears in the boundary conditions for the concentration. The proportionality coefficient is calculated by solving the spectral method.

These limiting and classical conditions are compared numerically on a physical problem. This paper is also dedicated to the extention of the particle simulation programs for the treatment of these inhomogeneous structures. In these devices, the dynamics are governed by the limiting conditions that need to be taken precisely into account. The geometry is one-dimensional in space and three-dimensional with axisymmetry in a wave vector. It is therefore necessary to solve the coupled Boltzmann–Poisson system in order to model a Schottky diode in the united and multi-dimensional cases, respectively. The numeric results obtained are explained later.

The system was solved by using a coupled Poisson–Boltzmann algorithm. Schottky BH is defined as the difference in energy between the Fermi level and the metal band majority carrier of a metal–semiconductor junction to the semiconductor contacts[1–4]. These include the particular distribution of interface states[2, 5], the series resistance[6–8], bias voltage[6–10] and temperature[1, 2, 6, 9, 11].

The theory of diffusion supposes that the driving force is distributed along the length of depletion layers. The theory of the thermionic emission-diffusion (TED) only applies to energetic carriers, which have energy equal to or bigger than the energy of the conduction strip on the interface of the metal–semiconductor. Quantum mechanics causes the current to pierce a tunnel through the gate, on account of the wave nature of the electrons. In a given junction, a combination of all three mechanisms could exist[12–14]. However, typically there is only one dominant current mechanism. The analysis reveals that the diffusion and thermionic emission-diffusion (TED) can

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be written in the following form[5, 7, 15]:

$$J_{\rm n} = qvN_{\rm c}\exp\left(-\frac{\phi_{\rm B}}{V_{\rm t}}\right)\left(\exp\frac{V_{\rm a}}{V_{\rm t}}-1\right). \tag{1}$$

This expression affirms that the current is the product of the electronic load, q, a speed, v, and the available carrier density in the semiconductor located next to the interface. Speed equals to the mobility multiplied by the electric field at the interface, the diffusion current and the speed of Richardson and the current of the thermionic emission-diffusion (TED)[16–18]. It ensures that the current is zero so no voltage is applied in thermal equilibrium.

The current tunnel is of a similar shape, to know:

$$J_{\rm n} = qv_{\rm R}n\Theta, \tag{2}$$

where $v_{\rm R}$ is the Richardson velocity, q the electronic charge, and n the density of carriers in the semiconductor. The current tunnel has the term of the probability Θ added since the total current depends on the carrier' flux arriving at the tunnel gate multiplied with the probability, Θ, that it pierces a tunnel through the gate.

This analysis supposes that the depletion layer is big compared to the middle free trajectory, so that the concepts of movement and diffusion are valid. The density currents are thus obtained as:

$$J_{\rm n} = \frac{q^2 D_{\rm n} N_{\rm c}}{V_{\rm t}}\sqrt{\frac{2q\left(\phi_{\rm i}-V_{\rm a}\right)N_{\rm d}}{\varepsilon_{\rm s}}}\exp\left(-\frac{\phi_{\rm B}}{V_{\rm t}}\right)\left(\exp\frac{V_{\rm a}}{V_{\rm t}}-1\right). \tag{3}$$

The current depends on the applied voltage, $V_{\rm a}$, and exponentially on the height of the gate, $\phi_{\rm B}$, therefore the prefactor can be consisted more easily if one rewrites it as function of the electric field on the interface of the metal–semiconductor $\varepsilon_{\max}$:

$$\varepsilon_{\max} = \sqrt{\frac{2q\left(\phi_{\rm i}-V_{\rm a}\right)N_{\rm d}}{\varepsilon_{\rm s}}}, \tag{4}$$

$$J_{\rm n} = q\mu n\varepsilon_{\max}N_{\rm c}\exp\left(-\frac{\phi_{\rm B}}{V_{\rm t}}\right)\left(\exp\frac{V_{\rm a}}{V_{\rm t}}-1\right), \tag{5}$$

so that the prefactor equals the current of the movement to the interface of the metal–semiconductor.

The theory of thermionic emission-diffusion (TED) supposes that electrons, with energy bigger than the summit of the gate, will cross the well-stocked gate that is displaced toward the gate. The real shape of the gate is ignored by this. The current can be expressed as:

$$J_{\rm MS} = A^{*}T^{2}\exp\left(-\frac{\phi_{\rm B}}{V_{\rm t}}\right)\left(\exp\frac{V_{\rm a}}{V_{\rm t}}-1\right), \tag{6}$$

where $A^{*} = \frac{4\pi q m^{*}K^{2}}{h^{3}}$ is the effective Richardson constant, q the electronic charge, k Boltzmann constant, T the absolute temperature, and $\phi_{\rm B}$ the height of the Schottky gate.

The expression for the current due to TED can also be written as function of the middle speed with which the electrons approach the gate interface. This speed is known as the Richardson speed and is given by:

$$v_{\rm R} = \sqrt{\frac{KT}{2\pi m}}. \tag{7}$$

So that the current density becomes:

$$J_{\rm n} = qv_{\rm R}N_{\rm c}\exp\left(-\frac{\phi_{\rm B}}{V_{\rm t}}\right)\left(\exp\frac{V_{\rm a}}{V_{\rm t}}-1\right). \tag{8}$$

The current tunnel is obtained with the product of the velocity and density. The velocity is the Richardson velocity. The carrier's density equals the available electron density, n, multiplied with the probability of piercing a tunnel, Θ, to give:

$$J_{\rm n} = qv_{\rm R}n\Theta. \tag{9}$$

Here the probability tunnel is obtained by:

$$\Theta = \exp\left(-\frac{4}{3}\frac{\sqrt{2qm^{*}}}{\hbar}\frac{\phi_{\rm B}^{3/2}}{\varepsilon}\right), \tag{10}$$

and the electric field equals $\varepsilon = \phi_{\rm B}/L$. Therefore the current tunnel exponentially depends on the height of gate, $\phi_{\rm B}$, to the 3/2.

A metal–semiconductor junction results in an Ohmic contact (a contact with voltage independent resistance) if the Schottky gate height, $\phi_{\rm B}$, is zero. In such case, the carriers are free to flow in or out of the semiconductor so that there is minimal resistance through the contact. For an n-type semiconductor, it means that the workfunction of the metal must be close to or smaller than the electron affinity of the semiconductor. A p-type semiconductor requires that the workfunction of the metal must be close to or bigger than the sum of the electron affinity and the bandgap energy. It can be problematic to find a metal that provides a p-type Ohmic contact with a semiconductor with a large bandgap such as GaN or SiC.

A more convenient contact is a tunnel contact. Such contacts have a positive gate to the metal semiconductor interface. If the width of the region of the depletion to the metal–semiconductor interface is very thin, of the order of 3 nm or less, the carriers can pierce a tunnel comfortably through such a gate. The required doping density for such contact is 10^{19} cm^{-3} or higher.

All sample or semiconductor structures are inevitably joined to metallic lines of current transportation. It is indispensable that contacts between the lines of transportation and the semiconductor allow the current in the two directions to pass and present the weakest resistances possible.

The resistance of a contact is defined by:

$$R = R_{\rm C}/S, \tag{11}$$

where $R_{\rm C}$ = specific resistor of contact ($\Omega\cdot$cm^2) (resistor of contact); S = surface of contact.

One can decrease this resistance while increasing the contact surface.

An ohmic contact on an SC'N' and SC'P' (Figs. 1, 2) is theoretically possible with a metal working at less than the output of a semiconductor. Unfortunately this ideal situation is rarely achieved. In practice, one decreases the resistance of a contact superficially by overdoping the region where one wants to achieve contact: we obtain a degenerate buffer layer (of 10^{19} to 10^{20} cm^{-3}).

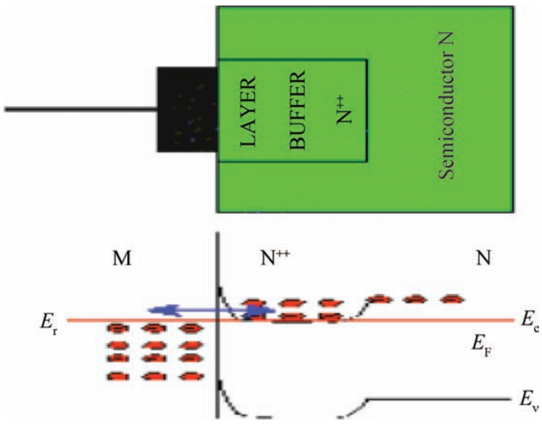

Fig. 1. Ohmic contact on semiconductor N.

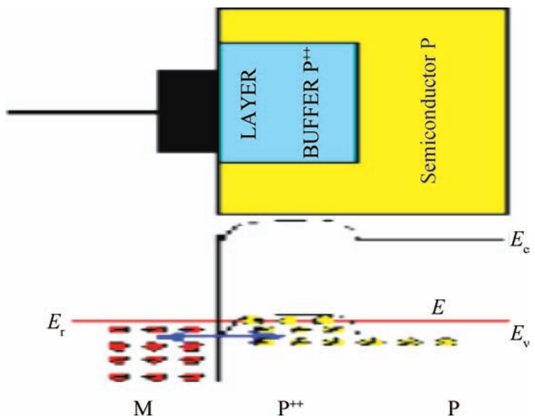

Fig. 2. Ohmic contact on semiconductor P.

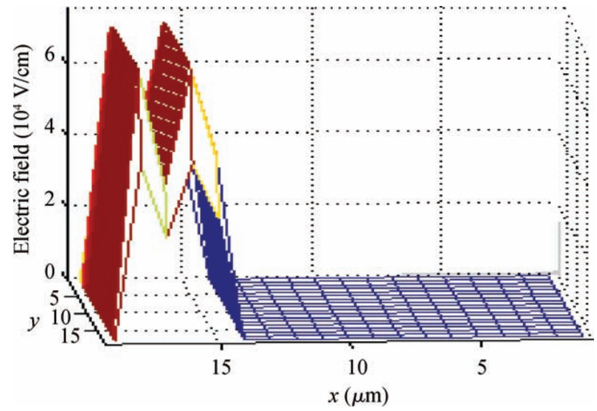

Fig. 3. Distribution of the potential to the out thermodynamic balance of an n-type Schottky diode in GaAs (Plan xoy, $z = 0.65$ μm).

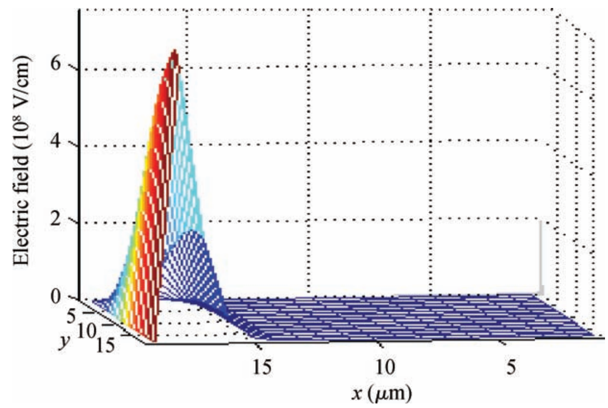

Fig. 4. Distribution of the potential to the thermodynamic balance of an n-type Schottky diode in GaAs (Plan xoy, $z = 0.65$ μm).

2. Results and discussion

We have used an SIM 3D simulator in our study, which studies devices with small geometry. The I–V characteristics of Schottky diodes are in the hypothesis of a parabolic summit.

The electric field generated by a voltage of polarization presents intensity and a specific direction in every point in the ZCE. However it is important to first determine all points of the electrostatic potential. The potential interest is the fact that the value of the electric field strength at a point drifts directly and affects the variation of the potential (Fig. 3).

The electric field is characterized in every point of the domain by a vector $E(x, y, z)$ with a direction and an intensity (Fig. 4). In a three-dimensional plot, it is marked by its three component scalar $E_x(x, y, z)$, $E_y(x, y, z)$, $E_z(x, y, z)$. The potential lines are generally given by closed lines (Fig. 5). They include the loads and are perpendicular to the lines of field.

The ZCE due to the metallurgic contact presents a width that varies from inversely proportional to the concentration the doping of the integrated layer. This ZCE is therefore important since it also presents an intensity considerable electric field due to the density of state of the center traps condensed at the surface of the metallurgic diode.

The simulation of the equilibrium state shows the influence of deep centers on I–V characteristics.

The density of state of the center traps evolving between 6×10^{16} and 3×10^{20} is inversely proportional to JTED (current thermionic emission-diffusion) that evolves between 2.1 $\times\ 10^{-8}$ and 8.1×10^{-8} A (Fig. 6–8).

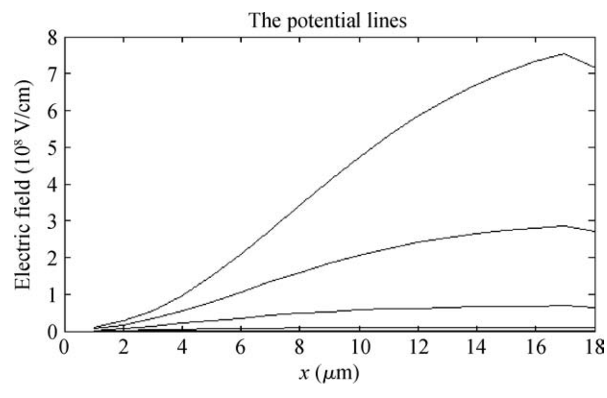

Fig. 5. Distribution of the potential lines of the thermodynamic balance of an n-type Schottky diode in GaAs (Plan xoy, $z = 0.65$ μm).

The deep centers involved in a recombination mechanism such as Shockley–Read is characterized by four new parameters that can vary independently from each other: n_{1t} (and p_{1t}) (cm^{-3}), which are functions of the energy level in the forbidden gap; τ_{nt} and τ_{pt} (s^{-1}) are related to the capture efficient sections for electrons and holes, and also to the density N_t (cm^{-3}) of the centers.

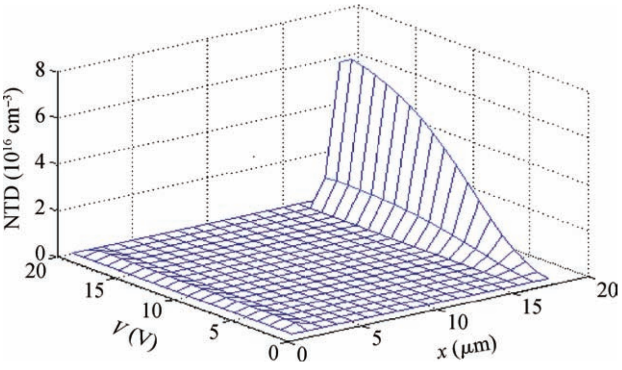

Fig. 6. Variation of the NTD according to the voltage of polarization.

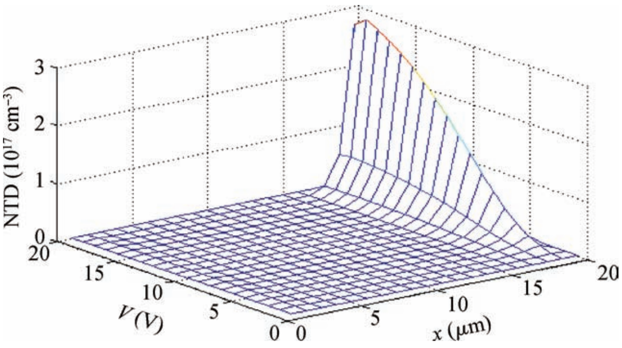

Fig. 7. Variation of the NTD according to the voltage of polarization.

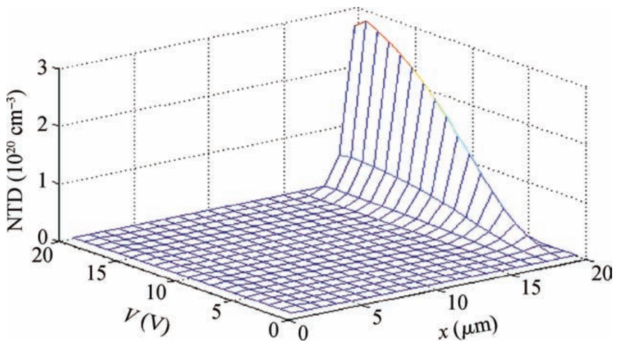

Fig. 8. Variation of the NTD according to the voltage of polarization.

The application of a forward bias voltage shows a reduction of the transistion region ZCE, and its variation depends on the deep trapping level $\Delta n_{\rm t}$. Because n-type semiconductors are always fully ionised, the second trap center has a negligible influence on the capture of carriers due to its low density. It can interfere in the recombination process because of its large capture coefficients due to its short lifetime ($\tau_{\rm nt}$ and $\tau_{\rm pt}$: 10^{-8} to 10^{-10} s). An increase of the density of electrons through the N^+ contact leads to an increase of $\Delta n_{\rm t}$ and consequently to an increase of the density of free holes through the P^+ contact leads to an increase of $\Delta p_{\rm t}$.

To achieve contact: one achieves a degenerated layer buffer (of 8×10^{16} to 3×10^{20} cm^{-3}). The ZCE of the gate formed between the layer buffer and the contact metal is so fine that the carriers can cross it by a tunnel effect. The contact is no longer a rectifier and the characteristic $I(V)$ is symmetrical.

The current through a metal–semiconductor junction is

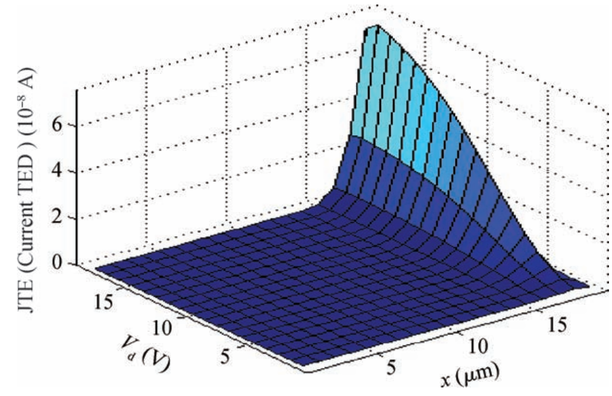

Fig. 9. Variation of the JTED current according to the voltage of polarization.

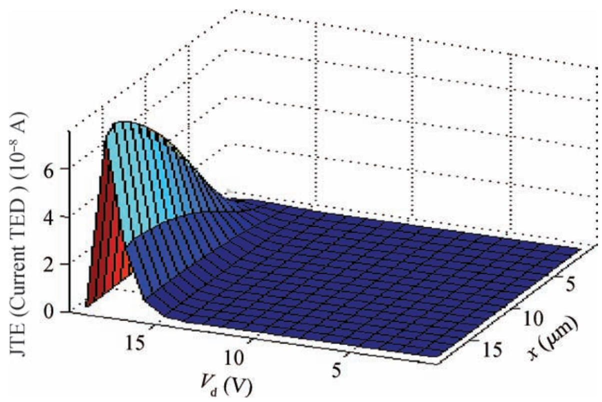

Fig. 10. Variation of the JTED current according to the voltage of polarization.

mainly due to majority carriers. Three distinctly different mechanisms exist in a Schottky diode: diffusion of the semiconductor carriers in metal, thermionic emission-diffusion (TED equation (6)) and a mechanical quantum that pierces a tunnel through the gate.

We conclude that the I–V characteristics of Schottky diodes are in the hypothesis of a parabolic summit of potential.

Two mechanisms can cause breakdown, namely avalanche multiplication or impact ionization of carriers in a high electric field. Neither of the two breakdown mechanisms is destructive. However heating is caused by the breakdown voltage and the diode may be destroyed unless sufficient heat sinking is provided. The breakdown in silicon can be predicted.

The introduction of deep centers in a semiconductor causes a disturbance of the characteristic $I(V)$.

The GaAs and its large concentration values of trap centers will participate in an increase in the process of thermionic electrons and holes, which will in turn act on the I–V characteristic of the diode, and it is the overflow maximum value [NT $= 3 \times 10^{20}$]. The characteristic $I(V)$ is shown in Figs. 9–11. One notices that the Jtunnel current varies between 1×10^{-13} and 5×10^{-13}. This range of variation is very small in relation to the one of JTED.

The current of thermionic emission-diffusion JTED is between 6×10^{-8} A and 5×10^{-13} A. The JTunnel current in

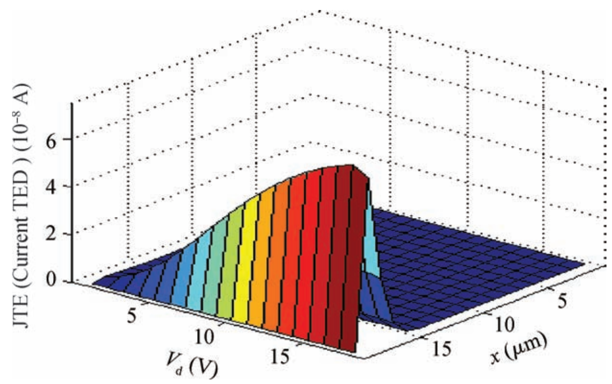

Fig. 11. Variation of the JTED current according to the voltage of polarization.

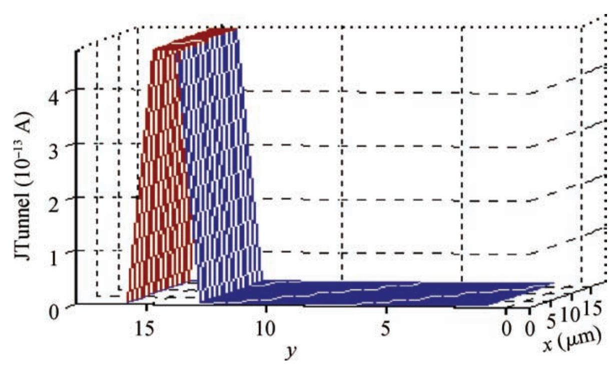

Fig. 12. Variation of the JTunnel current according to the tension of polarization.

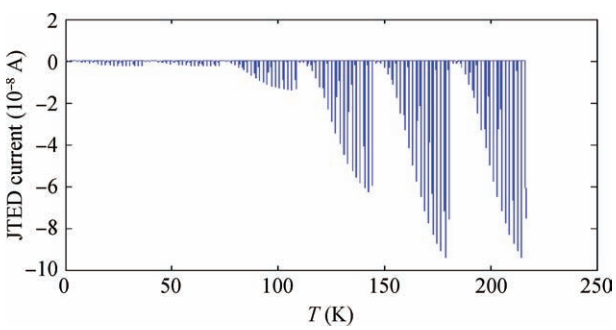

Fig. 13. Variation of the JTED current according to the temperature.

Fig. 12 (Eq. (9)) is inversely proportional to the density of trap centers, NT, whose values are located between 8×10^{16} and 3×10^{20} cm^{-3} and is going to influence the region of zone of desertion of carriers, act very quickly under the electric field effect. The electrons pulled out of the crystalline structure will be filled by other pairs of electron–holes created by the same phenomenon, this process repeats itself several times, until thermal saturation occurs, which leads to the straining of the diode.

The $\ln I$–V plots are generated at various temperatures and ideality factors, and are estimated by a (of 1 to 2) simulated fitting at all temperatures (50 to 250 K) in Fig. 13; this is the range of temperature that the thermionic emission-diffusion JTED current [of 6×10^{-8} A and 9.5×10^{-8} A] remained steady at for small values. Beyond this temperature, the current progresses in a brutal way until the Schottky diode are destroyed. Electron transport may occur via shallow traps, which are fewer in number, thus leading to relatively low ideality factor.

The interesting observation that the ideality factor increases above unity depending on decreasing temperature is almost identical to the reported variation of ideality factor obtained from the experimental data on MIS contacts[19, 20]. Thus, an increase in ideality factor with decreasing temperature is only possible if the interface state density is assumed to have inverse temperature dependence. Inverse temperature dependence implies that the interface states are effective at low temperature.

It can be further related to the available energy levels of the interface states. At higher energies there is a lower density of states, while at low energies more states are available.

Thus, more of the energy levels of the interface states will be at low energies. At low temperatures, electron transport may occur through deep level, trap states, whereas at high temperatures due to the high energies of electrons, shallow traps may participate in the conduction process at the interface.

Therefore, at low temperatures electron transport occurs via deep trap states, of which there are more, so the effective density of states is higher and hence the resulting ideality factor arising due to potential drop across the layer increases. On the other hand, at high temperatures electron transport may occur via shallow traps, which are fewer in number, thus leading to relatively low ideality factor. The similar inverse temperature dependence of interface state density derived from the experimental work on MIS Schottky diodes is also reported in Refs. [21–24]. The actual temperature dependence of interface state density at the MIS junction governs the rising trend of the ideality factor with decreasing temperature. The exact distribution of interface state density will shed more light on understanding the behaviour of MIS Schottky diodes, which requires more investigation and is open for future discussion.

3. Conclusions

The I–V characteristics of Schottky diodes with an interfacial insulator layer are studied by numerical simulation. The I–V data of the MIS Schottky diode are generated using the TED equation considering an interfacial layer parameter. The calculated I–V data are fitted into an ideal TED equation (6) to see the apparent effect of an interfacial layer on barrier parameters. It is shown that the mere presence of an interfacial layer at the MS interface makes the Schottky diode behave as an ideal diode of high apparent BH. The apparent BH is shown to decrease linearly with decreasing the temperature. However, the ideality factor and series resistance remain the same as that considered for a pure Schottky contact without an interfacial layer. It is shown that the bias coefficient of the tunneling barrier, however, increases the ideality factor, but makes the ideality factor decrease with decreasing temperature. It is considered that the potential drop across an interfacial layer also gives rise to high ideality factor, which remains constant at all temperatures. The inverse temperature dependence of interface states is suggested to be a possible reason for the increase in ideality factor with decreasing device temperature.

References

[1] Sze S M. Physics of semiconductor devices. 2nd ed. New York: Wiley, 1981

[2] Rhoderick E H, Williams R H. Metal–semiconductor contacts. 2nd ed. Clarendon Press, 1988

[3] Card H C, Rhoderick E H. Studies of tunnel MOS diodes I. Interface effects in silicon Schottky diodes. J Phys D, 1971, 4: 1589

[4] Turut A, Yalcin N, Saglam M. Metallic polythiophene/inorganic semiconductor Schottky diodes. Solid-State Electron, 1992, 35: 835

[5] Hackam R, Harrop P. Temperature dependence of the Schottky barrier height in gallium arsenide. Solid-State Commun, 1972, 11(5): 669

[6] Altindal S, Karadeniz S, Tugluoglu N, et al. The role of the interface insulator layer and interface states on the current-transport mechanism of Schottky diodes in wide temperature range. Solid-State Electron, 2003, 47: 1847

[7] Cova P, Singh A. Metallic polythiophene/inorganic semiconductor Schottky diodes. Solid-State Electron, 1990, 33: 11

[8] Chand S, Kumar J. Current transport in Pd_2Si/n-Si(100) Schottky barrier diodes at low temperatures. Appl Phys A, 1996, 63: 171

[9] Singh A, Reinhardt K C, Anderson W A. InP tunnel metal–insulator–semiconductor devices irradiated with 1 MeV electrons. J Appl Phys, 1990, 68: 3475

[10] Werner J H. Pressure dependences of silicide/silicon Schottky barrier heights. Appl Phys A, 1988, 47: 291

[11] Borrego, Guttmann R J. High barrier GaAs/metal Schottky junctions produced by electrochemical metal deposition. Solid-State Electron, 1979, 22: 621

[12] Chattopadhyay P, Daw A N. Energy distribution of interface state charge density in Cu-nSi Schottky diode with thin interfacial oxide layer. Solid-State Electron, 1986, 29: 555

[13] Hatori K, Torn Y. A new method to fabricate Au/n-type InP Schottky contacts with an interfacial layer. Solid-State Electron, 1991, 34(5): 527

[14] Dokme I, Altindal S. Temperature-dependent current–voltage characteristics of the Au/n-InP diodes with inhomogeneous Schottky barrier height. Semicond Sci Technol, 2006, 21: 1053

[15] Akkal B, Benamara Z, Bideux L, et al. Characterization of interface states at Au/InSb/InP(100) Schottky barrier diodes as a function of frequency. Microelectron J, 1999, 30: 673

[16] Cowley A M, Sze S M. Surface state and interface effects in Schottky barriers at n type silicon surfaces. J Appl Phys, 1965, 36: 3212

[17] Tseng H H, Wu C Y. Interpreting the nonideal reverse bias C–V characteristics and importance of the dependence of Schottky barrier height on applied voltage. Solid-State Electron, 1987, 30: 383

[18] Hudait M K, Kruppanidhi S B. The analysis of lateral distribution of barrier height in identically prepared Co/n-Si Schottky diodes. Solid-State Electron, 2000, 44: 1089

[19] Karatas S, Altindal S. Temperature dependence of barrier heights of Au/n-type GaAs Schottky diodes. Solid-State Electron, 2005, 49(6): 1052

[20] Karatas S, Altindal S. Temperature dependence of characteristic parameters of the Au/SnO_2/n-Si (MIS) Schottky diodes. Mater Sci Eng B, 2005, 122: 133

[21] Hudait M K, Kruppanidhi S B. The analysis of lateral distribution of barrier height in identically prepared Co/n-Si Schottky diodes. Solid-State Electron, 2000, 44: 1089

[22] Altindal S, Karadeniz S, Tugluoglu N, et al. Analysis of interface states and series resistance of MIS Schottky diodes using the current–voltage (I–V) characteristics. Microelectron Eng, 2008, 85(1): 233

[23] Dokme I, Altindal S. Simulation studies of current transport in-metal–insulator–semiconductor Schottky barrier diodes. Physica B, 2007, 390: 179

[24] Altindal S, Dokme I, Bulbul M M, et al. The distribution of barrier heights in MIS type Schottky diodes from current–voltage–temperature (I–V–T) measurements. Microelectron Eng, 2006, 83: 499