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Analytical Studies of Metal Insulator Semiconductor Schottky Barrier Diodes

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ABSTRACT

The current –voltage data of the metal –insulator semiconductor Schottky diode are simulated using thermionic emission diffusion equation taking into account the interfacial layer parameters. The computed current – voltage data are fitted into ideal thermionic emission diffusion equation to see the apparent effect of interfacial parameters on current transport.In presence of interfacial layer the Schottky contact behave as an ideal diode of apparently high barrier height. The behavior of apparent height and ideality factor with the presence of interfacial layer is discussed.

Key words: Interfacial parameters , Barrier height, Ideality factor.

INTRODUCTION

The metal–insulator–semiconductor (MIS) diode is themost useful device in the study of semiconductor surfaces.Since, the reliability and stability of all the semiconductordevices are intimately related to their surface conditions, anunderstanding of surface physics with the help ofMIS diodesis of great importance to device operation[1–6]. The barrierheight (BH) is an important parameter that determines theelectrical characteristics of metal–semiconductor (MS) contacts.Schottky BH is defined as the difference in the energybetween the metal Fermi level and band edge of thesemiconductor majority carriers at the junction for a metaland semiconductor in contacts[1–3]. In general, being aSchottky contact configuration, its performance and reliabilityis drastically determined by the interface qualitybetween the deposited metal and the semiconductor surface.It is well known that, unless specially fabricated, a Schottkybarrier diode posses a thin interfacial native oxide layerbetween metal and semiconductor. The existence of such aninsulating layer converts the MS device into a MIS deviceand has strong influence on its current–voltage (I–V)characteristics as well as the barrier parameters of Schottkydiode[3,7] There are several possible reasons of errorthat cause deviation of the ideal behaviour of Schottkydiodes with and without an interfacial insulator layer. Theseinclude the particular distribution of interface states[2,16],the series resistance[9,15,17], applied bias voltage[9,10,15,17,18] and device temperature[1,2,8–10]. In thispaper, we analyse effect of an interfacial layer on I–Vcharacteristics of Schottky diode using simulation studies.

BASIC THEORY

In the present paper, we consider a thermionic emission diffusion (TED) equation,the current through a Schottky diode as a function of applied voltage V is given by the expression[1–3]

$$I = AA^{*}T^{2}\exp\left(-\frac{q\phi_{b}}{kT}\right)\exp\left(\frac{qV}{\eta kT}\right)\left[1-\exp\left(-\frac{qV}{kT}\right)\right], \quad \ldots (1)$$

Where A is the diode area, A* the effective Richardsonconstant, q the electronic charge, k Boltzmann constant,T the absolute temperature, fb the BH at zero bias, Z is theideality factor which is measure of conformity of the

diodebehaviour to pure thermionic emission theory and is adimensionless factor introduced to account for deviationfrom TED theory. The deviation from pure thermionicemission may arise due to the presence of an interfacialinsulator layer between metal and semiconductor, surfacecharges and image force effects. For a Schottky diode withan interfacial insulator layer, Card and Rhoderick[2] reported that the relation between the applied bias V andcurrent I is same as Eq. (1), with an additional exponentialfactor dependent on interfacial layer parameter as given by

$$I = AA^{*}T^{2}\exp\left(-\frac{q\phi_{b}}{kT}\right)\exp(-a\sqrt{\chi}\delta)$$

$$\times\exp\left(\frac{qV}{\eta kT}\right)\left[1-\exp\left(-\frac{qV}{kT}\right)\right].$$

..(2)

The factor $(a\sqrt{c}d)$ is known as the electron tunnelingfactor, $a=(4\pi/h)(2m^{*})^{1/2}$ is a constant, m* = 0.067m_0 theeffective tunneling mass of electron, m_0 is the rest mass ofelectron, ^{c} is the mean tunneling barrier presented by thininterfacial layer which is expressed as energy differencebetween the conduction band edge of the semiconductorand that of the interfacial layer, ^{d} is the thickness of aninterfacial insulator layer.

The Eq. (2) is similar to standard thermionic emissionequation for Schottky diodes withexcept for the factorexp$(-a\sqrt{c}d)$, which is the tunneling probability and ischaracteristics of interfacial layer. Occurrence of exponentialfactor in the current equation yields the I–V curves ofdiode same as that of a diode without an interfacial layerbut shift the starting point of the I–V curves towards lowcurrent which corresponds to decreased value of thesaturation current and in turn give rise to high apparentBH. This apparent BH ^{f} , at temperature T, with aninterfacial insulator layer of thickness is given by

$$\phi_{ap}=\phi_{b}+\frac{akT\delta\sqrt{\chi}}{q}.$$

…(3)

If an interfacial layer is extremely thin, then exp is unity and BH of the diode remains unaltered by itspresence. In the usual analysis of the experimental orsimulated data of Schottky diode with an interfacial layerusing Eq. (2), the apparent BH and ideality factor aredetermined form the extrapolated current at zero bias andslope of the linear region of ln*I*–*V* curve, respectively,using fitting of *I*–*V* data into Eq. (1). The apparent BH andideality factor thus obtained, when analysed as a function of temperature reflects the effect of an interfacial layer onSchottky diode behaviour.Simulation of the *I*–*V* data of Schottky diodes with thepresence of an interfacial layer between the metal andsemiconductor has been performed by calculating the totalcurrent applying Newton–Raphson iteration method usingEq. (2). The *I*–*V* data thus obtained is fitted into ideal TEDEq. (1) to see the apparent effect of an interfacial layer onthe behaviour of diode parameters such as BH, idealityfactor and series resistance.

RESULTS AND DISCUSSION

Simulation of *I*–*V* data of Schottky diode with aninterfacial layer is performed for the Schottky diode areaA = 7.87 × 10^{-7} m^{-2}, corresponding to a 1mm diametermetal dot, effective Richardson constant A* = 1.12× 10^{6} Am^{-2} K^{-2} (for n-type silicon) and = 0.8V. Aninterfacial layer parameters taken for simulation of *I*–*V*data are = 0.58 eV and = 3 nm. These are typical valuesreported in the literature for experimentally fabricated MIScontacts [7,9,19,21]. The ln*(I)*–*V* plots thus obtained atvarious temperature are shown in Fig. 1. From Fig. 1 it isclear that behaviour of ln(I)–V curves is almost same asthat of a Schottky diode without an interfacial layer[20].These curves are linear over several orders of current atlower temperatures. To see the effect of an interfacial layeron barrier parameters the I–V data shown in Fig. 1 are fitted into Eq. (1) using least square method to deriveapparent BH, ideality factor and series resistance. Fig. 2shows the apparent BH obtained from the simulated dataat various temperatures. It is evident from Fig. 3that theapparent BH of Schottky diode with an interfacial layerincreases above the value of BH of pure MS contact.However, the ideality factor of the diodes, not shown here,remains unity at all temperatures. As shown in Fig. 4theapparent BH of MIS Schottky diode decreases linearlywith decreasing temperature and is consistent with Eq. (3).This clearly indicates that at a given temperature merepresence of an interfacial insulator layer yields increasedapparent BH, which decreases linearly

withdecrease intemperature, while the ideality factor of the diode remainsunity.

The interesting observation here is that presence of aninterfacial layer makes BH increase from its value (0.8 eV,here) that exists for a pure intimate MS contact without aninterfacial layer. At any temperature the BH increases byan amount $(\alpha K_i d\sqrt{c/q})$and obviously depends linearly ontemperature. The increase in value of apparent BH of MIScontact is more at room temperature and it approachesvalue of pure MS contact at 0K. This behaviour ofapparent BH with decreasing *T* is slightly different fromthe observed behaviour of experimentally fabricated MIScontacts[9,13,22,23]. In this paper, the apparent BH isshown to decrease linearly with decrease in temperature but the overall BH remains lower than BH of correspondingMS contact. The similarity in the results reported fromexperimental work and in our calculation is that BHdecreases linearly with decrease in temperature. However,the experimentally observed BH values varies over low BHrange than those shown in Fig. 2 obtained by numericalsimulation using the proposed theory of current conductionin Schottky diodes with an interfacial layer[7,9,22–27]. Similar linear decrease of BH with decreasing temperatureis also reported for Schottky diodes with inversely dopedsurface layer and the apparent BH is smaller than the BHconsidered for pure MS system[28].

There are other reports on current transport studies ofSchottky diodes with an interfacial layer[7,19]. Thevariation of BH as a function of T reported in thesestudies is non-linear and is inconsistent with the currenttransport theory of a Schottky contacts with an interfaciallayer[7,22–26]. The results reported on Schottky contactswith intentionally grown interfacial layer shows very smallincrease in BH of MIS diode as compared to the measuredBH of pure Schottky diode without an interfacial layer[20,21].Theseexperimental observations on high BH ofSchottky diode with an interfaciallayer are consistent withEq. (3).

The *I–V* data of Schottky diodes with differentinterfacial layer thickness and mean tunneling barrier χ were generated. The behaviour of the ln*(I)–V* plots fordifferent thickness and mean tunneling barrier is almost thesame. The apparent BH increases with increasing interfaciallayer thickness and mean tunneling barrier. Thecurrent depends on the tunneling probability $\exp(-\alpha\sqrt{\chi}d)$

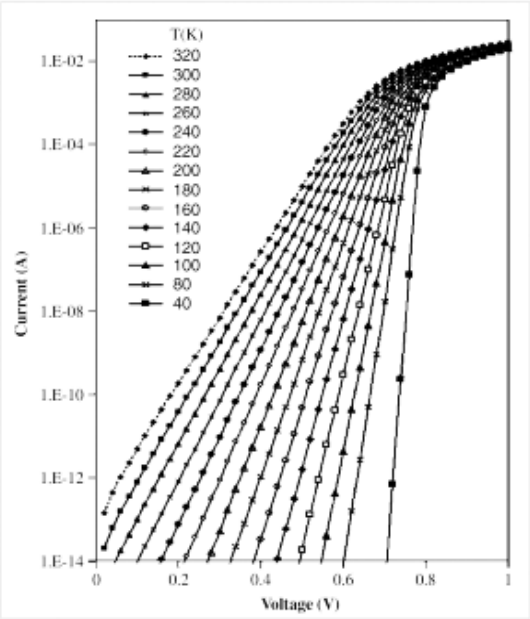

Fig. 1: Simulated *I–V* curves of a Schottky diode of BH, 0.8 eV with aninterfacial layer of thickness 3 nm and mean tunneling barrier of 0.58 eV,at various temperatures

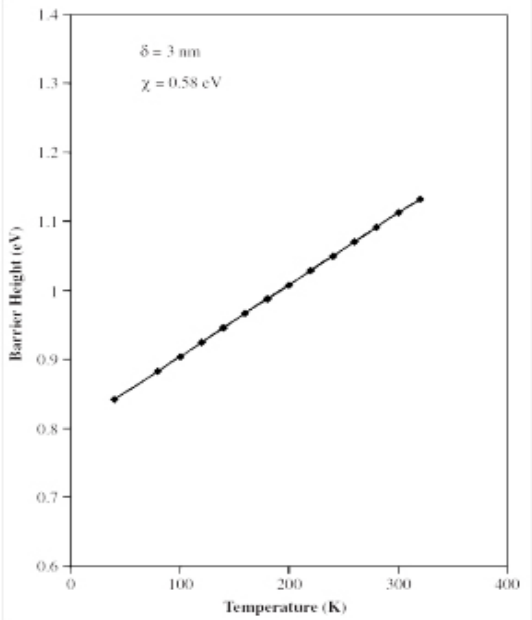

Fig. 2: Variation of apparent barrier height with temperature derivedfrom simulated *I–V* curves of Fig. 1

through an interfacial layer, because of which the currentdecrease with increasing interfacial layer thickness or meantunneling barrier and subsequently, the apparent BHincreases. Figs. 3 and 4 shows the apparent BH as obtainedfrom the simulated curves at different temperatures forvarious values of interfacial layer thickness and effectivemean tunneling BH, respectively. From these

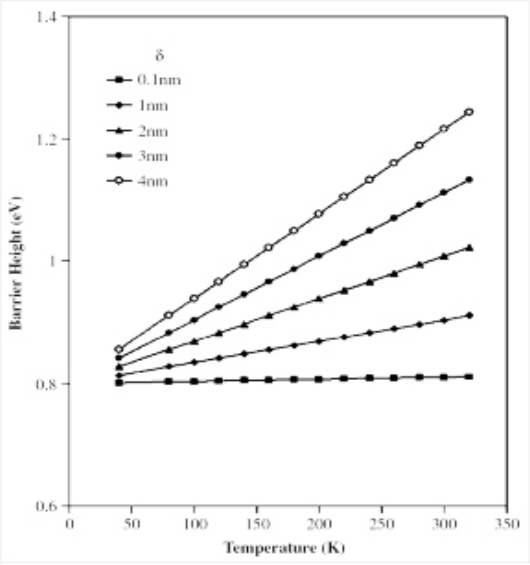

Fig. 3: Variation of apparent barrier height with temperature for variousinterfacial layer thicknesses and mean tunneling barrier of 0.58 eV.

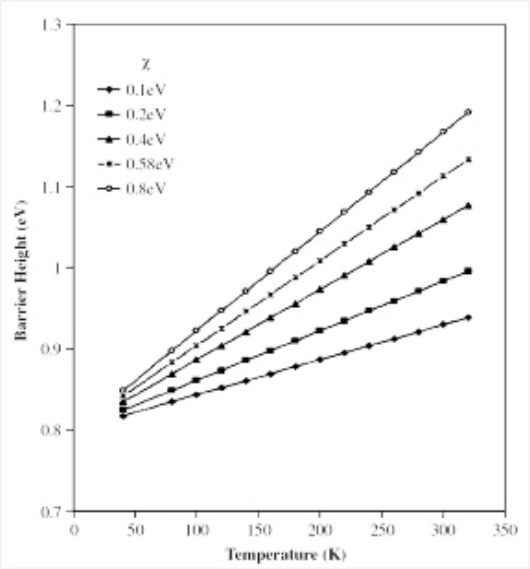

Fig. 4: Variation of apparent barrier height with temperature for variousmean tunneling barrier and interfacial layer thickness of 3 nm.

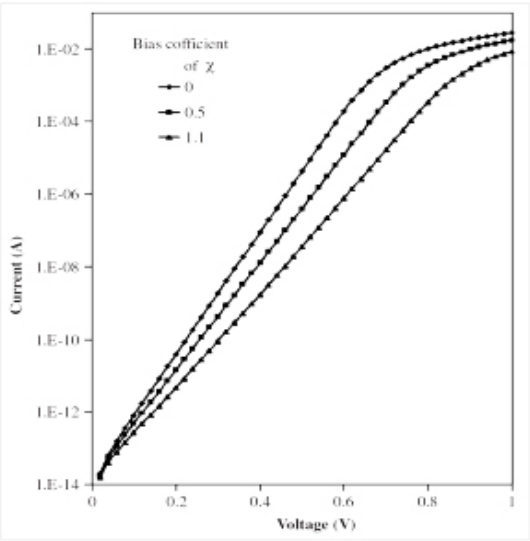

Fig. 5: *I–V* plots of MIS Schottky diode with bias coefficients of meantunneling barrier C as 0, 0.5 and 1.1. The corresponding values of idealityfactor for these bias coefficients are 1, 1.12 and 1.28, respectively.

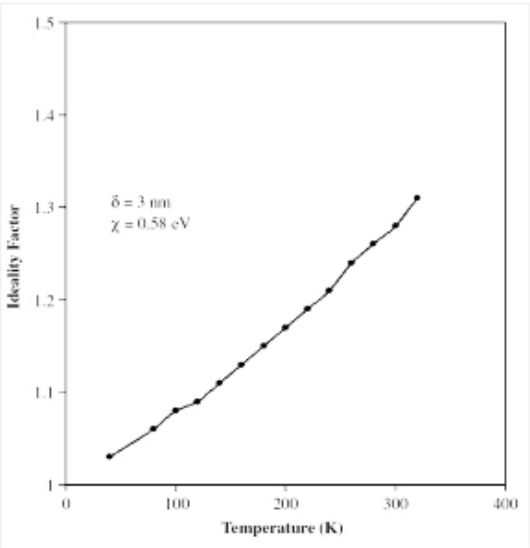

Fig. 6: Variation of ideality factor with temperature for bias coefficient of C equal to 1.1. It depicts that the ideality factor decreases almost linearlywith decreasing temperature.

figures, it isevident that increase in mean tunneling barrier or aninterfacial layer thickness makes the apparent BH increase.

It is obvious from the results obtained from thesimulated *I–V* data of a Schottky diode with an interfaciallayer that the value of ideality factor remain unity at alltemperatures. However, the experimental data reported inthe literature yields ln*(I)–V* plots having greater than unityideality factor [19,22,23,24]. Moreover, the reportedideality factor is temperature dependent. In order to havegreater than unity ideality factor from the simulatedcurrent–voltage data, we undertake the following analysis.

It is well established that BH is considered to be biasdependent, which give rise to high ideality factor inSchottky diodes[1,2]. In case of MIS contact meantunneling BH, $\bar{\chi}_c$ is a similar parameter which governs thecurrent transport across the diode according to Eq. (2). Asthe BH varies with applied bias, correspondingly the meantunneling barrier $\bar{\chi}_c$ should also be a function of bias.Therefore, we assume bias dependence of mean tunnelingbarrier and generate the ln(I)–V plots of the MIS contact. Fig. 5 shows the ln(I)–V plots of MIS contacts with

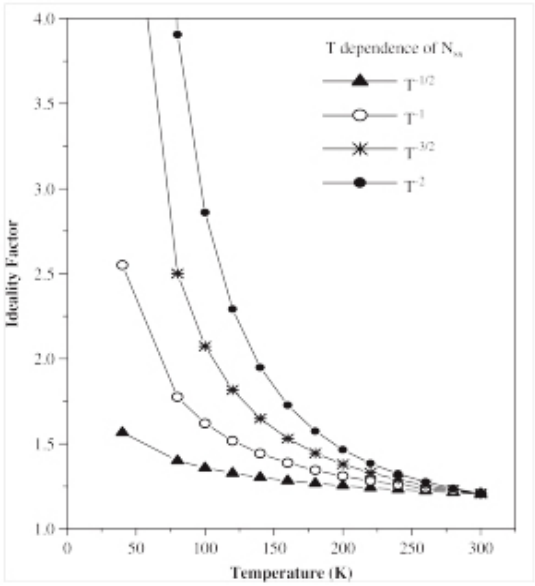

Fig. 7: Variation of ideality factor of MIS Schottky diodes withtemperature. Note different rising trend of ideality factors for differenttemperature dependence of interface state density

andwithout bias dependence of mean tunneling barrier $\bar{\chi}_c$.

It is clear from Fig. 5 that ln(I)–V plots with bias dependent $\bar{\chi}_c$ exhibit ideal shapes with less slopes and hence high idealityfactor. The least square fitting programme is used toextract BH, Z and RS. From the ln(I)–V curves with biasdependence of $\bar{\chi}_c$, it is observed that the value of BH and RSremains same as obtained from the curves withoutconsidering bias dependence of $\bar{\chi}_c$. The derived idealityfactor as a function of temperature is shown in Fig. 6. It isclear from Fig. 6 that the bias dependence of $\bar{\chi}_c$ gives rise tohigh ideality factor. However, the ideality factor decreaseswith decreasing temperatures. The experimental resultsreported in literature shows that ideality factor of MISdiodes increases with decreasing temperature, whereas theI–V data obtained by simulation using bias dependence of $\bar{\chi}_c$ yields linearly decreasing ideality factor with decreasingtemperature. Thus, the simulation result shows that thebias dependence of tunneling BH cannot account for highideality factor of MIS Schottky diode and consequently thetemperature dependence of ideality factor.

Potential drop across an interfacial layer is another causewidely cited in the literature, which is believed to give riseto high ideality factor in MIS diodes[3,5,9,23,24]. Wefurther simulated the I–V data of a MIS diode taking intoaccount potential drop across an interfacial layer. The dropacross an interfacial layer is modeled during numericalsimulation for generating I–V data of a MIS diode usingEq. (2). The forward voltage V applied across the devicepartially appears across the series resistance as IR_S, $V_i$across an interfacial layer and V_S across the device/ diodeand can be expressed as[23,24]

$$V = V_S + V_i + IR_S. \quad \ldots(4)$$

The voltage across an interfacial layer V_i is given by [23]

$$V_i = \frac{qN_{SS}\delta}{\varepsilon_i} V_S. \quad \ldots(5)$$

From Eqs. (4) and (5), the voltage across an interfaciallayer is given by

$$V_{\mathrm{i}} = \left(\frac{qN_{\mathrm{SS}}\delta}{\varepsilon_{\mathrm{i}} + qN_{\mathrm{SS}}\delta}\right)(V - IR_{\mathrm{S}}) \quad \ldots(6)$$

and the actual voltage that appears across the diode whichgoverns current flow through it, is given as

$$V_{\mathrm{S}} = \left(\frac{\varepsilon_{\mathrm{i}}}{\varepsilon_{\mathrm{i}} + qN_{\mathrm{SS}}\delta}\right)(V - IR_{\mathrm{S}}). \quad \ldots(7)$$

Thus, considering potential drop across an interfaciallayer, the voltage that actually appears across the device isless than the applied bias as given by Eq. (7). Clearly thisvoltage is function of interfacial layer thickness 'd',interface state density 'N_{ss}' and interfacial layer permittivity e_i. The ln*(I)–V* plots of MIS contact are simulated takinginto account the voltage drop across an interfacial layer.The ln*(I)–V* plots (not shown here), obtained by consideringvoltage drop across an interfacial layer exhibits lesserslope and thus correspond to high ideality factor. Theln*(I)–V* plots are generated at various temperatures andideality factor was estimated by fitting of simulated datainto Eq. (1) at all temperatures. The interesting observationis that the ideality factor increase above unity depending on the values of e_i, d and N_{ss} and attains same value at alltemperatures. As an example for $e_i = 7 \times e_o$, $d = 3$ nm and$N_{ss} = 4.0 \times 10^{16}$ eV^{-1} cm^{-2}, ideality factor attain value 1.30at all temperature. It is obvious from Eq. (7) that theideality factor is reciprocal of the factor $(e_i / (e_i + qN_{ss}d))$,which gives rise to voltage drop across an interfacial layer. Since, this factor does not contain temperature termtherefore ideality factor remains same when I–V data iscalculated at various temperatures. As the ideality factor isbelieved to be arising due to the voltage drop across aninterfacial layer, it will exhibit temperature dependenceonly if any of the factor in this expression is temperaturedependent. We have investigated this expression and are ofthe opinion that the parameter, which can be temperaturedependent is the interface state density 'N_{ss}'. So far, insimulating I–V data 'N_{ss}' is assumed to have constant valueand thus ideality factor remains constant at all temperatures.For ideality factor to vary with temperature theinterface state density must exhibit temperature dependence.Like the density of states in energy bands in solidhas $T^{3/2}$ dependence, we assume same temperaturedependence of interface state density 'N_{ss}'. The I–V dataof MIS Schottky diode thus generated at various temperaturesyield decreasing h with lowering temperature. Inorder to have high h at low temperatures N_{ss} should exhibitinverse temperature dependence. Thus, we assume inversetemperature dependence of 'N_{ss}' and simulated ln(I)–Vplots for different exponents of T.Fig. 7 shows variation inZ as a function of temperature for various exponent of T.Interestingly, the observed increase in ideality factor with decreasing temperature is almost identical to reportedvariation of ideality factor obtained from the experimentaldata on MIS contacts[12,13]. Thus, increase in idealityfactor with decreasing temperature is only possible if theinterface state density is assumed to have inverse temperaturedependence.

Inverse temperature dependence impliesthat more interface states are effective at low temperature.It can be further related to the available energy levels ofinterface states. At higher energies there is less density ofstates, while at low energies more states are available. Thus, more energy levels of interface states will be at lowenergies. At low temperature electron transport may occurthrough deep level, traps/states, whereas at high temperaturedue to high energies of electrons, shallow traps/statesmay participate in conduction process at the interface.Therefore, at low temperature electron transport occur viadeep traps/states, which are more, so effective density ofstates is more and hence the resulting ideality factor arisingdue to potential drop across the layer increases. On theother hand, at high temperature electron transport mayoccur via shallow traps/states, which are less in number,thus leading to relatively low ideality factor. The similarinverse temperature dependence of interface state densityderived from the experimental work on MIS Schottkydiodes is also reported in the literature[7,9,13,28]. Theactual temperature dependence of interface state density atthe MIS junction will governs the rising trend of idealityfactor with decreasing temperature. Exact distribution ofinterface state density will shed more light on understandingthe behaviour of MIS Schottky diodes, whichrequires more investigation and is open for futurediscussion.

CONCLUSION

The I–V characteristics of Schottky diodes with aninterfacial insulator layer are studied by numerical simulation.The I–V data of the MIS Schottky diode aregenerated using TED equation considering an interfaciallayer parameters. The calculated I–V data are fitted intoideal TED equation to see the apparent effect of aninterfacial layer on barrier parameters. It is shown thatmere presence of an interfacial layer at the MS interfacemakes Schottky diode behave as an ideal diode of highapparent BH. The apparent BH is shown to decreaselinearly with decreasing the temperature. However, theideality factor and series resistance remains same asconsidered for a pure Schottky contact without aninterfacial layer. It is shown that bias coefficient of meantunneling barrier, however, increases the ideality factor, but makes ideality factor decrease with decreasing temperature.Considering the potential drop across an interfaciallayer also give rise to high ideality factor, whichremains constant at all temperatures. The inverse temperaturedependence of interface states is suggested to be thepossible reason for causing increase in ideality factor withdecreasing device temperature.

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