Phonon-assisted tunneling in reverse biased Schottky diodes

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Reverse current–temperature (I_Γ/T) characteristics of Al–GaAs Schottky diodes with oxidized interfaces are measured in the temperature region of 250–400 K at various reverse bias voltage in order to elucidate a mechanism of carrier transport through the barrier. The I_Γ/T dependencies are explained on the basis of phonon-assisted electrons tunneling from interface states to the semiconductor model. The barrier height, evaluated from the I_Γ/T characteristics (activation energy) which depends on the applied voltage and temperature, is discussed. It is shown that these dependencies are due to the above-mentioned carrier transport through the Schottky barrier mechanism. The important of the phonon-assisted tunneling process on the current transport in the diodes is emphasized. © *1999 American Institute of Physics.* [S0021-8979(99)00824-5]

I. INTRODUCTION

It is well known that the current/voltage (I/V) characteristics of the Schottky barrier diodes cannot be described by the theory of the ideal metal-semiconductor contact. In the case of a moderately doped semiconductor, the current density under forward bias voltage V is given within the thermionic emission theory[1] as:

$$j=j_0(e^{qV/nkT}-1), \tag{1a}$$

where

$$j_0=A^*T^2e^{-q\Phi_{BO}/kT}. \tag{1b}$$

Here A^*, T, q, k, and Φ_{BO} are the effective Richardson constant, temperature, electronic charge, Boltzmann constant, and Schottky barrier height (SBH), respectively, and n is the ideality factor which describes the deviation of practical diodes from the pure thermionic-emission model characterized by $n=1$. The zero bias SBH Φ_{BO} is derivable from the density j_0 of the saturation current $I_0=j_0S$, where S the contact area, with the help of a semilogarithmic current/voltage plot by extrapolating the I/V curve from a regime $qV/nkT>1$ toward $V=0$.

A so-called Richardson plot of $\ln(j_0/A^*T^2)$ versus inverse temperature $1/T$ is often used to determine the SBH from the slope of the thermally activated behavior. According to Eq. (1b), one obtains:

$$\ln(j_0/A^*T^2)=-\frac{q\Phi_{BO}}{kT}, \tag{2}$$

and the plot of $\ln(j_0/A^*T^2)$ vs $1/T$ should yield a straight line with an activation energy $E_{act}=-q\Phi_{BO}$ if the SBH Φ_{BO} is independent of temperature. But in most cases these plots do not yield straight lines.[2–5] The curving in these plots is due to the temperature dependencies Φ_{BO} and n.

Temperature dependencies Φ_{BO} and n have been observed by many authors for a great variety of semiconductors and contacts.[2,3,6–9] Several authors remarked that SBH determined from capacitance/voltage (C/V) measurements was different from the one obtained from I/V measurements within the thermionic emission model.[3,7–9] For example, in measurements performed for Au/n-Si both the internal photoemission and the C/V showed a negative temperature dependence of the SBH, but the barrier height obtained from the I/V measurements strongly decreased from about 0.80 V at 300 K to 0.2 V at 7 K.[8] Levine[10] suggested that both Φ_{BO} and n should depend on a bias voltage. Actually, a strong decrease in the SBH with the increase of bias voltage was observed in Refs. 9,11–13. The apparent changes of the SBH from current–voltage/temperature ($I-V/T$) measurements with temperature and applied bias voltage can be quantitatively explained by neither the thermionic nor thermionic-field emission (TFE) theories. Therefore, to explain the dependence of the SBH on temperature and applied bias voltage, an additional carrier transport mechanism such as tunneling through the barrier[13,14] and carrier recombination processes in the depletion region were considered.[8,15] Nonideal I/Vcharacteristics of Si and GaAs Schottky barriers in Refs. 11,12, and 16 were attributed to changes in electron population of the interface states under applied bias voltage and accompanying change in barrier height. But contrary to this interfacial layer model,[12] the paper[9] points to the fact with references to Au/p-InP type diodes, that the charge trapped in the states of the interface layer is independent of reverse bias voltage in the range of 0–4 V, the SBH being strongly dependent on temperature and bias voltage for such diodes.

Recent models[3–5,7,17–20] explain the curvature of the Richardson plots and temperature dependent ideality factor n obtained from $I-V/T$ measurements by involving spatially inhomogeneous Schottky barriers. The nonideality according to this model is the result of the deformation of the spatial barrier distribution when a bias voltage is applied.[3] The main peculiarities of I/V characteristics measured in a wide temperature region for Al/n-GaAs[21] and Al/n-GaP[22] diodes have been explained by involving the phonon-assisted-tunneling processes[23,24] as a main carrier transport through the barrier mechanism.

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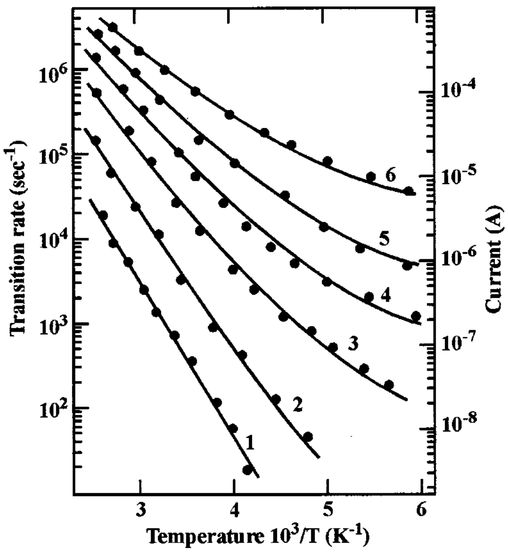

FIG. 1. Reverse current-temperature characteristics for the Al/n-GaAs Schottky diode (sample A) at different reverse bias voltages (closed circles) fitted with the theoretical $\ln W$ vs $1/T$ dependencies computed for $\Delta = 0.5$ eV, $m^* = 0.068 m_e$, $\hbar\omega = 36$ meV, $a = 6$ (solid lines). Voltage values for experimental data (1) 0.1, (2) 0.5, (3) 2, (4) 4, (5) 6, and (6) 8 V. Electric field F for theoretical curves (1) 13, (2) 20, (3) 26, (4) 29, (5) 32, and (6) 36 MV/m.

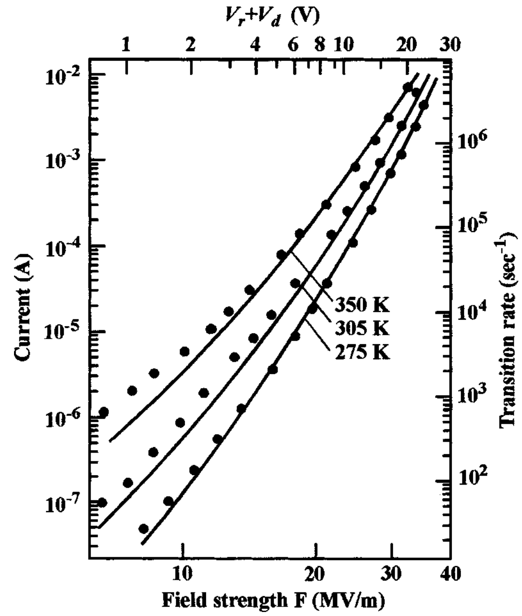

FIG. 2. The fit of current I dependencies on reverse bias voltages ($V_r + V_d$) at different temperatures (closed circles) with the computed transition rate $W(F)$ dependencies (solid lines) at different temperatures. The fitting parameters are the same as in Fig. 1.

In this article, we would like to show that the apparent SBH value dependence on applied voltage and temperature obtained from $I-V/T$ measurements may be caused by the peculiarities of the phonon-assisted tunneling mechanism which yield a current flow through a barrier. This proposition is confirmed: (i) by fitting the reverse current temperature dependence measured in Al/n-GaAs diodes at various voltages with an electron tunneling through the barrier rate W dependence on temperature computed for various field strengths; and (ii) by comparison of the apparent barrier height (energy activation) obtained from I/T characteristics for several Schottky junctions, not only own measurements but also previously published data for Schottky diodes on α-Si:H[11] and $CrSi_2$:Si[25] with a slope of the theoretical curves $\ln W(F,T)$ vs $1/T$ (theoretical ''energy activation'' E_{act}) dependence on field strength.

II. EXPERIMENTAL RESULTS AND COMPARISON WITH THEORY

The Schottky diodes were fabricated on a (100) GaAS n-type wafers with carrier concentration 5×10^{15} cm^{-3}. Two kinds of Schottky diodes were prepared. The surface of sample A was thermally oxidized at 500 °C for 10 min in a dry oxygen atmosphere, then Al was evaporated ($\phi = 0.8$ mm) as the Schottky contact. Sample B was prepared by evaporation of the Al electrode onto the surface without thermic treatment. Temperature dependent measurements were accomplished in darkness in a cryostat which was able to change the temperature from 100 to about 400 K.

The points in Fig. 1 represent a typical dependence of reverse current I_r on temperature obtained at various bias voltages V_r for such diode. It is seen that with increasing V_r the $\ln I_r$ vs $1/T$ curves become more curved and the linear region is less pronounced. With the increase of V_r, the curve slope is found to decrease and the bowing of curves is observed at lower temperatures. In Fig. 2 the $I(V)$ characteristics obtained at various temperatures are presented.

In the case of reverse bias voltage when $(qV/kT) \gg 1$ for the current density j_r from Eq. (1b) one obtains

$$j_r = A^* T_2 \exp(-q\Phi_{br}/kT). \tag{3}$$

The apparent SBH ϕ_{br} calculated from the gradient the Richardson plot lines will be lower due to lowering of the barrier height caused by image force. However, the experiment obtained a decrease in barrier height with an increase in the bias voltage larger than predicted by inclusion of the image-force lowering. This fact has been pointed out elsewhere.[3,9,13]

The $\ln I_r$ vs $1/T$ dependencies, exposed in Fig. 1 can be explained on the assumption that the main current transport mechanism is the phonon-assisted-electron tunneling from the states in the interface through the barrier. The electron population in the interface states is assumed to be independent of bias voltage due to the continuous filling of interface states from the Al electrode.

Under these conditions the reverse current density will be equal to $j_r = qN_S W$, where q is the electron charge, N_S is the electron density in the interface states, and W is the electron tunneling rate from these states, which is a function of field strength F and temperature T. Thus, $j_r \approx W(F,T)$ and we can fit the current dependencies obtained by measurements with the theoretical tunnel transition through the barrier rate dependencies on temperature. Computation of $W(F,T)$ was carried out using the multiphonon tunneling in an electric field theory[23] (see Appendix).

The total tunneling rate $W(F,T)$ through the Δ height barrier computed according to Eq. (A1) in the Appendix is the sum of contributions from the processes with participations of K phonon with K ranging from zero to $S_m \leqslant \Delta/\hbar\omega$. For the phonon energy $\hbar\omega$ the energy of LO phonon in GaAs was taken. The value of the electron-phonon coupling constant a was chosen so as to get the best fit on the assumption that the field strength at the junction is proportional to $\sqrt{V_r}$. The theoretical $\ln W$ vs $1/T$ dependencies computed for the various field strengths F are represented in Fig. 1 by solid lines. From Fig. 1 we can see that the theoretical $\ln W(T)$ vs $1/T$ curves mirror well the $\ln j_r$ vs $1/T$ dependencies. As seen from Fig. 2 a good fit of the theoretical $\ln W$ vs V_r dependencies with the $I(V)$ characteristics is obtained as well. From the measured current density j_r and calculated tunneling rate W, the electron density in interface states N_S can be determined. From the results presented in Fig. 1 or 2, N_S is equal to about $\cong 10^{12}$ cm^{-2}.

The fact that the $\ln W(F,T)$ vs $1/T$ dependencies are not linear at higher field strengths explains the apparent SBH as obtained from $I-V/T$ characteristics depends on temperature. Only at low field strength are these dependencies straight lines and only in this case is the simple TE valid. The decrease in slope of $\ln W(F,T)$ curves with an increasing field strength in our model yields a diminution in the apparent barrier height with applied voltage. The phonon-assisted theory predicts the same value of decrease in Φ_{br} as obtained from $I-V/T$ characteristics. The correctness of this assertion is evident from the good fit of theoretical curves with experimental data represented in Fig. 1 and should be confirmed once again by the comparison of the activation energy calculated from the gradient of theoretical lines as in Fig. 1. E_t with the activation energy E_{ex} is determined from the experimental ones. The activation energies were determined at higher temperature range where these dependencies are linear.

The dependencies of the energy activation E_t on field strength and experimental values of E_{ex} on voltage calculated from the lines in Fig. 1, are shown in Fig. 3. It is worth mentioning that the fast decrease in E_t with a field strength increase occurs only in a high field region. The similar decrease of effective barrier height (energy activation) with an increase in reverse bias voltage has been obtained elsewhere.[11,13] In Fig. 4 the reverse bias dependencies of the activation energy for Schottky diodes on α-Si:H,[11] and $CrSi_2$:Si[13] are fitted with theoretical E_t dependencies on field strengths.

III. DISCUSSION AND CONCLUSION

Theoretical $W(F,T)$ dependencies exhibit the peculiarities: strong temperature dependence in the lower field strength region and a decrease in energy activation with a field strength increasing—typical to experimental $I-V/T$ characteristics as well. In our model a strong temperature dependence of the apparent barrier height Φ_{br} as obtained from $I-V/T$ characteristics is explained by the peculiarities of the phonon-assisted tunneling which is revealed in nonlinearity of $\ln W$ vs $1/T$ curves and dependence of the energy activation on field strength. This nonlinearity implicates a temperature dependence of apparent SBH as measured from

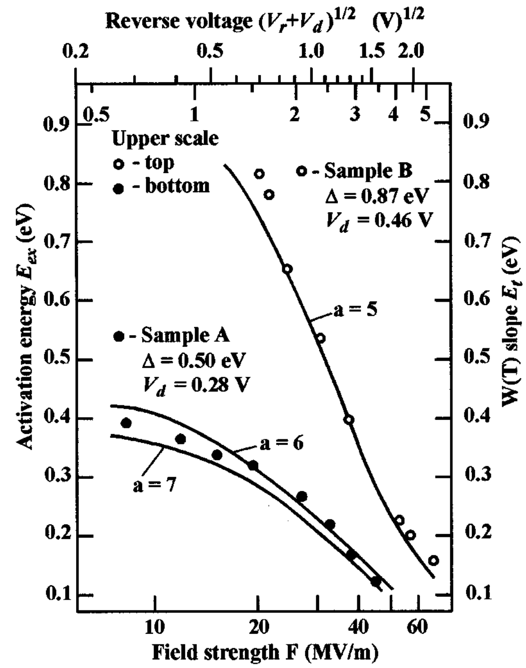

FIG. 3. Reverse voltage dependence of the activation energy E_{ex} evaluated from I/T characteristics as presented in Fig. 1 for sample A (closed circles) and the same dependence for sample B (open circles), respectively, fitted with a slope of the theoretical curves E_t dependence on field strength F (solid line). The upper scale indicates $\sqrt{V+V_d}$, where V_d diffusion potential: 0.28 V for sample A and 0.46 V for sample B.

$I-V/T$ characteristics. In reality, the "activation energy" of the tunneling process can be expressed roughly as $E_t = P\hbar\omega$, where P is an average number of phonons participating in the phonon-assisted tunneling process, which at low field strength is equal to $S_{max} = \Delta/\hbar\omega$ and thus $E_t = S_m\hbar\omega$ equals real barrier height (the case when the TE theory is valid). When the temperature decreases the number of phonons interacted with a center decreases according to Planck's law as a result of this is diminution in activation energy E_t and at the same time a decrease in measured Φ_{br}.

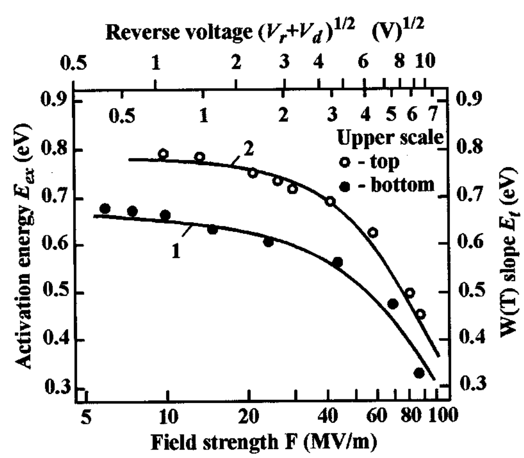

FIG. 4. The same dependencies as in Fig. 3 for α-Si:H Schottky diode from data Fig. 9 in Ref. 11 (closed circles); and for $CrSi_2$:Si diodes from Fig. 5 in Ref. 13 (open circles); solid lines - field strength F dependence of the slope E_t. $W(T)$ curves computed for the parameters $\Delta = 0.70$ eV (curve 1) and $\Delta = 0.80$ eV (curve 2), $m^* = 0.328 m_e$, $\hbar\omega = 52$ meV, and $a = 6$.

It is also evident from the phonon-assisted theory that at a higher field the phonon assistance in tunneling is less efficient and this is why the energy activation/barrier height decreases with increasing field strength.

Therefore, one can imagine that the tunneling of electrons from the interface states the semiconductor occurs through the barrier whose height in a complicated way depends on temperature and field strength.

In conclusion, the phonon-assisted-tunneling processes which were proved to be efficient in describing some electroluminescence phenomena in phosphors[24] or center ionization in semiconductors[25] seems to be applicable to the Schottky junctions. Assuming the domination of current flow by phonon-assisted-tunneling electrons from states in an interface allows to explain the temperature and voltage dependence of SBH evaluated from $I-V/T$ measurements (the problem of the curved behavior of Richardson plots falls away as well). The analysis of the influence phonon-assisted-tunneling processes on current flow through the barrier is carried out in this article for the reverse bias case only. Undoubtedly, including this mechanism carrier flow through the barrier injection may be fruitful in resolving similar problems in the forward-bias case as well.

APPENDIX: EXPRESSION FOR PHONON-ASSISTED TUNNELING RATE (REF. 23)

Center-to-band transition rate W as the function of temperature T and electric field F is given by

$$\begin{aligned} W(T,F) &= \exp[-a(2n+1)] \\ &\times \sum_{S=0}^{S_m} \sum_{K=0}^{K=S} \frac{eFa^S(n+1)^K n^{S-K}}{2\{2m^*[\Delta-\hbar\omega(S-2K)]\}^{1/2} K!(S-K)!} \\ &\times \exp\left(\frac{4\sqrt{2m^*}}{3e\hbar F}[\Delta-\hbar\omega(S-2K)]^{3/2}\right) \\ &\times (1-\zeta e^{\zeta^2}[1-\psi(\zeta)]\sqrt{\pi})^2, \end{aligned} \tag{A1}$$

where

$$\zeta = \frac{1}{2}\frac{\hbar\omega(S-2K)^4\sqrt{2m^*}}{\sqrt{e\hbar F}\sqrt[4]{\Delta+\hbar\omega(S-2K)}}. \tag{A2}$$

$\psi(\zeta)$ is the error integral, $n=[\exp(\hbar\omega/kT)-1]^{-1}$, $\hbar\omega$ is the energy of participating in the tunneling process phonon, a is the strength of the electron-phonon interaction, m^* is the electron effective mass, and Δ is the center depth (barrier height).

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