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On the existence of a distribution of barrier heights in Pd_2Si/Si Schottky diodes

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The current–voltage characteristics of Pd_2Si based Schottky diodes on both n- and p-type silicon measured over a wide temperature range (52–295 K) have been interpreted on the basis of thermionic emission-diffusion mechanism and the assumption of a Gaussian distribution of barrier heights. It is shown that while the occurrence of a distribution of barrier heights is responsible for the apparent decrease of the zero-bias barrier height (ϕ_{b0}) and nonlinearity in the activation energy plot, the voltage dependence of the standard deviation causes the unusual increase of ideality factor (η) at low temperatures. Also, it is demonstrated that the forward bias shifts the mean barrier height towards the higher side and causes narrowing of the distribution as well. A simple method, involving the use of ϕ_{b0} vs $1/T$ data, is suggested to gather evidence for the occurrence of a Gaussian distribution of barrier heights and obtain values of mean barrier height and standard deviation. The experimental results correspond to a mean barrier height of 0.80 V, standard deviation 0.05 V, and ideality factor 1.21 for Pd_2Si based Schottky barriers on n-type silicon; these values for p-type silicon are 0.38 V, 0.03 V, and 1.07, respectively. © *1996 American Institute of Physics.* [S0021-8979(96)02312-2]

I. INTRODUCTION

The analysis of the current–voltage ($I-V$) characteristics of Schottky barriers on the basis of thermionic emission-diffusion (TED) theory usually reveals an abnormal decrease of the barrier height and increase of the ideality factor with decrease in temperature.[1,2] These findings cannot be explained adequately by incorporating interface states or interfacial oxide layer, tunneling, image force lowering, and/or generation-recombination effects. The decrease in barrier height at low temperatures, in fact, leads to nonlinearity in the activation energy $\{\ln(I_s/T^2)$ vs $1/T\}$ plot; I_s and T being the saturation current at zero-bias and diode temperature in Kelvin, respectively. ''T_0 effect'' is advanced to explain the variation of ideality factor (η) with temperature.[3,4] This requires ηT vs T plot to be a straight line. Experimental results, however, do not always follow such a dependence and show deviation at very low temperatures.[2] Also, η is introduced in the denominator of the exponential term of the saturation current expression to account for the decrease of barrier height. A $\ln(I_s/T^2)$ vs $1/\eta T$ plot is then made to remove nonlinearity and obtain a straight line corresponding to a single activation energy.[3,4] Such a modification leads, no doubt, to extension of the linear portion, yet, fails to cover the entire temperature range.[2] The partial success appears to be somewhat accidental and/or due to nonavailability of $I-V$ data at very low temperatures. The incorporation of η in the expression for I_s seems to be artificial and without any proper justification. An attempt has, therefore, been made in this paper to explain the origin of the abnormal decrease of barrier height and increase of ideality factor with decrease in temperature and the nonlinearity of the activation energy plot. For case studies, Pd_2Si based Schottky barrier diodes on both n- and p-type silicon have been undertaken. The basis of explanation lies in assuming distribution of barrier heights around a mean value.

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II. EXPERIMENT

The Pd_2Si Schottky diodes were prepared on n-type (P-doped) and p-type (B-doped) silicon wafers of (100) and (111) orientation, respectively. The n/n^+ silicon wafers had a 8.2 μm thick epitaxial n layer of resistivity 2.6 Ω cm ($\approx N_D=1.35\times10^{21}$ m^{-3}) over the heavily doped n^+ region, whereas, p/p^+ silicon wafers had a 12–18 μm thick epitaxial p-layer of resistivity 2–3 Ω cm ($\approx N_A=5.16\times10^{21}$ m^{-3}) over the heavily doped p^+ region. The wafers were first degreased with soap solution and then cleaned with organic solvents viz., trychloroethylene, acetone, and methanol in succession in an ultrasonic cleaner, rinsed in deionized water and dried. Ohmic contacts were established on the back (i.e., n^+ and p^+) side of the silicon wafers by depositing aluminium (after usual cleaning and etching in dilute HF) and subsequent annealing in nitrogen at 450 °C for 30 min. Palladium film (thickness ~80 nm) was deposited by employing an electron beam evaporation source onto the epitaxial n and p layers (i.e., front side) of the precleaned silicon wafers through holes (1 mm diameter) in the metal mask and subsequently annealed at 450 °C in vacuum $\sim10^{-5}$ mbar for 2 h to form silicide based Schottky junctions. Before metal deposition, wafers were etched in dilute hydrofluoric acid ($HF:H_2O=1:10$) for removal of silicon dioxide layer usually formed on silicon. For measuring the $I-V$ characteristics of the Schottky diodes, use was made of a programmable voltage source model Keithley 230, an autoranging picoammeter Keithley model 485, and a personnel computer. For temperature dependence of the $I-V$ characteristics of the diodes in the range 52–295 K, a CTI-cryotronics close-cycle helium refrigerator model 22C equipped with a Lake Shore tempera-

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ture controller model 805 was employed. The actual temperature of the device was monitored by placing a copper-constantan thermocouple close to the device and measuring the e.m.f. with a millivoltmeter HIL model 2301. Rich Siefert ISO-Debyeflex 2002 x-ray diffractometer with CuKα radiation (λ=1.5418 Å) was used to identify the silicide phase formed during the heat treatment.

III. BASIC EQUATIONS

The current through a Schottky barrier at a forward bias V, based on the TED theory, is given by the relation[5]

$$I = A_d A^{**} T^2 \exp\left(\frac{-q\phi_b}{kT}\right)\left[\exp\left(\frac{q(V-IR_s)}{kT}\right)-1\right], \quad (1)$$

where A_d is the diode area, A^{**} is the effective Richardson constant, T is the temperature in Kelvin, k is the Boltzmann constant, q is the electronic charge, ϕ_b is the barrier height, and R_s is the diode series resistance. Since the barrier height invariably increases with the forward bias and if assumed to have linear dependence, one writes $\phi_b(V)=\phi_{b0}+\gamma V$, where ϕ_{b0} is the barrier height at zero-bias and $\gamma(=\partial\phi_b/\partial V)$ is positive.[5] Making this substitution and introducing a parameter (called ideality factor) $\eta=1/(1-\gamma)$, Eq. (1) becomes

$$I = I_s \exp\left(\frac{q(V-IR_s)}{\eta kT}\right)\left[1-\exp\left(\frac{-q(V-IR_s)}{kT}\right)\right], \quad (2)$$

where

$$I_s = A_d A^{**} T^2 \exp\left(\frac{-q\phi_{b0}}{kT}\right) \quad (3)$$

is the saturation current at zero bias.

IV. RESULTS AND DISCUSSION

X-ray diffraction analysis revealed the formation of Pd_2Si during the heat treatment. The Pd_2Si phase belongs to a hexagonal system and exhibits preferred orientation with its basal plane lying parallel to the underlying silicon substrate of (100) and (111) orientations.

A. Nature of *I–V* characteristics

The forward $I-V$ characteristics of Pd_2Si Schottky diodes on n-type Si(100) and p-type Si(111) at various temperatures are shown in Fig. 1. These ln(I) plots are indeed linear over several order of current at low temperatures. The least square fitting of the experimental $I-V$ data in Eq. (2) has been carried out using a computer program taking I_s, η, and R_s as adjustable parameters.[2] The effect of R_s is to deviate ln(I) vs V plot from a straight line at higher forward bias. Figure 2 shows the values of ϕ_{b0} determined from I_s value at each temperature (T) using Eq. (3) and taking the diode area A_d=7.87×10^{-7} m^2 and Richardson constant A^{**}=1.12×10^6 Am^{-2} K^{-2} or 3.2×10^5 Am^{-2} K^{-2} for n- or p-type silicon.[5] It depicts that ϕ_{b0} initially decreases slowly but later quite rapidly with fall in temperature. Moreover, activation energy, ln(I_s/T^2) vs 1/T, plot becomes nonlinear in nature. Figure 3, clearly demonstrates this fact for both n- and p-type diodes. Obviously, there exists no single activation energy in each case. Needless to say that the nonlinearity observed is a consequence of decrease of barrier height with fall in temperature.

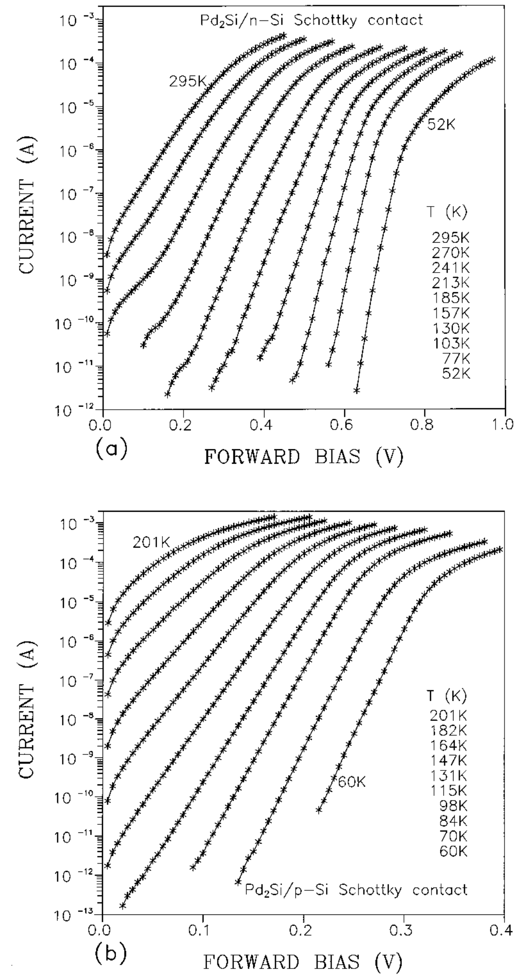


FIG. 1. Current–voltage characteristics of (a) Pd_2Si/n-Si and (b) Pd_2Si/p-Si Schottky contacts at various temperatures.

The nature of barrier height decrease suggests a temperature dependence of the type

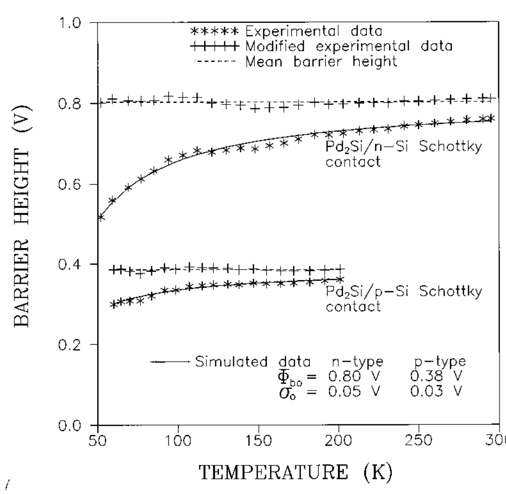


FIG. 2. Barrier height as a function of temperature for Pd_2Si/Si Schottky contacts.

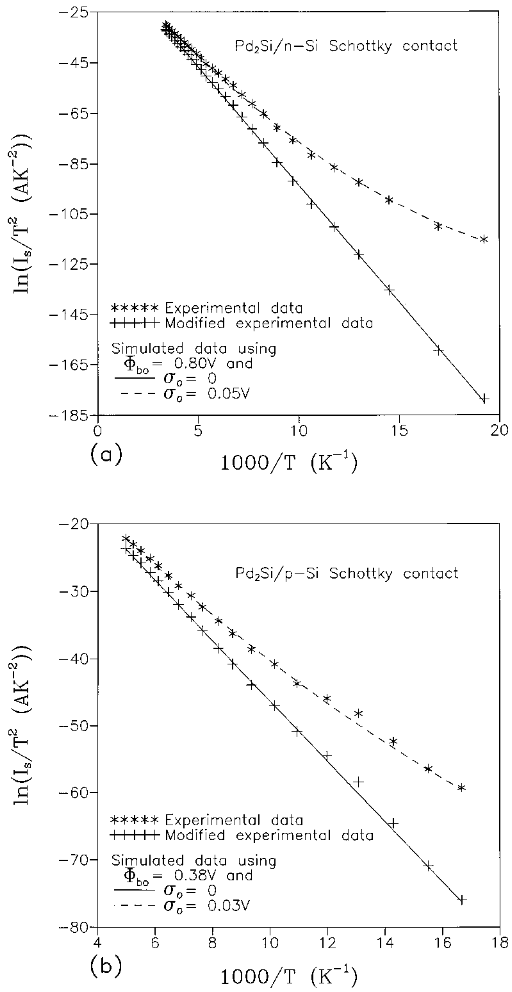


FIG. 3. $\ln(I_s/T^2)$ vs $1000/T$ plot (a) Pd_2Si/n-Si and (b) Pd_2Si/p-Si Schottky contacts.

$$\phi_{b0}(T)=A-\frac{B}{T^n}, \tag{4}$$

where A and B are constants and n stands for the exponent of T. Interestingly, ϕ_{b0} values for Pd_2Si/silicon Schottky barrier diodes follow Eq. (4) with $n=1$. Figure 4 shows straight line variation of ϕ_{b0} with $1/T$. The constants A and B can be determined from the intercept at the ordinate and the slope, respectively. It means that the temperature dependence of ϕ_{b0} is of the form $\phi_{b0}(T)=A-(B/T)$ and so $\phi_{b0}(T)$ should approach A with increase of temperature as (B/T) term progressively becomes negligible.

The variation of ideality factor η with temperature is shown in Fig. 5 for Schottky diodes fabricated on both n- and p-type silicon. Clearly, η increases initially rather slowly but very rapidly below ~100 K, attaining a significantly high value at ~50 K. Thus the observations that (i) $\ln(I)-V$ plots are linear over several orders of current even at low temperatures, and (ii) ϕ_{b0} decreases and η increases with decrease in temperature are *at first sight* indicative of deviation from the pure thermionic emission-diffusion theory. It may perhaps appear to be so due to excess current resulting by other processes, namely, tunneling through the barrier and/or recombination in the depletion region.

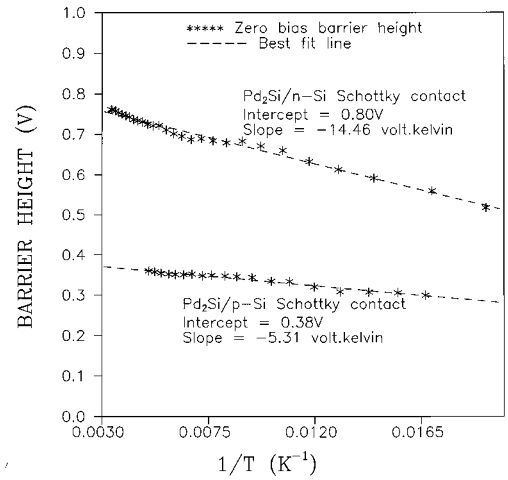


FIG. 4. Variation of the zero-bias barrier height as a function of inverse temperature.

The effective barrier lowering due to the tunneling current is given by[5]

$$\Delta\phi_t=(3/2)^{2/3}(E_{00})^{2/3}(V_d)^{1/3}\ \ \mathrm{V}, \tag{5a}$$

where E_{00} is the characteristic energy (determined by doping concentration N_D, effective mass of the carrier, and permittivity ϵ_s of the semiconductor), and V_d is the voltage corresponding to the band bending. For n-type silicon with doping concentration $N_D=1.35\times10^{21}\ \mathrm{m}^{-3}$, E_{00} comes out to be 0.188 meV and the effective barrier lowering $\Delta\phi_t$ amounts to 3.82 mV for a typical $V_d=0.7$ V. Similarly for the p-type silicon having $N_A=5.16\times10^{21}\ \mathrm{m}^{-3}$, E_{00} is 0.51 meV and the effective barrier lowering becomes 5.5 mV at V_d of 0.3 V. In contrast, barrier lowering of several hundred mV is actually observed. Also, the extent of lowering is found to depend on temperature as against a fixed value given by Eq. (5a). Also, the ideality factor η_t due to tunneling varies as[5]

$$\eta_t=\left(\frac{qE_{00}}{kT}\right)\coth\left(\frac{qE_{00}}{kT}\right). \tag{5b}$$

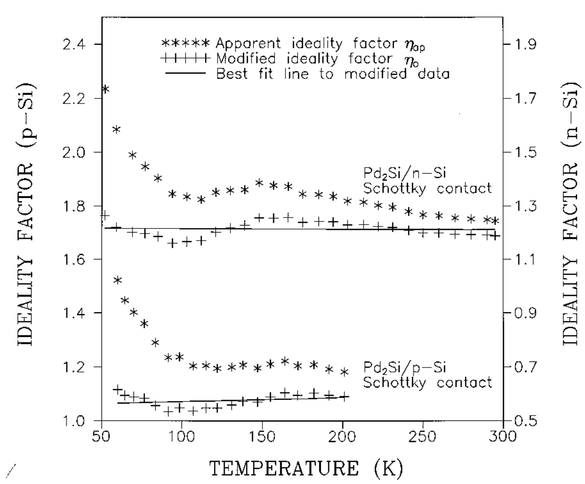


FIG. 5. Ideality factor as a function of temperature for Pd_2Si based Schottky contacts. Notice near constancy of η_0 over the entire temperature range.

This predicts η_t very close to unity for the entire temperature range (52–295 K), whereas the measured values are 1.344 at 185 K and 1.447 at 77 K for n-type, and 1.2 at 131 K and 1.4 at 70 K, for p-type samples. Obviously, the tunneling current is not responsible for the observed barrier lowering and high ideality factor.

Image force alone yields a barrier lowering of[6]

$$\Delta\phi_{imf}=\left[\left(\frac{q^3N_D}{8\pi^2\epsilon_s^3}\right)\left(\phi_{b0}-V-\phi_n-\frac{kT}{q}\right)\right]^{1/4}\ \mathrm{V}, \tag{6}$$

where $\phi_n=(kT/q)\ln(N_C/N_D)$ represents the penetration of the Fermi level in the semiconductor band gap. For Pd_2Si/n-Si Schottky diodes of zero-bias barrier height of 0.75 V at a typical forward bias voltage V=0.45 V, $\Delta\phi_{imf}$ is just 9.67 mV at 185 K and 10.94 mV at 77 K. Similarly, for Pd_2Si/p-Si diodes with zero-bias barrier height of 0.33 V and a bias of 0.15 V, $\Delta\phi_{imf}$ becomes 11.8 and 13.06 mV and 131 and 70 K, respectively. The ideality factor η_{imf} due to image force lowering[6] for n-type samples at a typical bias of 0.45 V turns out to be 1.017 and 1.012 at 185 and 72 K, respectively. Similarly, for p-type samples, η_{imf} values are 1.036 and 1.026 at 131 and 70 K, respectively. Thus the image force lowering effect is also insufficient and so fails to explain the observed changes in barrier height and ideality factor.

The recombination current can be described by[7]

$$I_r=I_{r0}\left(\exp\left(\frac{qV}{2kT}\right)-1\right) \tag{7a}$$

with

$$I_{r0}=qn_iA_dw/2\tau, \tag{7b}$$

where w is the thickness on the depletion region, τ is the effective minority carrier lifetime in the depletion region, $n_i=(N_CN_V)^{1/2}\exp(-E_g/2kT)$ is the intrinsic carrier concentration with E_g the energy band gap and N_C and N_V are the effective conduction and valence band density of states, respectively. Such a current must be comparable to or in excess of that produced by majority carriers at low forward bias for generation-recombination process to become meaningful. However, the saturation current I_{r0} as calculated from Eq. (7b) with a typical $\tau=1\times10^{-5}$ s comes out to be 1.07×10^{-25} A at 185 K and 1.02×10^{-58} A at 77 K for n-type and 7.0×10^{-28} A at 131 K and 1.19×10^{-47} A at 70 K for p-type cases. These current levels are excessively low compared to those actually observed in experiments. Also, generation-recombination causes the ideality factor to be close to 2. However, the maximum value of ideality factor is 1.735 at 52 K and 1.52 at 60 K on n- and p-type Si, respectively.

The band gap of silicon has a negative temperature coefficient (-9.025×10^{-5} eV/K in the range 150–300 K), i.e., it increases with decrease in temperature.[8] However, the barrier height decreases with a fall in temperature. Therefore, temperature dependence of the band gap of silicon can in no way account for the decrease of barrier height at low temperature in the present Pd_2Si/Si Schottky diodes.

All the above considerations together with the observed linearity in $\ln(I)-V$ plots over several orders of current in the temperature range 52–295 K suggest that the TED mechanism is indeed operative in the Pd_2Si/Si diodes even at very low temperatures. Therefore, increase in η and decrease in ϕ_{b0} are possibly caused by some other effects giving rise to extra current such that the overall characteristics continue to remain consistent with the TED process.

B. Concept of barrier inhomogeneities

One way to account for the abnormal behavior of barrier height at low temperatures is to assume the existence of yet another barrier of low ϕ_{b0}. But, this requires the corresponding area fraction[9,10] to be extremely small ($\sim<5\times10^{-5}$). In such cases, one expects an activation energy plot to fit well with two straight lines, the slope of each giving the corresponding value of barrier height and the intercept at the ordinate the value of Richardson constant. However, $I-V$ characteristics of Pd_2Si/Si diodes lead to continuous variation in the activation energy plot (Fig. 3) and hence do not match with this very description. Moreover, simulation studies of Freeouf *et al.*[11,12] on mixed-phased Schottky contacts revealed that below a critical size low BH region is ''pinched-off'' and only high barrier remains effective. According to Sullivan *et al.*,[13] pinch-off actually occurs at some depth (~0.03 μm) in the semiconductor from the metal–semiconductor (MS) interface. At this stage, potential contours beneath the low and high BH regions become essentially the same. Further, with increase of size (say, beyond 0.06–0.1 μm), pinch-off ceases and low BH region begins to be operative as well. Consequently, the extra current passing through them leads to apparent changes in the barrier height and ideality factor. Also, Tung[14] found that when the variation of BH occurs on a scale smaller than a certain value (say, the depletion region width), interaction between patches leads to pinch-off of the conduction path from the low BH regions leaving only high BH areas to be operative. In fact, BH varies on a scale much smaller than or comparable to the depletion region width and so only high BH areas be essentially effective.[15]

Another way to explain the abnormal behavior of ϕ_{b0} and η is to assume the existence of barrier inhomogeneities and describe them with some suitable distribution function. Earlier, Johnson *et al.*[16] invoked multicontact concept and suggested the possibility of exponential distribution function for contact potential at the metal–semiconductor interface to understand the temperature dependence of the $I-V$ characteristics. Also, numerous evidences have been reported on the existence of barrier inhomogeneities.[17–22] According to Henisch,[23] fluctuations in barrier heights are unavoidable as they exist even in the most carefully fabricated systems. Needless to say that inhomogeneities may be due to variation in thickness and composition of silicide layer, nonuniformity of the interfacial charges, and locally defective hot regions.[24] Various types of distribution functions have been proposed to describe barrier inhomogeneities, e.g., a Gaussian or normal[1,25] or log–normal.[26] Already, a Gaussian distribution function has been utilized to explain (i) the difference in barrier heights obtained from $C-V$ and $I-V$ measurements in Al/p-InP[25] at 285–384 K and PtSi/Si[1] at 76–344 K; (ii) nonlinearity in the Arrhenius plot and findings of photoresponse measurements in PtSi/p-Si Schottky barriers[24] in the temperature range 77–120 K; (iii) influence of distribution parameters and temperature on the barrier height and ideality factor of Schottky diodes using numerical simulation.[27] Palm *et al.*[15] have even shown direct images of Schottky barrier height fluctuations in Au–Si contacts using ballistic electron emission microscopy techniques and represented them with a Gaussian distribution function. One may therefore assume a Gaussian distribution of barrier heights, with a mean value of $\overline{\phi_b}$ and standard deviation σ, having the form[1,24,25,27]

$$P(\phi_b)=\frac{1}{\sigma\sqrt{(2\pi)}}\exp\left[-\left(\frac{(\phi_b-\overline{\phi_b})^2}{2\sigma^2}\right)\right], \tag{8}$$

where the pre-exponential term is the normalization constant. The total current across the Schottky contact at a forward bias is then given by

$$I(V)=\int I(\phi_b,V)P(\phi_b)\,d\phi_b, \tag{9}$$

where $I(\phi_b,V)$ is the current for a given barrier ϕ_b and bias voltage V. Substituting $I(\phi_b,V)$ and $P(\phi_b)$ from Eqs. (1) and (8) and performing the integration (9) from $-\infty$ to $+\infty$, one gets

$$I(V)=A_dA^{**}T^2\exp\left[\frac{-q}{kT}\left(\overline{\phi_b}-\frac{\sigma^2q}{2kT}\right)\right]\exp\left(\frac{q(V-IR_s)}{kT}\right)\times\left[1-\exp\left(\frac{-q(V-IR_s)}{kT}\right)\right]. \tag{10}$$

However, the barrier height is known to depend on the electric field and hence on the applied bias; the possible causes being the presence of an interfacial layer, image force lowering, and/or effects due to penetration of electrons wave functions into the semiconductors.[5] This has already been incorporated in Eq. (2) by assuming linear bias dependence of the barrier height. Now, since barrier heights are represented by a Gaussian distribution, the entire profile should be affected by the applied bias. Hence, extending the linear bias dependence to distribution parameters viz., mean barrier height ($\overline{\phi_b}$) and standard deviation (σ) both, one writes $\overline{\phi_b}=\overline{\phi_{b0}}+\gamma V$ and $\sigma=\sigma_0+\xi V$ (where γ and ξ are positive derivatives, and $\overline{\phi_{b0}}$ and σ_0 are mean barrier height and standard deviation at zero-bias, respectively). Making these substitutions and neglecting the term involving ξ^2V^2, Eq. (10) gets modified to

$$I(V)=I_s\exp\left(\frac{q(V-IR_s)}{kT\eta_{ap}}\right)\left[1-\exp\left(\frac{-q(V-IR_s)}{kT}\right)\right] \tag{11}$$

with

$$I_s=A_dA^{**}T^2\exp\left(\frac{-q\phi_{ap}}{kT}\right). \tag{12}$$

Here, I_s is the observed saturation current, ϕ_{ap} and η_{ap} are the apparent barrier height and ideality factor, respectively. ϕ_{ap} and η_{ap} are given by

$$\phi_{ap}=\overline{\phi_{b0}}-\frac{\sigma_0^2q}{2kT}, \tag{13}$$

$$\frac{1}{\eta_{ap}}=(1-\gamma)+\frac{\sigma_0q\xi}{kT}. \tag{14}$$

Equation (11) is of the form (2) but contains ϕ_{ap} and η_{ap} in place of ϕ_{b0} and η, respectively. Therefore, fitting of experimental $I-V$ data into Eq. (11) can still be carried out in the usual way,[2] but the values of ϕ_{ap} and η_{ap} derived should be interpreted in terms of Eqs. (13) and (14), respectively. It is interesting to note that ϕ_{ap} depends on the distribution parameters $\overline{\phi_{b0}}$ and σ_0 and temperature T. Obviously, decrease in barrier height is caused by mere existence of distribution and its effect becomes pronounced at low temperatures. On the other hand, η_{ap} is a function of rate of change of $\overline{\phi_b}$ and σ with bias.

C. Interpretation of experimental data

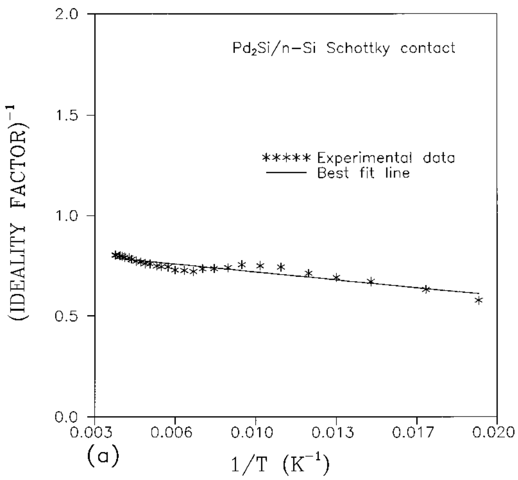
The diode parameters derived from fitting of the experimental data in Eq. (11) can therefore be interpreted using Eqs. (13) and (14). Thus the ϕ_{ap} vs $1/T$ plot should be a straight line giving $\overline{\phi_{b0}}$ and σ_0 from the intercept at the ordinate and the slope, respectively. This is equivalent to finding out constants A and B of Eq. (4) for $n=1$. Thus $A=\overline{\phi_{b0}}$ and $B=\sigma_0^2q/2k$. Now ϕ_{ap} is calculated by substituting the values of $\overline{\phi_{b0}}$ and σ_0 in Eq. (13). Its variation with temperature is shown in Fig. 2 by a continuous line (notice that the line almost lies on the experimental data points). Also, the correction to the experimental data can now be made using Eq. (13). For this, $\overline{\phi_{b0}}$ is calculated back using value of ϕ_{ap} and σ_0. The values of $\overline{\phi_{b0}}$ thus obtained are marked as modified experimental data in Fig. 2.

Combining Eqs. (12) and (13), one may write

$$\ln(I_s/T^2)-(q^2\sigma_0^2/2k^2T^2)=\ln(A^{**}A_d)-q\overline{\phi_{b0}}/kT. \tag{15}$$

Thus the conventional activation energy equation gets modified under the assumption of Gaussian distribution of barrier heights. The nonlinearity in the activation energy plot can be understood on the basis of Eq. (15). The factor $\ln(I_s/T^2)-(q^2\sigma_0^2/2k^2T^2)$ is calculated to modify the experimental data and plotted as a function of $1/T$ to obtain a straight line corresponding to a single activation energy around $\overline{\phi_{b0}}$. The slope now gives $\overline{\phi_{b0}}$ accurately. Taking $\overline{\phi_{b0}}$, I_s is estimated from Eq. (12) for $\sigma_0=0$ and a particular σ_0 (i.e., 0.05 and 0.03 V for n- and p-type Si, respectively) and $\ln(I_s/T^2)$ vs $1/T$ plots are produced. These are shown by continuous and broken lines in Fig. 3. Undoubtedly, they match well with the experimental results. The intercept of the straight line corresponding to $\ln(I_s/T^2)-(q^2\sigma_0^2/2k^2T^2)$ vs $1/T$ plot at the ordinate gives the Richardson constant itself. The values obtained being 1.61×10^6 Am^{-2} K^{-2} and 3.13×10^5 Am^{-2} K^{-2} for diodes on n- and p-type silicon, respectively. These clearly show close agreement with the known theoretical values (see, e.g., Sec. IV A).

The temperature dependence of the ideality factor (η_{ap}) can be understood on the basis of Eq. (14). It indicates that $1/\eta_{ap}$ vs $1/T$ plot should yield a straight line with slope giving $\sigma_0q\xi/k$ and intercept $(1-\gamma)$. The $1/(1-\gamma)$ factor (or say η_0) is solely determined by the rate of change of the BH with bias and corresponds to the ideality factor of a Schottky di-



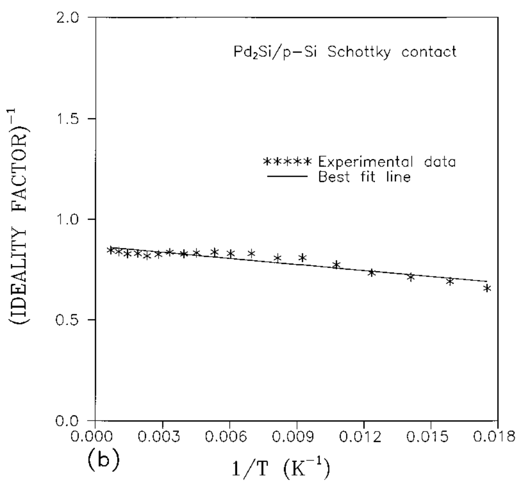


FIG. 6. Variation of inverse ideality factor as a function of inverse temperature in (a) Pd_2Si/n-Si and (b) Pd_2Si/p-Si Schottky contacts.

ode having a homogeneous barrier of height $\overline{\phi}_{b0}$. The increase of η_{ap} with fall in temperature arises due to the term containing ξ (i.e., rate of change of σ with bias). The plot of $1/\eta_{ap}$ vs $1/T$ (Fig. 6) corresponds to a negative slope in the present Pd_2Si based Schottky diodes and so ξ is essentially negative; the values being -0.0192 and -0.0414 for n- and p-type cases, respectively. These experimental results coupled with the positive values of γ ($\sim$0.18 and 0.07) revealed that the increase of ideality factor is caused by the voltage dependence of σ (through ξ); also the contribution becomes significant at low temperatures. The overall effect is that the bias increases the mean barrier height but decreases the standard deviation, i.e., *forward bias makes the distribution function dynamic in the sense that it shifts towards higher energy side and becomes narrow at the same time*. Knowing ξ from the $1/\eta_{ap}$ vs $1/T$ plots, the term $1/(1-\gamma)$ (say, η_0) can be estimated over entire temperature range using Eq. (14). Figure 5 shows both the ideality factors (η_{ap} and η_0) as a function of temperature for Pd_2Si Schottky diodes. Notice that the unusual increase of ideality factor with decrease of temperature ceases if distribution of barrier heights is believed to exist. The term $\eta_0 = 1(1-\gamma)$ can be taken as a *characteristic* value of a Schottky diode independent of the effect of barrier heights distribution; the values being 1.21 and 1.07 for diodes on n- and p-type silicon, respectively.

The studies on many other simultaneously fabricated diodes revealed slight variation in values of the mean barrier height and standard deviation at zero bias. Such observations are primarily attributed to the local chemistry and conditions of the interface. For same reasons, the Schottky diodes on n-type and p-type silicon are believed to exhibit different standard deviation. Interestingly, the standard deviation always lie within 7%–12% of the mean barrier height.

Due to similarity in the empirical relation (4) with $n=1$ and expression (13), the former can be used to check the occurrence of the distribution of barrier heights in Schottky diodes. Accordingly, ϕ_{b0} vs $1/T$ plot should correspond to a straight line (having nonzero slope) if a Schottky diode indeed possesses a Gaussian distribution of barrier heights. The intercept of the line with ordinate then yields the zero-bias mean barrier height $\overline{\phi}_{b0}$ and the slope gives the zero-bias standard deviation σ_0. The modified activation energy $\{\ln(I_s/T^2) - (\sigma_0^2 q^2/2k^2T^2)\}$ plot can subsequently be made from distribution parameters to find out the value of $\overline{\phi}_{b0}$ and A^{**} for a given diode area.

V. CONCLUSIONS

(a) $I-V$ characteristics of the Pd_2Si based Schottky diodes over a wide temperature range can be successfully explained on the basis of TED mechanism by incorporating the concept of Gaussian distribution of barrier heights.

(b) The values of various parameters are zero-bias mean barrier height 0.80 V (0.38 V), standard deviation 0.05 V (0.03 V), and characteristics ideality factor 1.21 (1.07) for Pd_2Si based diodes on n-type (p-type) silicon wafers.

(c) The linearity of ϕ_{b0} vs $1/T$ plot itself provides evidence for the occurrence of a Gaussian distribution of barrier heights, with the intercept at the ordinate and the slope giving the values of zero-bias mean barrier height and standard deviation, respectively.

(d) The distribution concept not only explains the temperature dependence of ideality factor η adequately, but also avoids the practice of artificial introduction of η in the saturation current expression to account for the unusual decrease of barrier height at low temperatures.

(e) The effect of forward bias is to make the distribution of barrier height dynamic in nature, i.e., it causes shift of the distribution towards higher energy and at the same time makes that narrow.

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