Temperature anomalies of Schottky-barrier diodes on \(n\)-type silicon

D. Jäger and R. Kassing

*Institute of Applied Physics, University of Münster, 4400 Münster, Federal Republic of Germany*

(Received 29 March 1977; accepted for publication 25 May 1977)

Experimental investigations of the temperature dependence of \(I-V\) and \(C-V\) characteristics of Schottky-barrier diodes lead to deviations from the thermionic-emission model. The barrier height and the ideality factor determined from forward \(I-V\) plots of Al, Au, and Pt Schottky contacts on \(n\)-Si strongly depend on temperature. Experimental results of forward \(I-V\) characteristics, Richardson plots, and reverse \(C-V\) data are given. An excess temperature is used as a parameter to describe the observed anomalies according to Levine’s analysis.

PACS numbers: 73.30.+y, 85.30.Hi, 73.20.−r

A substantial amount of work on the Schottky-barrier height \(\phi_B\) of metal-semiconductor contacts has been reported for the past decade. If, as usual, thermionic emission of electrons over the top of the barrier is expected to be the dominant transport mechanism, the barrier height is obtained from measured \(I-V\) characteristics given by

\[
I = I_0 \exp\left(\frac{V}{V_0}\right) - 1
\]

(1)

with

\[
I_0 = A A^* T^2 \exp(-\phi_B/V_0),
\]

(2)

where \(A\) denotes the contact area, \(A^*\) is the Richardson constant, \(V_0 = kT/q\) is the thermal voltage, \(T\) is the absolute temperature, and \(I_0\) is the saturation current. The following methods are commonly used: an evaluation (a) from \(I_0\) extrapolated from the semilog \(I-V\) plot and (b) from the Richardson plot \(\ln I_0/T^2\) versus \(1/T\). A third method (c) is based upon the measurement of reverse \(C-V\) characteristic

\[
C/A = \left[\frac{eqN_p}{2(V_p - V)}\right]^{1/2},
\]

(3)

where the diffusion voltage \(V_p = \phi_B - E_{CF}/q\) is determined from the plot \(C^2\) versus \(V\). \(N_p\) signifies the doping concentration (here \(n\)-type material), \(\varepsilon\) is the semiconductor permittivity, and \(E_{CF}\) is the depth of the Fermi level below the conduction band.

It is the purpose of this paper to present experimental results obtained from Al, Au, and Pt Schottky barriers on \(n\)-type silicon within a temperature range of about 20–320 K using the formulas as above. \(Si\) substrates with carrier concentrations between \(10^{14}\) and \(5 \times 10^{16}\) \(cm^{-3}\) have been used. The Schottky contacts were prepared by either electron gun or resistive evaporation on chemically cleaned surfaces. The Ohmic contacts were formed by alloying Au/Sb. In Figs. 1–3, some typical results of Al-Si barriers are shown with \(N_p = 3 \times 10^{16}\) \(cm^{-3}\) and \(A = 2 \times 10^{-3}\) \(cm^{2}\). Similar results have been obtained for other doping concentrations, independent of evaporation technique (vacuum < \(10^{-6}\) Torr oil-free or < \(10^{-5}\) Torr oil-diffusion pump system) and annealing temperatures (\(450 \leq T_i \leq 600^\circ\) C). Au-Si and Pt-Si barriers exhibited quite the same behavior.

In Fig. 1, the results of investigations on forward \(I-V\) characteristics are given: the barrier height as determined from the extrapolated saturation current using \(A^* = 120\ A cm^{-2} K^{-2}\) and the ideality factor \(n\) defined by \(V/V_0 = qV/nkT\). The value of \(n\) has been calculated from the slope of the semilog \(I-V\) plot at a constant current density of \(10^{12}\ A cm^{-2}\). The deviations from thermionic-emission theory are evident; both \(n\) and \(\phi_B\) strongly depend on temperature. Figure 1 shows another important result: the product \(n\phi_B\) is almost independent of temperature, so that the \(I-V\) relationship according to Eq. (1) may be rewritten in the following form:

\[
I = A A^* T^2 \exp(-q\phi_B/nkT)\left[\exp(qV/nkT) - 1\right],
\]

(4)

where \(\phi_B\) is a constant. From the experimental results, the following expression for the temperature dependence

---

**Fig. 1.** Measured temperature dependence of ideality factor \(n\) and barrier height \(\phi_B\) from forward \(I-V\) characteristics. Calculated product \(n\phi_B\) versus \(T\), Al-\(n\)-Si barrier.

**Fig. 2.** Richardson plot (a) versus \(1/T\) and (b) versus \(1/nT\) (sample of Fig. 1).
of the ideality is always found to be valid:

$$n = a + \frac{T_o}{T}.$$  \hspace{1cm} (5)

In the case of Al–nSi barriers, a typical example of which is shown in Fig. 1, one gets $\phi_p = 0.69$ V, $a = 0.88$, and $T_o = 59$ K.

Figure 2 shows the Richardson plots $\ln(I/AT^2)$ versus $1/T$ [Fig. 2(a)] as well as versus $1/nT$ [Fig. 2(b)]. Obviously, the common plot versus $1/T$ does not yield a straight line over the whole range of temperatures. If, therefore, one would ignore the experimental values below 200 K from the slope of the straight line in Fig. 2(a), one would deduce $\phi_p = 0.57$ V and the zero axis intercept would give $A* \approx 1 \text{ A cm}^{-2} \text{ K}^{-2}$, neglecting the small temperature dependence of the semiconductor energy gap. According to Eq. (4), however, the plot versus $1/nT$ in Fig. 2(b) yields a straight line and the proper values $\phi_p = 0.72$ V and $A* \approx 100 \text{ A cm}^{-2} \text{ K}^{-2}$, thus confirming the validity of Eq. (4).

In Fig. 3, the results of reverse $C$-$V$ characteristics measured at 100 kHz—where no frequency dependence is observed—are shown, i.e., the diffusion voltage $V_D$ and the “apparent” doping concentration $N_D$ determined from the voltage intercept and the slope of $C$-$V$ plots, respectively. One observes the following typical behavior: a stronger temperature dependence of $V_D$, than would be expected from the variation of the semiconductor Fermi level; a corresponding barrier height $\phi_p \approx 0.84$ V, essentially that later than that evaluated from $I$-$V$ characteristics; and a decreasing value of $N_D$ when temperature is reduced. Carrier freeze-out can be neglected.

The presented results obtained from Al-, Au-, and Pt-nSi Schottky barriers establish those which have been found at Ni-, Cr-, and Au-Si,\textsuperscript{1,2} and at Au\textsuperscript{3} and Ni-GaAs\textsuperscript{4} Schottky barriers. It is also demonstrated that $C$-$V$ data deviate from the basic depletion-layer model at lower temperatures. It is therefore concluded that the observed anomalies reveal a fundamental peculiarity of those Schottky-barrier diodes and that the anomalies should be considered if the ideality factor deviates from unity. As pointed out, this is particularly valid if the Richardson plot is evaluated as has been shown by other authors\textsuperscript{5,6} as well as in this paper. Consequently, it should be noted that the $T_o$ anomaly must be taken into account if, for example, $A*$ is calculated, a fact which has not been discussed in a very recent paper.\textsuperscript{6}

Until now, no satisfactory explanation for the observed temperature anomalies has been given. The only theory which exists for an $I$-$V$ characteristic of the form given in Eq. (4) is that of thermionic field emission\textsuperscript{7} which, however, is not expected to be valid in case of our low-concentration semiconductors. Other theories on the basis surface states and interfaces,\textsuperscript{9} deep levels,\textsuperscript{8} screening effects,\textsuperscript{9} quantum-mechanical tunneling,\textsuperscript{10} or image forces explain, until now, only some individual peculiarities but not the whole set of experimental results. Levine,\textsuperscript{11} however, suggests an attractive surface-state model with the proper temperature dependence, which has very recently been tracked back to Bardeen’s interface model.\textsuperscript{12} Although Levine did not explain the origin of surface states, his results lead to the observed $I$-$V$ anomalies. Additionally, our experiments are in accordance with the reverse $C$-$V$ characteristics derived by Levine, i.e., the “apparent” doping concentration is given by $N_D/n^2$ where, however, $T_o$ should be much less than under forward-bias conditions: the measured temperature dependence as given in Fig. 3 yields $T_o \approx 3$ K at a reverse bias of $-0.5$ V in agreement with the predicted voltage dependence of $T_o^3$. In the case of the presented results on Al–nSi Schottky barriers, Levine’s characteristic voltage $E_o$ for the surface–state distribution is found to be $E_o = 0.1$ V, and agreement between $I$-$V$ and $C$-$V$ data is established. A more detailed analysis of our Schottky-barrier results is in progress and will be given in a forthcoming paper. As a concluding remark, it should be anticipated that the results of Pellegrini’s analysis\textsuperscript{10} are in many respects similar to those of Levine’s, which would imply that the surface states are the quantum-mechanical tails of the wave functions of the metal electrons.

We wish to thank R. Bäumer, I. Landmann, and W. Wehrmann for the experimental investigations.