Conduction mechanisms in erbium silicide Schottky diodes

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Conduction mechanisms in erbium silicide Schottky diodes on n-type silicon have been studied over a temperature range of 25 to 160 K. Thermionic emission is the dominant carrier transport mechanism above 70 K. Below this temperature, deviations are apparent in the zero-bias barrier height and ideality factor. However, the flat-band barrier height is shown to remain constant over the entire temperature range. The Fermi level is demonstrated to be pinned to the conduction band. A new quantity, the flat-band saturation current (I_s^f) is defined. Plots of $n\ln(I_s^f/T^2)$ vs $1/T$ are found to give an excellent fit to the data over 28 orders of magnitude. From these plots the flat-band barrier height and the modified Richardson constant are obtained directly. This technique provides a completely self-consistent and more reliable way of obtaining these parameters than do previous methods. For low temperatures and low forward bias, recombination via tunneling through surface states becomes the dominant conduction mechanism.

I. INTRODUCTION

Erbium silicide is a promising new infrared detector material. As a family, the rare-earth elements have the lowest Schottky barrier heights known on n-type silicon. In the case of erbium silicide the barrier height is ~ 0.28 eV, corresponding to an infrared wavelength cutoff of ~ 4.4 μm. This is intermediate between platinum silicide [0.24 eV, 5.2 μm (Ref. 1)] and palladium silicide [0.35 eV, 3.5 μm (Ref. 2)], both of which are used on p-type silicon. Erbium silicide is thus well suited to take advantage of the 2 to 5 μm atmospheric transmission window.

Essential to the understanding of any metal-semiconductor contact is a knowledge of the conduction mechanisms involved in allowing the charges (electrons in an n-type substrate) to move across the Schottky barrier in response to an applied driving voltage. This understanding then allows the Schottky barrier height to be accurately determined.

The most common means of investigating Schottky diodes is to assume that ideal thermionic-emission theory applies and to measure the forward current-voltage (IV) characteristics of the diode at a single temperature. With low barrier diodes this temperature is usually that of liquid nitrogen, 77 K. Although this approach is adequate for many purposes, more information on the nature of the barrier and conduction mechanisms can be obtained by studying the behavior of the Schottky diode over a range of temperatures.

In this study we have investigated the conduction mechanisms in erbium silicide on n-type silicon over the temperature range 25 to 160 K. As expected, the dominant conduction mechanism is thermionic emission. However, serious deviations from ideal thermionic-emission theory increasingly manifest themselves as the temperature drops below 70 K.

II. EXPERIMENTAL SETUP

Erbium was chosen for this study because it is the easiest to handle of those rare-earth metals known to produce low barrier heights on n-type silicon, and as such is the most likely to be useful from an applications point of view. The diodes were made on ⟨100⟩, 10 Ω cm ($N_D=4.45\times10^{15}$ cm^{-3}), n-type silicon wafers. Following the diffusion of n^{++} guard rings, a 300-nm-thick masking layer of SiO_2 was thermally grown. A series of 1000-μm-diam holes was then etched through this masking layer. An 80-nm-thick layer of erbium was thermally evaporated through a mechanical mask and through the holes in the SiO_2. The silicide was then produced by sintering the wafer in vacuum at 410 °C. A fuller description of the fabrication process can be found in Unewisse and Storey.[3]

The IV characteristics of the erbium silicide Schottky diodes were measured by supplying a controlled voltage and then measuring the current with a Keithley 617 electrometer, while monitoring the voltage with a Prima 5000 DVM. These instruments were connected to an IBM XT compatible computer, to allow automated measurements. With multiple sampling and other noise reduction techniques, currents down to 1×10^{-13} A were measurable.

The diodes used in these experiments were tested in an RMC LST-22-IR cryo-cooler, with an available temperature range of 10 to 300 K, which was also interfaced to the computer. To minimize errors due to thermal gradients within the cold head a separate Lake Shore Cryotronics DRC-80C temperature controller was used to monitor the temperature. Fully automated testing of current-voltage-temperature (IVT) characteristics was possible, and IV characteristics were thus taken over a wide range of temperatures. However, due to the low Schottky barriers involved, temperatures over 200 K did not give useful results.

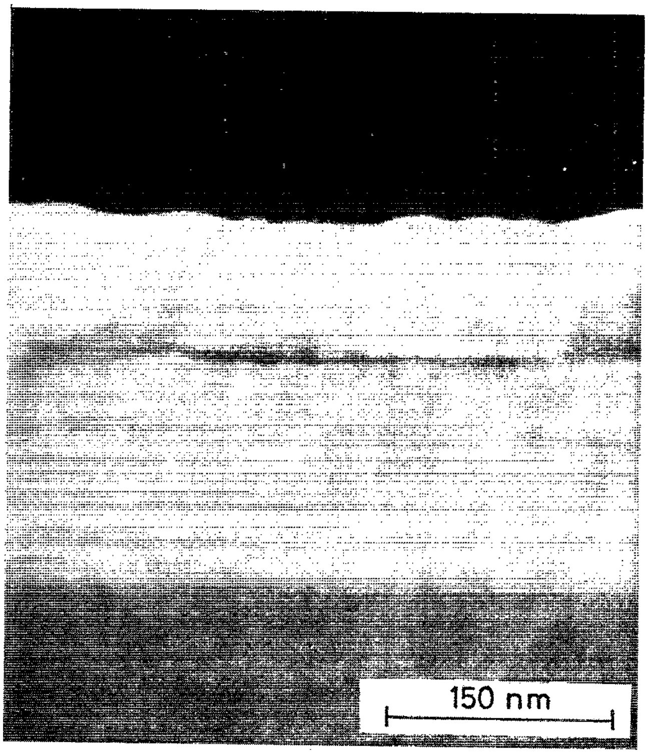

FIG. 1. 200 000× electron micrograph of the cross section of an erbium silicide diode.

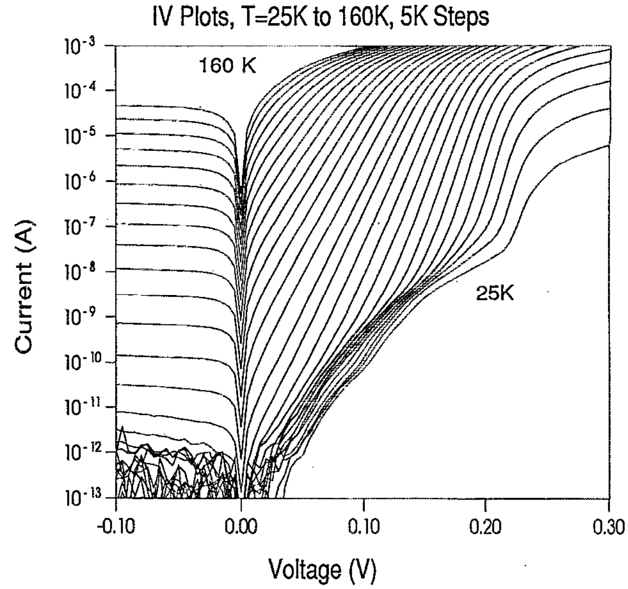

FIG. 2. IV characteristics of $ErSi_2$ over a temperature range of 25 to 160 K in 5 K steps. Each curve consists of about 80 data points and is therefore shown as a solid line.

III. ERBIUM SILICIDE-SILICON INTERFACE

The Schottky barrier height is controlled to some extent by the detailed structure of the metal-semiconductor interface. Figure 1 shows a 200 000 times magnification electron-micrograph, taken with a Hitachi S-900 field emission electron microscope, of a vertical cross section through the top surface of a cleaved erbium silicide diode. At the bottom is the silicon, followed by the erbium silicide. The erbium silicide is then overlayed by any residual erbium. Exactly where this interface is located is uncertain, but we believe that it is about 50 nm above the silicon. Above the erbium is a 95-nm-thick capping layer of aluminum.

Note that the boundary between the silicon and erbium silicide layer is very smooth, unlike the surface morphology reported in many of the early studies of thermally evaporated erbium silicide.[4] The smooth interface is characteristic of erbium silicide diodes with a low barrier height of 0.28 eV. In addition, it makes the diode area calculations more reliable than would be the case with a "rough" interface. Close examination of the boundary between the silicon and the erbium silicide shows that there does not appear to be any interfacial layer between them.

During the course of our investigations into erbium silicide we also found that sintering the wafer at a somewhat higher temperature ($\sim$450 °C) resulted in rough surfaces similar to the diodes reported by Lao *et al.*[4] and Knapp *et al.*[5] For these "rough" diodes a barrier height of $\sim$0.36 eV was measured. This is again in agreement with the results of many of the vacuum annealed erbium silicide diodes previously reported. Erbium silicide diodes with barrier heights of 0.28 and $\sim$0.4 eV have both been show to be $ErSi_{2-x}$ $(0<x<0.5$, usually 0.3).[6,7] Thus a more detailed surface analysis will be required to fully understand what the difference is between these two types of erbium silicide. Such measurements are, however, beyond the scope of this paper.

IV. FORWARD *IV* CHARACTERIZATION

For an ideal Schottky diode, thermionic emission-diffusion theory gives the relationship between current and voltage.[8,9] If the effects of image force lowering are included, this relationship is given by Eq. (1):

$$I=I_s \exp\left(\frac{qV}{nkT}\right)\left[1-\exp\left(-\frac{qV}{kT}\right)\right]. \tag{1}$$

Here I is the diode current, V is the voltage across the diode, k is Boltzmann's constant, q is the electronic charge, T is temperature, and n is the ideality factor. I_s is the saturation current given by[10]

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

where A_d is the area of the diode, A^{**} is the modified Richardson constant, and ϕ_{b0} is the zero-bias Schottky barrier height. Once I_s is known, the barrier height is easily determined. The saturation current is found from the intercept at $V=0$, while the ideality factor comes from the slope of the IV plot.

Figure 2 shows a series of IV plots for temperatures ranging from 24.5 to 160 K. Above 160 K it becomes increasingly difficult to extract the barrier height and ide-

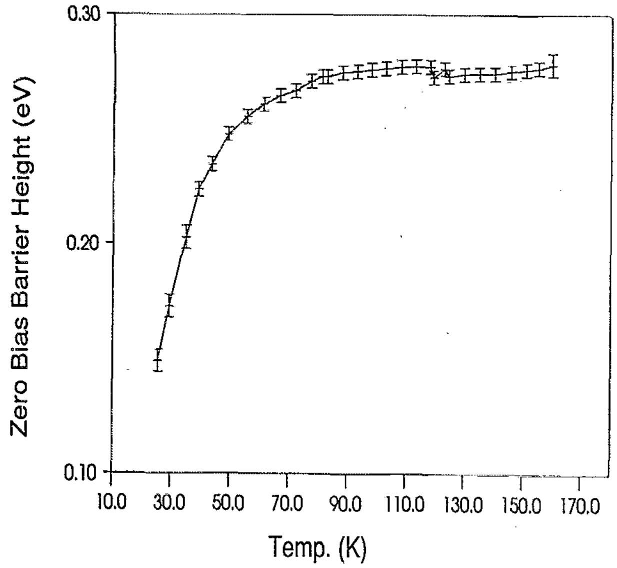

FIG. 3. Variation of the zero-bias barrier height with temperature. Note the significant deviation below 70 K.

ality information, and so the data taken in this region were discarded. As can be seen in Fig. 2 the slope increases and the *IV* curve shifts to the right as the temperature is decreased, in accordance with Eqs. (1) and (2). In addition, there is change from exponential increase to linear increase of current with voltage as the current becomes large enough for the series resistance, found in all real diodes, to have a significant effect on the *IV* curve. To correct for this effect a modeling program for the *IV* data, based in part on the work of Boutrit *et al.*,[11] was written. This program models the data using a series resistance and a shunt resistance (the latter proved to be completely negligible for the erbium silicide diodes on *n*-type silicon) as free parameters and then calculates I_s and n. The model uses a modified

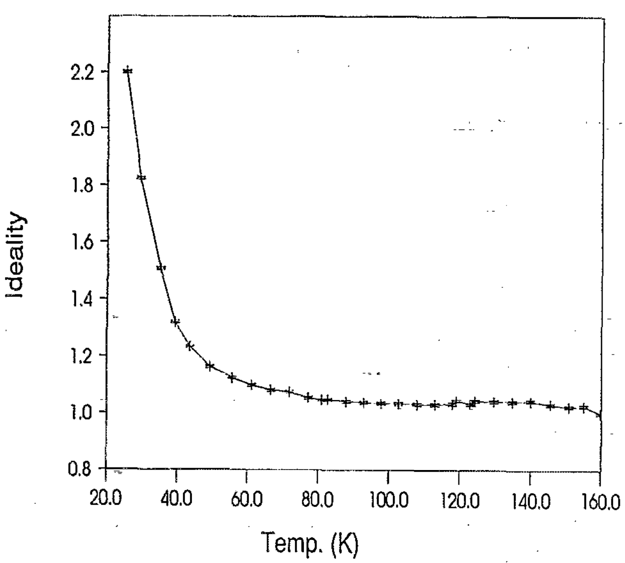

FIG. 4. Temperature dependence of the ideality factor. The plot demonstrates the large increase in "n" as the temperature falls below 70 K.

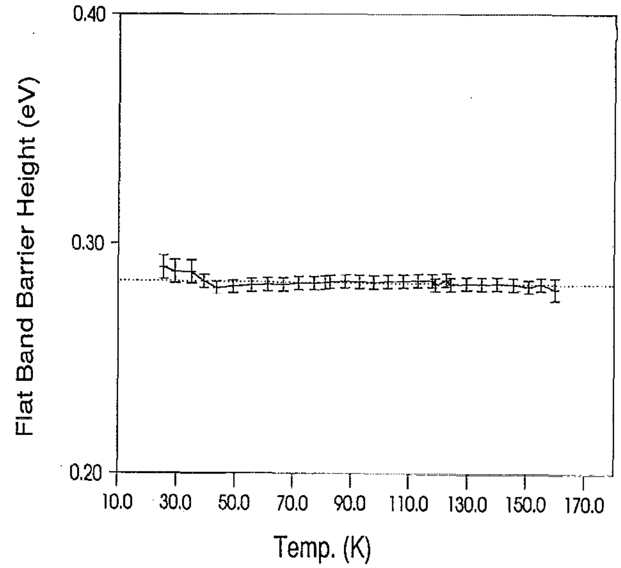

FIG. 5. Plot showing that the flat-band barrier height for $ErSi_2$ is essentially constant with temperature, with a temperature coefficient of approximately 1.5×10^{-5} eV/K.

Richardson constant of 110 $A/cm^2/K^2$.[12] At low temperatures and forward bias the *IV* curves seem to hit a region which is very different, i.e., with very high ideality factor, from that described by the thermionic emission-diffusion model. This region will be discussed later in the paper.

Values for I_s and n were thus determined from the *IV* curve at each temperature, using the data lying above the "kink" in Fig. 2 (below this kink the ideality factor becomes very large). The zero-bias barrier height, calculated from I_s, is plotted against temperature in Fig. 3. It can clearly be seen that there is a significant drop in ϕ_{b0} as the temperature falls below 70 K. Above 70 K the ϕ_{b0} is about 0.274 eV, reducing to a value of 0.149 eV at 25 K. When the ideality factor n is plotted against temperature, as in Fig. 4, it too shows a deviation from the ideal value of 1, increasing significantly below 70 K. Both of the these results are indicative of deviations from thermionic emission theory.

The flat-band barrier height is often a better measure of the barrier height than the zero-bias barrier height. It can be determined using the relation[13,14]

$$\phi_{bf}=n\phi_{b0}-(n-1)\left(\frac{kT}{q}\right)\ln\left(\frac{N_C}{N_D^+}\right), \qquad (3)$$

where ϕ_{bf} is the flat-band barrier height, and N_C and N_D^+ are the effective density of states in the conduction band and the ionized donor density, respectively. Note that it was necessary to modify Eq. (3) to take into account the large fall in the density of ionized donor atoms as the temperature falls below 50 K, hence the use of N_D^+ instead of N_D. Both N_C and N_D^+ are functions of temperature. When the flat-band barrier height is plotted as a function of temperature it is found to have a constant value of (0.283 ± 0.003) eV, as shown in Fig. 5. This indicates that, despite conduction mechanisms other than ideal thermi-

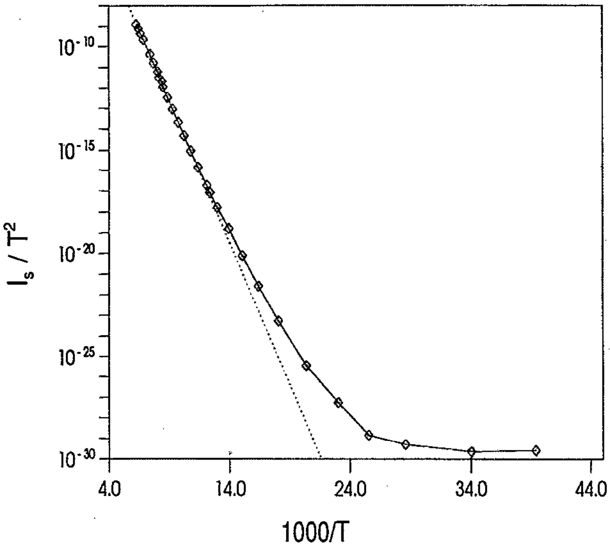

FIG. 6. Plot of $\ln(I_s/T^2)$ vs $1/T$. Note that the result is linear down to moderately low temperatures ($\sim$80 K), below which there is an increasingly large deviation from a straight line. From the linear region a zero-bias barrier height (0.276 eV) and Richardson constant can be estimated ($\sim$85 A cm^{-2} K^{-2}).

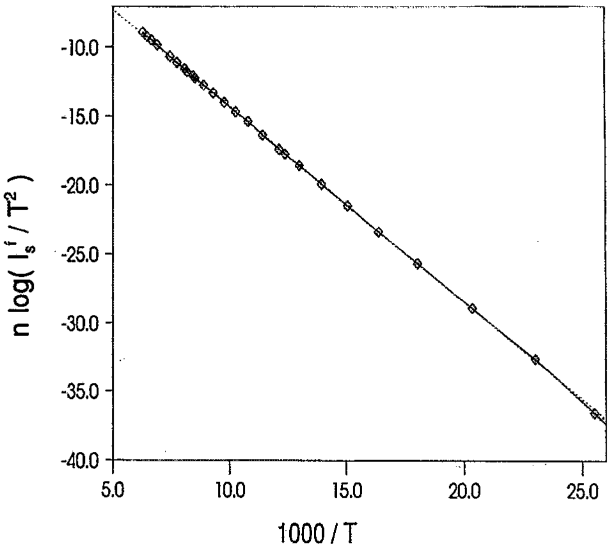

FIG. 7. $n \log(I_s^f/T^2)$ vs $1/T$ for an erbium silicide diode, giving: ϕ_{bf} =0.283 eV, A^{**}=88 A cm^{-2} K^{-2}. Note that the plot gives a linear fit over 28 orders of magnitude.

onic emission becoming significant at low temperatures (manifested as deviations in the zero-bias barrier height and ideality factor), the actual barrier height of the erbium silicide Schottky diode is essentially constant with temperature. Clearly the flat-band barrier height is a significantly better measure of the barrier height at low temperatures than is the zero-bias barrier height. In addition, the fact that the barrier height is independent of temperature over a range where the bandgap of silicon has varied significantly shows that the Fermi level is pinned to the bottom of the conduction band. This agrees with the result of Duboz *et al.*,[15] who used photoemission data at somewhat higher temperatures.

Further information can be obtained if $\ln(I_s/T^2)$ is plotted against $1/T$. From Eq. (2) it can be seen that the slope of such a plot should give the barrier height, and the intercept will give the Richardson constant. In Fig. 6 this is plotted over the temperature range 25 to 150 K. Fitting a straight line, to the data above 80 K, then gives a barrier height of (0.276±0.005) eV and an A^{**} of (85±20) A cm^{-2} K^{-2}. However, the plot begins to increasingly curve away from a straight line as the temperature falls below 70 K. Consequentially the derived Richardson constant, in particular, is very dependent on the selection of the range of temperature values. The deviation from a straight line indicates a deviation from thermionic emission-diffusion theory. Several possible mechanisms have been considered in order to explain these deviations. The electron micrograph of Fig. 1 shows that there is either no or a very small interfacial layer, making this unlikely as an explanation. The barrier height is much too low for recombination to be the explanation. Arrhenius plots [$\ln(I_s)$ vs $1/T$] confirm this as they show that the data do not form a second straight line, indicative of lower activation energy recombination current, at lower temperature. In addition the doping level is far too low for thermionic field emission or field emission tunneling to be significant.

Previous workers have modeled this effect by the introduction of a new parameter, T_0.[16–18] While this effect is not yet fully explained, it appears to be due to a combination of a particular distribution of interface states and a nonuniformly doped layer near the surface of the substrate.

It was observed above (compare Figs. 3 and 5) that ϕ_{bf} is essentially constant with temperature whereas ϕ_{b0} is not. If the expression for ϕ_{b0} from Eq. (3) is substituted into Eq. (2) then a new quantity called the flat-band saturation current (I_s^f) can be defined:

$$I_s^f = A^{**} A_d T^2 \exp\left(\frac{-q\phi_{bf}}{nkT}\right), \tag{4}$$

where I_s^f is related to I_s by

$$I_s^f = I_s/\exp\left[\frac{(n-1)}{n} \ln\left(\frac{N_D^+}{N_C}\right)\right]. \tag{5}$$

A plot of $n \ln(I_s^f/T^2)$ vs $1/T$ should thus be a straight line even at low temperatures, with the slope directly giving ϕ_{bf}. In addition, the increased temperature range over which the plot is linear provides a more reliable measure of A^{**}. Thus, this plot allows all the information readily obtained from IV plots (n, I_s, and T) to be combined in the one curve, and the fundamental parameters (ϕ_{bf} and A^{**}) easily and accurately determined. Figure 7 shows such a plot for an erbium silicide diode, from which a ϕ_{bf} of (0.281±0.002) eV and an A^{**} of (88±5) A cm^{-2} K^{-2} are obtained. Note that the plot is linear over 28 orders of magnitude.

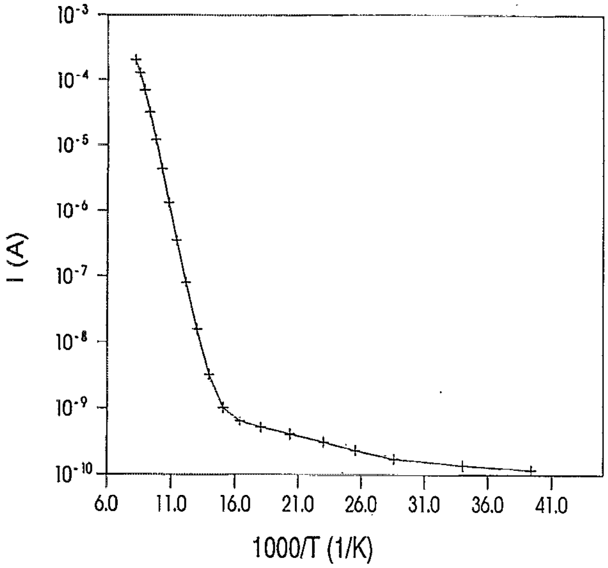

FIG. 8. Plot demonstrating the large temperature dependence of forward current, I, for thermionic emission ($T>75$ K) and the very small temperature dependence shown at low temperatures (<70 K), at low bias (0.1 V).

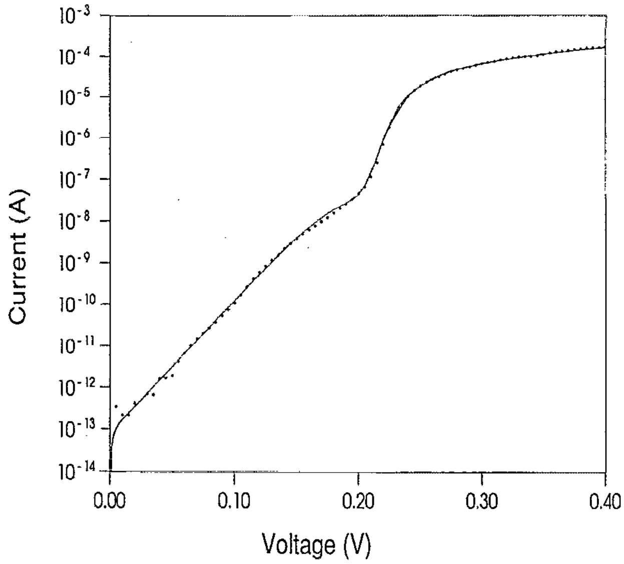

FIG. 9. An example of the quality of the fit, with two exponentials, to the IV data. The points represent the data (100 individual data points) taken at a temperature of 30 K, while the line is the fitted model.

The Schottky barrier height can be taken to be linear to first order with temperature, such that the temperature modified barrier height (ϕ_b') is given by

$$\phi_b' = \phi_b^0 + \alpha T, \tag{6}$$

where ϕ_b^0 is the zero temperature barrier height and α is the temperature coefficient of the barrier height. From Fig. 5 a value for α of 1.5×10^{-5} eV/K is obtained.

The Richardson constant can also be modified according to

$$A^{**\prime} = A^{**} \exp\left(-\frac{\alpha q}{k}\right). \tag{7}$$

When the experimental value of A^{**}, 88 A cm^{-2} K^{-2}, is compared with the commonly accepted value of approximately 110 A cm^{-2} K^{-2} an α of $\sim 2\times10^{-5}$ eV/K is obtained. Given the uncertainty in the usual value of A^{**}, this is consistent the value for α of 1.5×10^{-5} eV/K obtained from the flat-band versus temperature plot of Fig. 5. This value is much smaller than the temperature coefficient of the bandgap, providing further evidence that the Fermi level is pinned to the bottom of the conduction band.

A particularly interesting feature of the erbium silicide diodes studied is their response at low temperature and small forward bias. Looking again at Fig. 2 it can be seen that the IV plots are completely dominated at low temperature and bias by some current transport mechanism other than thermionic emission. This mechanism is characterized by almost parallel IV lines (see Fig. 2) with very weak temperature dependence, as shown in Fig. 8. Such small temperature dependence implies that a form of tunneling is operating. However, it is neither thermionic-field emission nor field emission, as both mechanisms give far too small a contribution to the current at the doping level involved. Similar low-bias IV characteristics have been observed in many heterojunction solar cells and in Schottky barriers.[19–24] We believe that the mechanism responsible is recombination via trap-assisted tunneling. The origin appears to lie in the generation of surface and near-surface interface states during the production of the diodes.

The complete IV curve, including the low bias region, can be well modeled by using a second exponential. However, unlike previous models of the low bias IV (Ref. 23) data, it was found necessary to introduce a separate series resistance in order to model the bending of the $\ln(I)$ vs V curve seen below 60 K (see Fig. 2). Figure 9 gives an example of the excellent fit of the double exponential model to the data. Another feature which can be seen in Fig. 2 is some additional structure in the very low temperature (<40 K), low bias region. While we do not yet have a clear explanation for this structure it is interesting to note that it is similar to that found for $YSi_{1.7}$ on p-type silicon at 180 K.[24] More measurements, in particular CV measurements, will be needed to clarify the understanding of these low forward bias, low current features.

V. REVERSE *IV*

Additional information on the current transport mechanisms in erbium silicide Schottky diodes can be obtained by examining their reverse bias behavior. This is especially important if the diodes are to be used as infrared detectors, since these are normally operated in reverse bias. From Fig. 2 it can be seen that the low temperature, low forward bias transport mechanism does not produce as large a current in the reverse bias mode. It is assumed that the mechanism is working but that its effect is largely lost in the noise at these very low currents.

Nevertheless, there is a steady increase of the reverse bias current with voltage. Ideally this increase in current

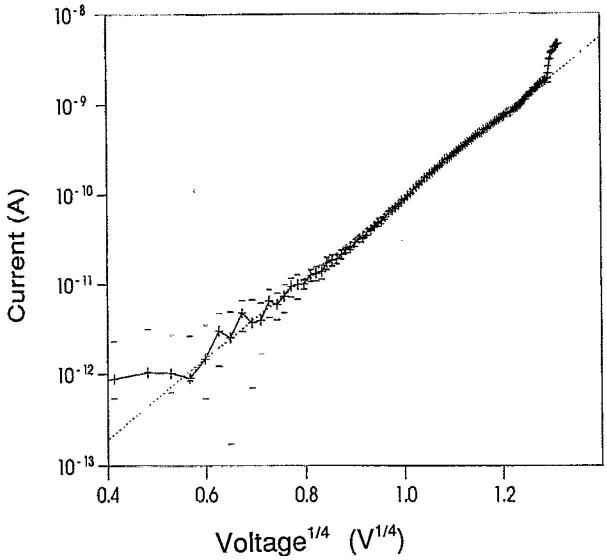

FIG. 10. Ln(I) vs $V_r^{1/4}$, demonstrating that the reverse bias current follows the reduction in the Schottky barrier height due to image force lowering for an erbium silicide diodes at 79 K.

should be due to a reduction in the barrier height caused by image-force lowering. The amount that the barrier is lowered ($\Delta\phi_{\rm bi}$) is given by[25]

$$\Delta\phi_{\rm bi}=\left[\frac{q^3N_D}{8\pi^2\epsilon_s^3}\left(\phi_b-V-\xi-\frac{kT}{q}\right)\right]^{1/4}, \tag{8}$$

where ϵ_s is the permittivity of silicon and ξ is the position of the Fermi level relative to the bottom of the conduction band. Thus, if the increase in reverse bias current with voltage is due to image force lowering, a plot of $\ln(I)$ vs $V_r^{1/4}$ should give a straight line. In Fig. 10 it can be seen that, at least to moderate voltages, this is true. At greater voltages this relation breaks down. We believe that the deviation from image force lowering controlled behavior is due to imperfections in the diode guard rings, and may represent the onset of breakdown. Thus more careful lithographic processing should result in better reverse bias performance.

VI. DISCUSSION AND CONCLUSIONS

The IV response of erbium silicide diodes on n-type silicon has been characterized over a wide range of temperatures (25 to 160 K). The results have demonstrated the general dominance of thermionic emission, in particular at the temperatures normally used for infrared detection (77 K). However, they have also shown a significant deviation from ideal thermionic emission-diffusion theory at low temperatures (<70 K). This deviation has been previously observed in other materials, and modeled by the introduction of a parameter, T_0.

The zero-bias barrier height was found to drop significantly as the temperature fell below 70 K, while the ideality factor increased at the same temperatures. The flat-band barrier height was, however, found to be a much better measure of the Schottky barrier at low temperatures, remaining essentially constant down to at least 25 K. With this in mind a new method of plotting the variation of the saturation current with temperature was developed. By plotting $n \ln(I_s^f/T^2)$ vs $1/T$, the flat-band barrier height and the Richardson constant can be directly and more accurately determined than by either the $\ln(I_s/T^2)$ vs $1/T$ or Arrhenius plots. In addition all of the available data can be used, with the result that the values derived for ϕ_{bf} and A^{**} do not depend on an arbitrary choice of data set. Using this technique, a ϕ_{bf} of (0.281 ± 0.002) eV and an A^{**} of (88 ± 5) A cm^{-2} K^{-2} were obtained.

Investigation of the variation of ϕ_{bf} with temperature has shown that the Fermi level of erbium silicide is pinned to the bottom of the conduction band. This result was confirmed by calculating the temperature coefficient of the Schottky barrier height from the variation in A^{**}. Erbium silicide has a Fermi level well above the band-gap center while most Schottky contacts have a Fermi level near or below the band-gap center and are pinned to the valence band. Thus these results support the suggestion by Duboz *et al.*[15] that the Fermi level is pinned to the nearest band. Many of the theories of Schottky barrier formation[26–28] argue that the pinning of the Fermi level is completely dominated by the surface states; however, these results indicate that both the barrier height and temperature dependence of the contact may be substantially affected by the metal. Such dependence on the metal is not unique, as other researchers[29,30] have demonstrated that the pinning of the Fermi level on GaAs is affected by the metal. Duboz *et al.*[15] have suggested some possible mechanisms by which the metal may determine the band to which the Fermi level is pinned. However, more work will be required in order to achieve a better understanding of the fundamental mechanisms involved in the pinning of the Fermi level and the determination of the Schottky barrier height.

Low temperature measurements (<60 K) demonstrated that thermionic emission was dominated for small forward bias by some other transport mechanism. It is believed that this mechanism is recombination via tunneling through surface and near-surface states.

Reverse bias measurements indicated that, at least to moderate voltages, the increase in the reverse bias current is due to image force lowering of the Schottky barrier height. At higher voltages there is some breakdown of this ideal behavior. It should be possible to greatly increase this breakdown voltage with more careful processing of the diodes. Many of the other deviations from ideal behavior might also be either eliminated or greatly reduced with more stringent processing. These deviations from ideality do, however, highlight the need for great care in device processing, especially with regard to surface defects, if very low temperature operation is desired.

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