On the Richardson constant for aluminum/gallium arsenide Schottky diodes

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Measurements have been made of the Richardson constant (A^{**}) for Al/GaAs Schottky diodes in which the aluminum is deposited epitaxially by molecular beam epitaxy. These diodes are the nearest to ideal that have yet been reported. The value of (A^{**}) for n-type GaAs, after allowing for the temperature variation of the barrier height and for the effect of tunnelling, was found to be $(0.41 \pm 0.15) \times 10^4$ A m $^{-2}$ K^{-2}. This is much lower than the previously accepted value, and confirms the low value reported by Srivastava, Arora, and Guha. Since there is no possibility of an interfacial layer in our diodes, we believe the low value of A^{**} to be an intrinsic property of the Al/GaAs interface. The value of A^{**} for Al/p-GaAs was found to be $(7.0 \pm 1.5) \times 10^4$ A m^{-2} K^{-2}, which is lower than the theoretical value, though the discrepancy is not so large as for n-type GaAs. Because of the uncertainty in A^{**}, values of barrier hights obtained from C^{-2} vs V plots are likely to be more reliable than those deduced from I/V characteristics.

I. INTRODUCTION

A reliable value of the Richardson constant is vital if one is to obtain accurate values of Schottky barrier heights from I-V measurements. Unfortunately, the value of the Richardson constant for GaAs is still open to debate.

For semiconductors with spherical constant-energy surfaces the Richardson constant is independent of crystal orientation and is given[1] by

$$A^* = 1.2 \times 10^6 (m^*/m) \text{A m}^{-2} \text{ K}^{-2},$$

where the effective mass ratio m^*/m has the value 0.067 for GaAs.[2] This yields a value of 8×10^4 A m^{-2} K^{-2} for A^*. According to Crowell and Sze[3] the effects of quantum-mechanical reflection at the interface and of phonon scattering should reduce this to a value A^{**} which is less than A^* by about 50%, and most recent workers have assumed values between 4×10^4 and 8×10^4 A m^{-2}K^{-2}. The Richardson constant is always assumed not to depend on the metal.

Experimental determinations of A^{**} can be made by measuring the saturation current density J_0 as a function of temperature and assuming the relationship

$$J_0 = A^{**} T^2 \exp(-q\varphi_b/kT) \tag{1}$$

which should hold provided the current is limited by pure thermionic emission. (All barrier heights are expressed in eV.) There is a complication if, as is usually the case, the barrier higher φ_b depends on temperature. Assuming a linear dependence of the form $\varphi_b(T) = \varphi_b(0) + \alpha T$, Eq. (1) can be written in the form

$$\ln\left(\frac{J_0}{T^2}\right) = \ln A^{**} - \frac{q\varphi_b(0)}{kT} - \frac{q\alpha}{k} \tag{2}$$

so that the correct value of the Richardson constant, A_c^{**}, can be obtained from the intercept on the vertical axis of an Arrhenius plot of $\ln(J_0/T^2)$ vs $1/T$, thus:

$$\ln A_c^{**} = \left[\ln\left(\frac{J_0}{T^2}\right)\right]_{\text{intercept}} + \frac{q\alpha}{k}.$$

If the dependence of φ_b on T is ignored, an uncorrected value A_{uc}^{**} is obtained such that

$$\ln A_{\text{uc}}^{**} = \left[\ln\left(\frac{J_0}{T^2}\right)\right]_{\text{intercept}}$$

and

$$A_c^{**} = A_{\text{uc}}^{**} \exp(q\alpha/k). \tag{3}$$

It is important to realize that the temperature dependence of φ_b cannot be obtained from the I/V characteristics unless the accurate value of A_c^{**} is known. This requires a knowledge of the parameter $\alpha(= d\varphi_b/dT)$, which can only be obtained from photoelectric or C/V measurements. If some inaccurate value A_i^{**} is used, then an incorrect value of the barrier height $\varphi_b'(T)$ will be obtained from the I/V measurements if one uses Eq. (1), such that

$$\varphi_b'(T) = \varphi_b(T) + \frac{kT}{q} \ln(A_i^{**}/A_c^{**}),$$

and a false temperature dependence of φ_b will be obtained. In particular, if the uncorrected value A_{uc}^{**} [Eq. (3)] is used, then $\varphi_b'(T) = \varphi_b(0)$, and the barrier height obtained from the I/V characteristics will show no temperature dependence.

It is essential when making C/V measurements to use the full expression for the barrier height

$$\varphi_{bCV} = V_I + \frac{kT}{q} + \xi,$$

where V_I is the intercept of the C^{-2} vs V plot on the voltage axis and $\xi = E_C - E_F$. The temperature dependence of the last two terms is positive, and opposite in sign to dV_I/dT.

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A careful series of measurements of A^{**} and α has been reported by Srivastava, Arora, and Guha[4] for gallium arsenide Schottky diodes with contacts of gold and aluminum. These diodes were prepared by etching the GaAs and then evaporating the metal in a conventional vacuum system at a pressure of 10^{-5} Torr, so that one would expect a thin oxide layer to exist between the gallium arsenide and the metal. For both metals the temperature coefficient α, obtained from C/V characteristics, had the value $-(3.5\pm0.3)\times10^{-4}$ eV K^{-1}. The intercepts of the $\ln(J_0/T^2)$ vs $1/T$ plots led to values of A^{**}_{uc} in the range $(55–95)\times10^4$ A m^{-2} K^{-2} for gold and $(19–45)\times10^4$ A m^{-2} K^{-2} for aluminum, yielding values of A^{**}_c in the range $(0.95–1.64)\times10^4$ A m^{-2} K^{-2} for Au and 0.32 to 0.78×10^4 A m^{-2} K^{-2} for Al. Srivastava *et al.* suggest that the lower values for the Al/GaAs diodes may arise from the presence of an interfacial layer brought about by a chemical reaction between the aluminum and the native oxide on the surface of the gallium arsenide. The values for both gold and aluminum are significantly below the theoretical values.

II. EXPERIMENT

In an attempt to shed further light on the discrepancy, we have made measurements of the Richardson constant for Al/GaAs diodes in which the aluminum is deposited epitaxially by molecular beam epitaxy,[5] with a background pressure in the mid 10^{-10} Torr range. We can confidently assume the absence of an interfacial oxide layer. The aluminum film was an almost perfect single crystal, and the I/V characteristics were the most close to ideal that have yet been reported.[5] Diodes were made using both n- and p-type GaAs, with $N_d=1.4\times10^{22}$ m^{-3} and $N_a=3.0\times10^{22}$ m^{-3}, respectively. I/V and C/V characteristics were measured over a range from 200 to 400 K, the capacitance measurements being made at a frequency of 1 Mhz. The ideality factors for the I/V characteristics (defined[1] by expressing the characteristics in the empirical form $J=J_0\exp(qV/nkT)\{1-\exp(-qV/kT)\}$) were not greater than 1.03 over the entire temperature range, and the C^{-2} vs V plots were indistinguishable from straight lines. The quality of the diodes is demonstrated by the electrical characteristics shown in Figs. 1 and 2.

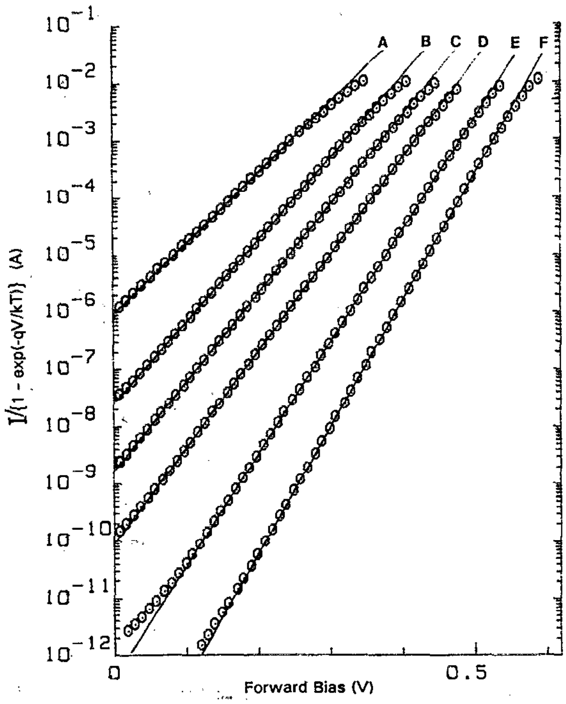

FIG. 1. Logarithmic plots of $I/\{1-\exp(-qV)$ vs forward bias for n-type Al/GaAs diodes at various temperatures. A: 402 K, $n=1.002$, B: 352 K, $n=1.005$, C: 322 K, $n=1.008$, D: 292 K, $n=1.01$, E: 252 K, $n=1.02$, F: 222 K, $n=1.03$.

For the n-type diodes, φ_{bCV} was found to decrease linearly with temperature with $\alpha=-(3.8\pm0.3)\times10^{-3}$ eV

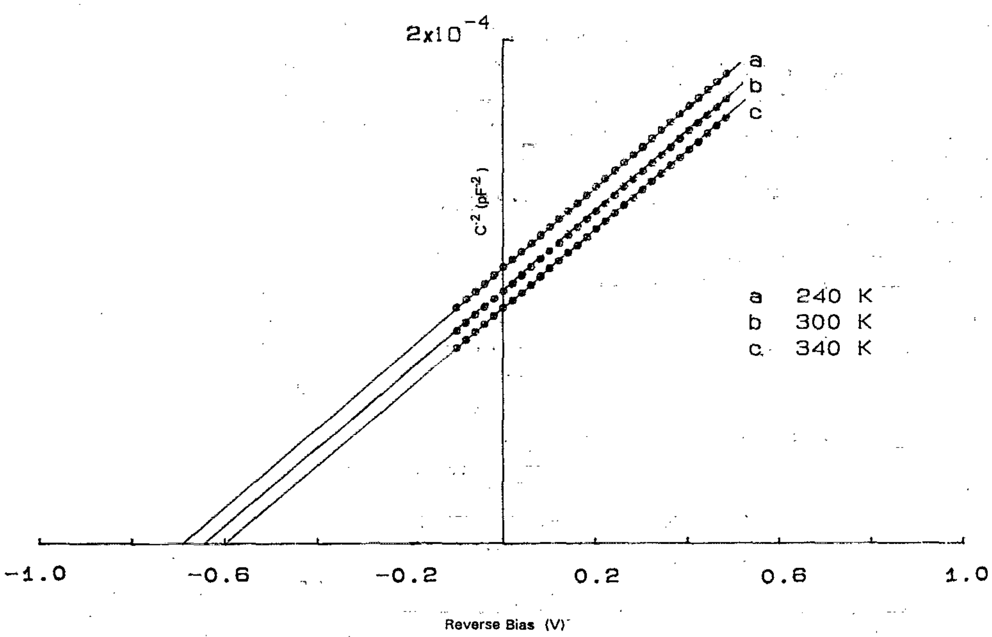

FIG. 2. Plots of C^{-2} vs V for n-type Al/GaAs diodes at various temperatures. a: 240 K, b: 300 K, c: 340 K.

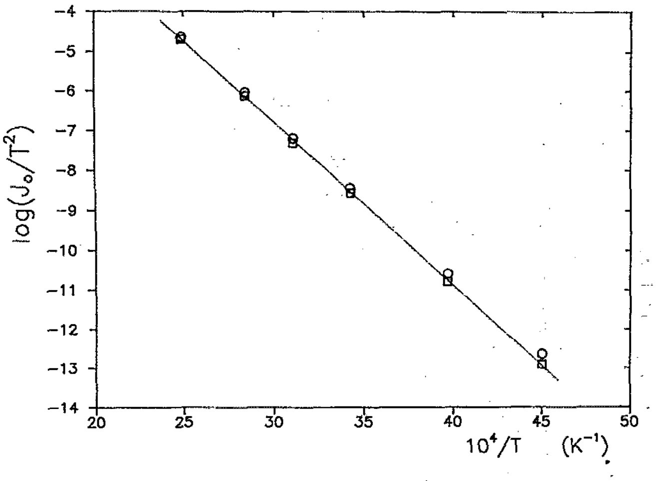

FIG. 3. Plot of $\log(J_0/T^2)$ vs $10^4/T$ for n-type Al/GaAs diodes. ○: raw data, □: corrected for tunnelling.

K^{-1}, in good agreement with Srivstava *et al.* The Arrhenius plots of $\ln(J_0/T^2)$ vs $1/T$, represented by circles in Fig. 3, were linear and yielded a value 21.2×10^4 A m^{-2} K^{-2} for A^{**}_{uc}, leading to $A^{**}_c=(0.27\pm0.05)\times10^4$ A m^{-2} K^{-2}. This value is not significantly lower than the lower limit of the range obtained by Srivastava *et al.* for aluminum. Since we can be confident that there is no interfacial layer in our diodes, it seems that the low value of A^{**}_c is an intrinsic property of the Al/GaAs interface and not an artefact.

For p-type material we found that φ_b was much less dependent on temperature than for n-type, giving $\alpha=-(1.6\pm0.2)\times10^{-4}$ eV K^{-1}. The intercept of the plot of $\ln(J_0/T^2)$ vs $1/T$ gave $A^{**}_{uc}=45\times10^4$ A m^{-2} K^{-2} leading to a value of 7.0×10^4 A m^{-2} K^{-2} for A^{**}_c. This compares with the theoretical value $A^*=60\times10^4$ A m^{-2} K^{-2} obtained by using the heavy-hole effective mass.

III. THE EFFECT OF TUNNELLING

For our n-type diodes the tunnelling parameter E_{00} (using the nomenclature of Padovani and Stratton[6]) has the value 2.4×10^{-3} eV, so that the ratio kT/qE_{00} exceeds seven over the entire temperature range, and one would expect the effect of tunnelling to be negligible.[1] However, Rideout and Crowell[7] have calculated the effect of tunnelling through a Schottky barrier modified by the effect of the image force, and their analysis predicts that for lightly-doped material tunnelling may cause a significant increase in the magnitude of the forward current even though there is little change in the ideality factor. They show that if the current is limited by almost pure thermionic emission, the effect of tunnelling is to increase the forward current by a factor F, where

$$F=\frac{1}{kT}\int_{-qV_m}^{\infty}\frac{\exp(-U/kT)}{1+\exp(-U/E_t)}dU.$$

Here U is the energy of an electron measured with respect to the maximum of the image-lowered barrier, $E_t=(E_{00}/\pi)(8E_b/\Delta\varphi_{bi})^{1/2}$ where E_b is the diffusion-voltage ignoring the image-force lowering $\Delta\varphi_{bi}$, and V_m is the maximum band-bending after allowing for the image force, so that $V_m=E_b-\Delta\varphi_{bi}$. [The lower limit for the integral given here differs from that in Rideout and Crowell's Eq. (38) because in their equation the integration is with respect to E, where $E=U+qV_m$.]

The lower limit of the integral corresponds to those electrons which tunnel through the barrier with energies equal to that of the bottom of the conduction band in the bulk semiconductor. For the light doping used in these experiments the probability of tunnelling for such electrons is completely negligible, and we may therefore take the lower limit of integration to be $-\infty$ without perceptible error. Making use of the identity[8]

$$p\int_{-\infty}^{\infty}\frac{e^{-px}}{1+e^{-qx}}dx=\frac{p\pi}{q}\operatorname{cosec}\left[\frac{p\pi}{q}\right]$$

which holds for $q>p>0$, we may write

$$F=\left[\frac{\pi E_t}{kT}\right]\operatorname{cosec}\left[\frac{\pi E_t}{kT}\right].$$

The effect of tunnelling may therefore be taken into account by constructing an Arrhenius plot of $\ln(J_0/FT^2)$ vs $1/T$. Since F increases with decreasing temperature, the effect of including F is to increase the (negative) slope of the Arrhenius plot and to increase the magnitude of the intercept on the vertical axis. The incorporation of the correction factor F into our results is represented by the squares in Fig. 3, and increases A^{**}_{uc} to 32.2×10^4 A m^{-2} K^{-2} and A^{**}_c to 0.41×10^4 Am^{-2} K^{-2}, showing that the effect of tunnelling is small but not negligible. For the p-type specimens the effect is smaller because of the smaller value of E_{00}. The values A^{**}_{uc} and A^{**}_c shown in Table I are corrected for the effect of tunnelling.

IV. BARRIER HEIGHTS

From Eq. (2) (modified to allow for the effect of tunnelling), the slope of a plot of $\ln(J_0/FT^2)$ vs $1/T$ is equal to $-q\varphi_b(0)/K$. The value of $\varphi_b(0)$ for n-type samples obtained in this way, which we denote by $\varphi_{bact}(0)$, is 0.82

TABLE I. Results for n-type and p-type Al/GaAs diodes. All barrier heights are in eV.

Type	N_d,N_a (m^{-3})	$\Delta\varphi_{bi}$	α (eV K^{-1})	A^{**}_{uc} (A m^{-2} K^{-2})	A^{**}_c (A m^{-2} K^{-2})	$\varphi_{bact}(0)$	$\varphi_{bact}(0)+\Delta\varphi_{bi}$	$\varphi_{bCV}(0)$	$\varphi_{bIV}(300)+\Delta\varphi_{bi}$	$\varphi_{bCV}(300)$
n	1.4×10^{22}	0.026	$-(3.8\pm0.3)\times10^{-4}$	32×10^4	$(0.41\pm0.15)\times10^4$	0.82	0.84_6	0.87	0.72_9	0.76
p	3.0×10^{22}	0.029	$-(1.6\pm0.2)\times10^{-4}$	45×10^4	$(7.0\pm1.5)\times10^4$	0.62_5	0.65_4	0.68	0.60_9	0.64

eV, as shown in Table I. This would be the notional barrier height at absolute zero as encountered by an electron crossing into the metal, and includes the image-force reduction $\Delta\varphi_{bi}$. To compare this with the barrier height (φ_{bCV} (0) obtained from the capacitance measurements we must add on $\Delta\varphi_{bi}$, and this comparison is shown in columns 8 and 9 of Table I. Both $\varphi_{\mathrm{bact}}(0)$ and $\varphi_{bCV}(0)$ are notional barrier heights in the sense that they are the values that would be obtained if the barrier height continued to increase linearly with decreasing temperature down to absolute zero. This, however, cannot be so. The barrier height is related in a complicated way to the band gap, which does not increase linearly with decreasing temperature but follows an approximately parabolic temperature dependence. The agreement between the two values obtained from the I/V and C/V characteristics is imperfect, but does not greatly exceed the experimental error, which is about ± 0.01 eV in each case.

The value of A_c^{**} deduced from the Arrhenius plot enables us to calculate the barrier height at any temperature from the I/V characteristics, using Eq. (1). A comparison between $\varphi_{bIV} + \Delta\varphi_{bi}$ obtained in this way and φ_{bCV} at 300 K is shown in columns 10 and 11 of Table I. The agreement is not especially good, but is only just outside the experimental error, which is about ± 0.02 eV for φ_{bIV} and ± 0.01 eV for φ_{bCV}. (The apparently good agreement between φ_{bIV} and φ_{bCV} which we claimed previously[5] was based on a value of 3×10^4 Am^{-2} K^{-2} for A^{**}.)

It is instructive to compare the value of the sum $\varphi_{bn} + \varphi_{bp}$ obtained by the two methods with the band gap E_g, since, if the same set of interface states determine the barrier height in each case, the sum of the two barrier heights should equal E_g.[1] At 300 K the agreement between the sum of the barrier heights and the band gap (1.42 eV) is better for the C/V data (1.40 eV) than for the I/V data (1.34 eV). The agreement in the case of the I/V values could be improved by adopting larger values of A_c^{**}, but if this were done the temperature variation of the barrier height as deduced from Eq. (1) would no longer agree with that obtained from the C/V data. There is no point in making a similar comparison at absolute zero, since, as we have already pointed out, both $\varphi_{\mathrm{bact}}(0)$ and $\varphi_{bCV}(0)$ are notional values and not true values.

V. DISCUSSION AND CONCLUSION

The most important result of this work is the confirmation of the very low value of A^{**} for Al/n-GaAs Schottky diodes reported by Srivastava, Arora, and Guha, which is very much lower than the theoretical value. Since our measurements were made on almost perfect diodes in which the aluminum is deposited epitaxially by molecular beam epitaxy in an ultrahigh vacuum, it would appear that this result is an intrinsic property of Al/GaAs contacts, and not an artefact due to the presence of an interfacial oxide layer as proposed by Srivastava *et al.*

We have not yet been able to make measurements with other metals, but plan to do so at the earliest opportunity. If it should turn out that for other metals on GaAs the Richardson constant has a value closer to the theoretical value, as was found by Srivastava *et al.* for gold, this would be a most important result, since it would mean that the Richardson constant depends on the metal as well as on the semiconductor. R. H. Williams (private discussion) has suggested that such a dependence on the the metal could arise if the conduction band of the metal were to have forbidden gaps in certain directions in k space, as is known to happen with some metals. If the k direction associated with one of these gaps were to be normal to the plane of the interface, an electron could not easily pass from the semiconductor into the metal. Such an effect could only appear if the metal were a single crystal, as is indeed the case with our diodes. However, the diodes used by Srivastava *et al.* were polycrystalline, yet they also observed a low value for Al.

Using this low value for A^{**}, the values of φ_b deduced from the I/V characteristics are slightly lower than those obtained from the C/V data, but by an amount which is only just outside the experimental error. The reliance of the I/V barrier heights on an accurate value of A^{**} suggests that C/V determinations of φ_b are more reliable, provided the C^{-2} vs V plots are good straight lines and independent of frequency.

The value of A^{**} was also found to be lower than the theoretical value for Al/p-GaAs diodes, thought the discrepancy is not so great as for the n-type case.

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