Correlation between current-voltage and capacitance-voltage Schottky barrier height on (100) and (110) GaAs and (110) InP surfaces

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(Received 28 August 1989; accepted for publication 13 June 1990)

Recently, systematic studies of the electrical properties of both n- and p-type Schottky diodes formed by a large number of metals on GaAs of both (100) and (110) orientation and on (100)-oriented InP have been reported. Current-voltage (I-V) and capacitance-voltage (C-V) measurements were carried out and the barrier heights were evaluated in these studies. In this paper, these I-V zero-bias barrier heights have been correlated with the ideality factors of these diodes. Resulting from this modified barrier height approach is a more fundamental flat-band (zero-field) barrier which compares remarkably well with the reported values from the C-V measurements. In addition, the sum of the modified n- and p-type flat-band barrier heights for the GaAs (100) and InP (110) Schottky diodes is in better agreement with the band gap for each of the different metals used than the initially reported results.

I. INTRODUCTION

Electrical studies of Schottky diodes on GaAs and InP surfaces have been of considerable interest for the past 20 years.[1–7] Recently there has been a considerable expansion of information on the properties of these diodes for a large range of metals.[8–11] These thorough and systematic studies of the electrical properties of a vast number of metal/GaAs and metal/InP diodes (both n and p type, with different crystal orientation, formed under ultrahigh vacuum conditions with *in situ* cleavage and metal deposition) have enabled the evaluation and verification of an analytical method correlating the barrier height determined from current-voltage (I-V) measurements with that obtained from the capacitance-voltage (C-V) method.

This analytical approach was first developed by Wagner *et al.* to analyze n-type PtSi Schottky diodes[12] and further extended by Chin *et al.*[13] to test its validity on p-type PtSi Schottky diodes. It was found that this approach works remarkably well. The barrier height of a Schottky diode is field dependent and consequently bias dependent, which results in a correlation between the diode ideality factor and the measured barrier height. Since the barrier height is field dependent, it is fundamentally more rigorous to specify it under a standard field condition to allow comparison between different metals and substrates evaluated using different measurements. The flat-band (zero-field) barrier height is introduced to serve this purpose.

Hence, the aim of the present paper is twofold. First, it is to show that this relatively simple method does indeed give consistent results not only with Si-based Schottky diodes but III-V semiconductor-based Schottky diodes as well. Second, it is to tabulate the zero-field barrier heights of a large number of metals on GaAs and InP to investigate substrate orientation effects upon these fundamental barrier heights, and to investigate a possible correlation between the sum of these barrier heights on n- and p-type substrates and the substrate band gap.

II. METHOD OF ANALYSIS

The standard expression for analyzing the forward-biased I-V data for a moderately doped Schottky diode is given by[14]

$$I = aA^{**}T^2 \exp\left(\frac{-q\phi_{b,i}}{kT}\right) \times \left[\exp\left(\frac{q}{kT}(V-IR)\right)-1\right], \qquad (1)$$

where the various terms are as follows: a is the area of the diodes (cm^2), A^{**} is the effective Richardson constant (A/cm^2 K^2), T is the temperature (K), q is the electronic charge (C), k is Boltzmann's constant (J/K), $\phi_{b,i}$ is the flat-band barrier height [subscript i denotes n or p type (eV)], V is the forward voltage (V), and R is the contact and bulk resistance (Ω). This expression is based on a

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combined thermionic emission and diffusion theory formulation of current flow in the diode. The modified Richardson constant, A^{**}, includes the effects of quantum mechanical reflection and transmission of carriers negotiating the barrier, and phonon scattering of carriers between the top of the barrier and the surface of the metal. Due to the high effective resistance of the depletion region, the voltage drop across the contact and bulk resistance is usually insignificant (except at high current) and thus the IR term in the square bracket can be neglected. Both the A^{**} and $\phi_{b,i}$ terms in Eq. (1) are, in general, field dependent and thus bias dependent. However, the theoretical analysis of Crowell and Sze[15] shows that A^{**} is essentially constant over the range of fields where diodes operate. Consequently, A^{**} is regarded as a constant in this analysis. The barrier height can then be expanded to give

$$\phi_{b,i}(V)=\phi_{b0,i}+\frac{\partial\phi_{b,i}}{\partial V}V+\dots . \tag{2}$$

Neglecting the small dependence of A^{**} on field as described above and hence on bias, the effective barrier height, $\phi_{b,i}(V)$, can be related to the zero-bias barrier height, $\phi_{b0,i}$, and the ideality factor n, of the diode, by neglecting the higher-order terms in Eq. (2).[16,17] The relationship between $\partial\phi_{b,i}/\partial V$ and n is given by the expression

$$\frac{\partial\phi_{b,i}}{\partial V}=1-\frac{1}{n}. \tag{3}$$

Since $\phi_{b,i}$ would be expected to increase with V due to reduced image force barrier lowering effects, the ideality factor n would be expected to be slightly greater than unity and be virtually constant over the limited forward voltage range. Using Eqs. (2) and (3), the thermionic emission equation for moderate forward bias (where $V>3kT/q$) can be written as

$$I=aA^{**}T^2\exp\left(-\frac{q\phi_{b0,i}}{kT}\right)\exp\left(\frac{qV}{nkT}\right). \tag{4}$$

Equation (4) indicates that the barrier height obtained experimentally from I-V measurements using the normal approach[18] is $\phi_{b0,i}$, the zero-bias barrier height. The flat-band or zero-field barrier height, ϕ_{bn} or ϕ_{bp}, can be calculated by deriving two diode parameters, n, the ideality factor, and $\phi_{b0,i}$, the zero-bias barrier height from the I-V measurements. The flat-band value given by[12,13]

$$\phi_{bn}=n\phi_{b0,n}-(n-1)(kT/q)\ln(N_C/N_D), \tag{5a}$$

$$\phi_{bp}=n\phi_{b0,p}-(n-1)(kT/q)\ln(N_V/N_A). \tag{5b}$$

The terms N_C, N_D, N_V, and N_A are the effective density of states in the conduction band, donor density, effective density of states in the valence band, and acceptor density, respectively. It is known that the barrier height obtained from the C-V measurement gives essentially the flat-band barrier.[19] Therefore, Eqs. (5a) and (5b) provide a simple way to compare the barrier height obtained from the two experimental methods, and to test the consistency of this analytical approach.

TABLE I. Physical constants and parameters used in the flat-band barrier calculations.

	GaAs[a]			InP[a]	
	n-type (110)	n-type (100)	p-type (100)	n-type (110)	p-type (110)
m^*	0.067	0.067	0.471	0.077	0.64
$N_C(\mathrm{cm}^{-3})\times10^{17}$	4.0	4.0		5.0	
$N_V(\mathrm{cm}^{-3})\times10^{16}$			760		2.0
$N_D(\mathrm{cm}^{-3})\times10^{16}$	5.0,2.0	6.0		0.6	
$N_A(\mathrm{cm}^{-3})\times10^{16}$			8.0		2.0
T(K)	293	300	300	298	298

[a]Values are obtained from Ref. 32.

III. RESULTS

Experimental data for the barrier height, obtained from both I-V and C-V measurements, and the corresponding ideality factors (n) for n-type (110), both n- and p-type (100) GaAs Schottky diodes and both n- and p-type (110) InP Schottky diodes for a large range of metals are obtained from Refs. 8–11, respectively. The (110) GaAs and (110) InP samples were prepared by *in situ* deposition of various metals on clean surfaces by cleavage in ultrahigh vacuum (UHV), whereas the (100) GaAs samples are fabricated in UHV onto clean GaAs surfaces at room temperature. Table I is a list of the values assigned to the parameters required in the calculation. Using these values, the more fundamental flat-band barrier height can be determined with the results described below.

A. n-type GaAs (110)

The flat-band barrier heights determined from the I-V zero-bias barrier are tabulated in Table II for two different donor densities. The zero-bias barrier heights, the ideality factors n, and the barrier height determined from C-V measurements where available (from Ref. 8) are also listed in the table. It is observed that the calculated flat-band barrier height, ϕ_{bn}, and the C-V barrier, ϕ_{CV}, are in excellent agreement for all metals except Ag and Au (for N_D of 5×10^{16}

TABLE II. Calculated flat-band barrier heights ϕ_{bn} compared to C-V barrier heights ϕ_{CV} for n-type (110) GaAs Schottky diodes for two donor densities. Also shown are experimental zero-bias barrier heights ϕ_{b0} and the ideality factors, n. All barrier heights have units of eV, and ϕ_{CV} has an uncertainty of ±0.05 eV.

	$N_D=5\times10^{16}\ \mathrm{cm}^{-3}$				$N_D=2\times10^{17}\ \mathrm{cm}^{-3}$			
Metal	ϕ_{b0}[a]	n[a]	ϕ_{CV}[a]	ϕ_{bn}[b]	ϕ_{b0}[a]	n[a]	ϕ_{CV}[a]	ϕ_{bn}[b]
Cu	0.87	1.05	0.94–1.08	0.91	0.83	1.10	0.89	0.91
Pd	0.85	1.05	0.88	0.89	0.80	1.09	0.84	0.87
Ag	0.89	1.05	0.97	0.93	0.85	1.08	0.89	0.92
Au	0.92	1.05	1.02	0.96	0.88	1.10	0.95	0.97
Al	0.80–0.85	1.05	0.85–0.89	0.84–089	0.73	1.09	0.77	0.79
Mn	0.72	1.05	0.75	0.75	0.72	1.09		0.78
Ni	0.77	1.06	0.82	0.81	0.73	1.09	0.77	0.79
Sn	0.77	1.06	0.83	0.81	0.72	1.09	0.81	0.80
Cr	0.67	1.06	0.72	0.71	0.64	1.09	0.73	0.70

[a]From Ref. 8. Note the zero-bias barrier height excludes image force.
[b]This work.

TABLE III. Calculated flat-band barrier heights, ϕ_{bn} and ϕ_{bp} for n-type and p-type (100) GaAs Schottky Diodes. Also shown are experimental zero-bias barrier heights ϕ_{b0} and ideality factors n. All barrier heights have units of eV, and ϕ_{CV} has an uncertainty of ± 0.05 eV.

	n-type				p-type		
Metal	ϕ_{b0}[a]	n[a]	ϕ_{CV}[b]	ϕ_{bn}[a]	ϕ_{b0}[b]	n[a]	ϕ_{bp}[b]
Cu	0.92	1.05	0.96	0.96	0.42	1.24	0.49
Pd	0.87	1.03	0.93	0.90	0.47	1.21	0.55
Ag	0.86	1.03	0.89	0.88	0.47	1.21	0.55
Au	0.85	1.03	0.87	0.87	0.47	1.15	0.53
Al	0.81	1.07	0.84	0.86	0.58	1.06	0.60
Ti	0.79	1.03	0.83	0.82	0.53	1.37	0.68
Mn	0.77	1.07	0.89	0.82	0.53	1.18	0.61
Pb	0.76	1.03	0.91	0.78	0.49	1.13	0.54
Bi	0.73	1.03	0.79	0.75	0.58	1.08	0.62
Ni	0.73	1.15	0.91	0.83	0.59	1.13	0.65
Cr	0.73	1.04	0.81	0.76	0.53	1.09	0.57
Co	0.72	1.08	0.86	0.77	0.58	1.19	0.67
Fe	0.68	1.02	0.75	0.69	0.57	1.23	0.68
Mg	0.58	1.03	0.66	0.61	0.52	1.44	0.70

[a]From Ref. 9. Note the zero-bias barrier height excludes the image force.
[b]This work.

cm^{-3}) where the differences are in excess of 0.03 eV. Although this is still well within the limit of experimental uncertainty, this difference will be commented on in more detail later. For N_D of 2×10^{17} cm^{-3}, the barrier heights agree to within 0.03 eV. This is again well in the limit of experimental uncertainty.

B. n- and p-type GaAs (100)

Similarly, the flat-band barrier height of both n- and p-type GaAs (100) Schottky diodes on various metals are calculated from I-V barrier heights and the corresponding ideality factors. The results are presented in Table III. Again, the n-type flat-band barrier heights, ϕ_{bn}, obtained are in good agreement with C-V measurements, ϕ_{CV}, except for Pb, Ni, and Co contacts where the differences are in the order of 0.1 eV. At this stage, it is not clear why the correlation is not good for these metals. However, it should be pointed out that the accuracy of the diode ideality factor measurement is important in establishing an accurate flat-band barrier height. For p-type barriers, no comparison can be made as C-V barrier heights were not measured on the corresponding diodes.

C. n- and p-type InP (110)

The flat-band barrier heights of n- and p-type InP(110) Schottky diodes for a large number of metals have also been calculated from previous experimental data. They are tabulated together with the I-V zero-bias barriers, diode ideality factors, and C-V barriers, where available, in Table IV. It is observed that the flat-band barrier height evaluated from Eq. (5) again compares reasonably well (to within experimental uncertainty) with the C-V measurements although not as well as in the case of GaAs.

TABLE IV. Calculated flat-band barrier heights, ϕ_{bn} and ϕ_{bp}, for n- and p-type (110) InP Schottky diodes. Also shown are experimental zero-bias barrier heights ϕ_{b0} and the ideality factors n. All barrier heights have units of eV, and ϕ_{CV} has an uncertainty of ± 0.05 eV.

	p-type(110)				n-type(110)		p-type(100)	
Metal	ϕ_{b0}[a]	n[a]	ϕ_{CV}[a]	ϕ_{bp}[b]	ϕ_{b0}[c]	n[c,d]	ϕ_{bn}[b]	ϕ_{CV}[e]
Ag	0.76	1.04	0.77	0.784	0.54	1.02	0.55	0.86
Cr	0.82	1.04	0.74–0.82	0.874	0.45	1.10	0.48	
Cu	0.90	1.04	0.86	0.93	0.42	1.03	0.43	
Au			0.86		0.42	1.03	0.43	0.93
Pd	0.87	1.03	0.87	0.890	0.41	1.03	0.42	0.90
Sn					0.35	1.04	0.36	
Mn	0.94	1.05	0.95	0.979	0.35	1.10	0.37	
Al	0.98	1.08	0.97–1.00	1.046	0.325	1.0	0.33	1.12
Ni	0.93	1.10	0.96	1.007	0.32	1.0	0.32	1.14

[a]From Ref. 10.
[b]This work.
[c]From Ref. 11.
[d]Only average values are listed here.
[e]From Ref. 37, these Schottky contacts are prepared on chemically etched p-type InP.

D. Sum of n- and p-type barriers

According to Schottky's original model,[20] the barrier height is very much dependent on the metal work function, and the barrier height on n- and p-type substrates is expected to add up to the band gap of the semiconductor.[20] From the results of Tables II, III, and IV, little or no correlation between the metal work function and the barrier height can be established. For a variety of semiconductors, several workers[8,10,21–22] have found that the barrier height is essentially independent on the metal work function and the position of the Fermi level is pinned. Numerous models have been proposed to explain the above behavior.

The influence of localized surface states on determining the Schottky barrier height was first discussed by Bardeen.[23] When the metal is brought into contact with the semiconductor, equilibrium of the Fermi level is reached by the exchange of charges between the metal and the surface states. If the surface state density is large enough, the barrier height is then solely dependent on the surface states and becomes independent of the metal work function. Heine[24] and, more recently, Louie and Cohen[25] have instead argued that the metal-induced gap states (MIGS) and not semiconductor surface states that are responsible for the pinning of the Fermi level. The MIGS arise from the penetration of the tails of metal electronic wavefunction into the band gap of the semiconductor at the interface, with an attenuation length of the order of a few angstroms or a bond length. Spicer *et al.*[26,27] have also proposed a model of barrier height formation on III-V compound semiconductor based on the formation of defect levels caused by the deposition of foreign metals. These defects give rise to donor and acceptorlike interface states in the band gap of the semiconductor which are able to pin the Fermi level.

The physical mechanism that causes the pinning of the Fermi level and thus the barrier height is still under considerable debate as shown above. However, it should be emphasized that the fundamental pinning mechanisms proposed have similar elements, i.e., the existence of some type of interface state during or before the metal deposition that results in the observed pinning.

Using the simplest qualitative picture provided by Bardeen's theory, Cowley and Sze[28] have shown that for n-type semiconductor, the barrier height can be approximated by

$$\phi_{bn}=\gamma(\phi_m-\chi_s)+(1-\gamma)(E_g-\phi_0), \tag{6}$$

where the various terms are defined as ϕ_m, the metal work function (eV), $\gamma=\epsilon_i/(\epsilon_i+q\delta D_s)$, χ_s, the electron affinity of the semiconductor (eV), E_g, the energy gap of the semiconductor (eV), ϕ_0, the neutral level for the surface states (eV), and D_s, the density of surface state ($\mathrm{eV}^{-1}/\mathrm{cm}^{-2}$). It is observed that when γ approaches 1, the original Schottky model prevails and when γ approaches 0, the interface states play a major role in determining the Schottky barrier. Also note that the above expression is valid only if the charge in the surface states is very much greater than the charge in the diode depletion region. It also assumes the presence of a very thin interfacial film exists between the metal and semiconductor. The corresponding expression for the p-type semiconductor is[29]

$$\phi_{bp}=\gamma(\chi_s-\phi_m+E_g)+(1-\gamma)\phi_0. \tag{7}$$

By adding the two previous expressions, we again find that $\phi_{bn}+\phi_{bp}=E_g$ as in the Schottky model, assuming the same surface-state parameters in both cases. While the precise mechanism determining Schottky barrier height is still under some debate, there are some grounds for expecting that the sum of the n- and p-type barrier heights to add up to the band gap. Previous work[30] suggest this is a reasonable approximations for Si. This is also found to be true for Al and Sb on GaAs Schottky diodes.[31]

To investigate this aspect for GaAs and InP, the sum of $\phi_{bn}+\phi_{bp}$ has been calculated with the results listed in Table V. The band gap of GaAs is reported to be 1.424 eV.[33] With the exception of Mg, the sum of $\phi_{bn}+\phi_{bp}$ for all other metals is randomly scattered within 0.1 eV of the value of the band gap. The mean value is 1.408 ± 0.06 eV, in close agreement with the band gap. Waldrop[9] has also tabulated the sum of $\phi_{bn}^{IV}+\phi_{bp}^{IV}$,[34] the image force corrected barrier heights and his results are also presented in Table V. This sum is consistently lower than the bandgap with an average value of 1.365 ± 0.065 eV. The sum of $\phi_{bn}+\phi_{bp}$ for InP is also shown in Table V. The results are in good agreement with the accepted value of the band gap of InP of 1.344 eV.[33] The average $\phi_{bn}+\phi_{bp}$ from the present analysis and from the corresponding analysis by Newman *et al.*[9] are 1.342 ± 0.020 and 1.338 ± 0.023 eV, respectively.

TABLE V. The sum of flat-band barrier height $\phi_{bn}+\phi_{bp}$ evaluated from the *I-V* measurements. Also included are the results from the initial reports.

Metal	GaAs(100) $\phi_{Bn}+\phi_{Bp}$ [a] (eV)	GaAs(100) $\phi_{b0,n}^{IV}+\phi_{b0,p}^{IV}$ [b] (eV)	InP(100) $\phi_{bn}+\phi_{bp}$ [a] (eV)	InP(100) $\phi_{b0,n}^{IV}+\phi_{b0,p}^{IV}$ [c] (eV)
Cu	1.46	1.41	1.36	1.37
Pd	1.44	1.41	1.31	1.33
Ag	1.43	1.40	1.33	1.35
Au	1.40	1.39		
Al	1.47	1.46	1.37	1.355
Ti	1.48	1.39		
Mn	1.43	1.37	1.35	1.34
Pb	1.32	1.32		
Bi	1.37	1.38		
Ni	1.48	1.39	1.33	1.30
Cr	1.33	1.33	1.33	1.32
Co	1.44	1.37		
Fe	1.37	1.32		
Mg	1.31	1.17		
Average	1.410 ± 0.060	1.365 ± 0.065	1.341 ± 0.02	1.338 ± 0.023

[a]This work.
[b]From Ref. 9, Table II.
[c]From Ref. 10, Table I.

E. Further discussions

It can be seen that the flat-band barrier height ϕ_{bn} for the n-type (100) GaAs Schottky diodes (Table III) is slightly larger than the ϕ_{bn} of n-type (110) GaAs Schottky diodes for all metals except Ag and Au (Table II). However, as mentioned earlier, the measurement of the flat-band barrier of n-type (110) GaAs Schottky diodes for Ag and Au using *I-V* and *C-V* methods gives the least consistency. If little weight is given to this data on this account, it can be concluded that the orientation of the semiconductor crystals does indeed have a slight effect on the barrier height. This is in contradiction with the conclusions of Newman *et al.*[8] However, there is additional support for an orientation dependence of barrier height since it has been reported that quantum efficiency is enhanced (by approximately two times) for Schottky diodes made using different crystal orientations in Pd_2Si infrared diodes.[34] This could well be a direct result of a slightly different barrier for different substrate orientations. An orientation dependence is also apparent for the InP Schottky diodes of Table IV. This slight dependence on crystal orientation for the barrier height could be due to the dangling bond density being different on the two planes after cleavage.[36] Alternatively the deposited metal may crystallize in different sizes and orientations depending on substrate orientations.

Nevertheless, it should be emphasized that this slight difference in barrier height due to substrate orientation is by no means conclusive. This is because the preparation methods utilized to fabricate these samples on different crystal orientations are not identical. The (100) samples are prepared by heat cleaning above the decomposition temperature of GaAs prior to metal deposition in UHV. In the other case, the (110) GaAs samples are cleaved in UHV. Similarly, the (110) InP samples are fabricated by *in situ* deposition on clean surfaces prepared by cleavage in UHV, whereas the (100) InP Schottky diodes are fabricated on chemically etched surfaces. Since the physics of the formation of Schottky diodes and the effect of the barrier height due to different preparation techniques are not completely understood, the observed difference may be also due to the different preparation method used in the fabrication of these samples.

IV. SUMMARY

By relating the ideality factor n and the zero-bias barrier height determined from I-V measurements, we have calculated fundamental "flat-band" barrier heights for GaAs and InP Schottky diodes for a large number of metals. The flat-band barrier height provides a normalized comparison of Schottky barriers between different metals and substrates. The calculated flat-band barrier heights are compared with the barrier heights from C-V measurements, where available, and shown to be very well correlated.

For (100) GaAs Schottky diodes the sum of the fundamental barrier height, $\phi_{bn} + \phi_{bp}$, is well within 0.1 eV of the band-gap energy except Mg($\cong$0.12 eV). The mean value of the sum is 1.408 ± 0.06 eV compared to the accepted value of the band gap of 1.424 eV. The average sum of $\phi_{bn} + \phi_{bp}$ for InP is 1.341 eV also found to be very much in agreement with the accepted value of the band gap of InP of 1.344 eV. It is also observed that the barrier height (or at least the flat-band barrier height) appears to be dependent on the orientation of the semiconductor crystals. However, the possibility of the different sample preparation methods having some effects on the barrier height cannot be ruled out.

ACKNOWLEDGMENTS

This work is supported by the Australian Research Council and the Defense Research Centre, Salisbury. The Joint Microelectronics Research Centre is supported by the Commonwealth Special Research Centres Scheme.

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