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A SELF CONSISTENT APPROACH TO *IV*-MEASUREMENTS ON RECTIFYING METAL–SEMICONDUCTOR CONTACTS‡

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Abstract—An experimental procedure is presented for the determination of the barrier height of metal–semiconductor contacts that avoids the use of the so called "ideality factor" n, common in the fit of experimental *IV*-data.

We choose the commonly experienced case where the deviation of n from 1 is caused by a combination of recombination current contribution and the influence of series resistance. These effects are introduced into a computer fitting to the experimental forward *IV* data.

We report on very good fitting of theory and experiment. Also, the discrepancy in the ϕ_B values determined by ordinary deduction from *IV* measurements and those obtained from photoelectric measurements practically vanishes if our procedure is used.

1. INTRODUCTION

Many methods have been developed through the years for the determination of the barrier at metal–semiconductor interfaces.

An enumeration of all the methods and their refinements would be rather extensive; the methods may be broadly divided into *IV*, *CV* and photoelectric.

All of the methods have their typical limitations and great care should be used when comparing the results not only emanating from different laboratories but also from the different methods used for the determination of the barrier ϕ_B.

For the same metal, on the same semiconductor, quite different values for ϕ_B are reported, a fact that depends both on the preparation of the diode and on the method of determination of the barrier.

The simplest and the most commonly used method uses forward *IV* measurement.

Several models have been developed to describe current flow through the metal–semiconductor contact (Ref. [1] presents a good summary).

In practice, the most common approach for the fitting of the experimental *IV*-data is based on pure thermionic emission, according to which the current may be described by:

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

$$I_s = AA^{++}T^2\exp(-\phi_B/kT) \tag{2}$$

is the saturation current, A is the area of the diode, and A^{++} is the modified Richardson constant (112 and $32 \times 10^4\,\mathrm{Am^{-2}\,K^{-2}}$, for n and p-silicon respectively, Ref. [2]).

When attempts are made to fit a set of experimental points by a straight line using this equation (or approximations thereof), it is clearly seen that there is a discrepancy.

Because of this, an "ideality" factor n has been introduced (Ref. [1], p. 87) that somewhat improves the fitting.:

$$I = I_s\exp(qV/nkT)[1 - \exp(-qV/KT)]. \tag{3}$$

Including the effect of series resistance we obtain:

$$I = I_s\exp\left(\frac{q(V - IR_s)}{nkT}\right)\left[1 - \exp\left(-\frac{q(V - IR_s)}{kT}\right)\right]. \tag{4}$$

Here R_s is just one of the physical effects that causes deviation from the pure emission model, while n is a nondescript number that is introduced to describe a number of others[3–7]. Among these are 1. recombination current; 2. Schottky barrier lowering (even for an "ideal diode" this gives $n \approx 1.01$–1.02; 3. oxide interface layers; 4. tunnelling through the barrier; 5. minority carrier injection and 6. edge effects. Their relative importance depends largely on the fabrication parameters. In the experimental part of this paper we will concentrate on a case which often occurs in practice: the dominant effects are due to recombination current and series resistance.

The poor fitting of experimental data for a number of such diodes to eqn (4) is demonstrated in Fig. 1. The range in which the fit can be carried out satisfactorily is limited and, sometimes, there exists too high a degree of subjectivity in the choice of a proper range of fitting.

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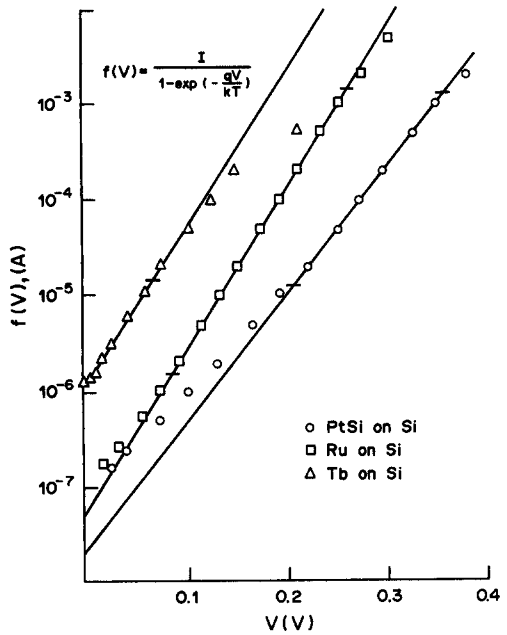

Fig. 1. The common semilogarithmic plot of IV-data [according to eqn (4)]. The region for the least squares fit is marked with short line segments.

2. OUR APPROACH

The question is whether the "ideality" factor n should be used at all, or rather is it an artefact, brought into the equations without any physical fundament?

We would rather see existing models used to explain the data.

It has traditionally been common practice for experimental physicists to fit the data by straight lines. This was the only practical approach possible in the days of the slide rule where least squares fit was possible but seldom done in practice.

The addition of a microcomputer to both control the experiment and to process the data can lead to a substantial saving in time and operator effort.

It is now possible to solve complex equations in a very short time and it is therefore a simple matter to account for the recombination current as well as series resistance at the same time.

We have implemented such an approach in the form of a computer program as described below.

The equation used is

$$I = I_s\{\exp[q(V - IR_s)/kT] - 1\} + I_g\{\exp q(V - IR_s)/2kT - 1\} + (V - IR_s)/R_{sh}, \quad (5)$$

with I_s given by eqn (2) and I_g given by:

$$I_g = \frac{qn_i w}{2\tau}, \quad (6)$$

where n_i is the intrinsic carrier concentration, w the depletion width and τ the effective carrier lifetime.

The small term at the end of eqn (5) which is due to a leakage resistance R_{sh} is more important in the low voltage ranges ($qV \ll kT$) where the first two terms almost vanish. For a "normal" range of IV measurements, this term will be negligible.

On the other hand, this term may be very important in some special cases, which will be shown in a forthcoming article.

We have found that the experimental data may be well fitted over a wide range of applied voltages, starting from the very low region (less than kT/q) to the region where the influence of the series resistance R_s is quite significant.

On the other hand, using the "n value approach", much depends on how the line is drawn. This changes the intercept and hence the deduced value of the barrier height. False conclusions about physical parameters may thus result. On the contrary, increased physical information may be gained by using the computer fit method.

3. EXPERIMENTAL PROCEDURE

We have developed a flexible program, written in BASIC for an Apple II desk computer. The steps of the procedure will now be described.

1. An ordinary IV-measurement is done. A wide range of voltages may be used (not limited to $V > 3\,kT/q$).

2. The data is plotted in a semilogarithmic graph

$$\log \frac{I}{[1 - \exp(-qV/kT)]} \text{ vs } V.$$

This is the plot (Fig. 1) of a "straight line" whose intercept with the y-axis gives $\log I_s$. As seen from the Fig. 1, there is a high degree of subjectivity in the choice of range for a straight line. After choosing such a range, a least squares fit is made in order to somewhat minimize the subjectivity involved. The common practice is to stop here and derive the values for ϕ_B and n, from the obtained intercept (I_s) and from the slope. Instead, we added the following steps:

3. The extrapolated value of I_s may be defaulted (together with default $I_g = 0$ and $R_s = 0$) in the program as a first approximation for the iteration of fitting the data.

4. The process of iteration involves finding the adequate combination of I_s, I_g and R_s that fits the experimental points over a wide range with a minimum deviation. The final value of I_s is often clearly different from the starting one.

5. From I_s, the value of ϕ_B is evaluated. The determination of ϕ_B is of course influenced by the precise knowledge of actual area and temperature and by the choice of value for A^{++}. The sensitivity of the process (of determination of ϕ_B) is primarily dependent on the knowledge of the temperature but also, now that we are discussing greater accuracy in the measurements, it is important that the proper value for A^{++} be introduced in the equations.

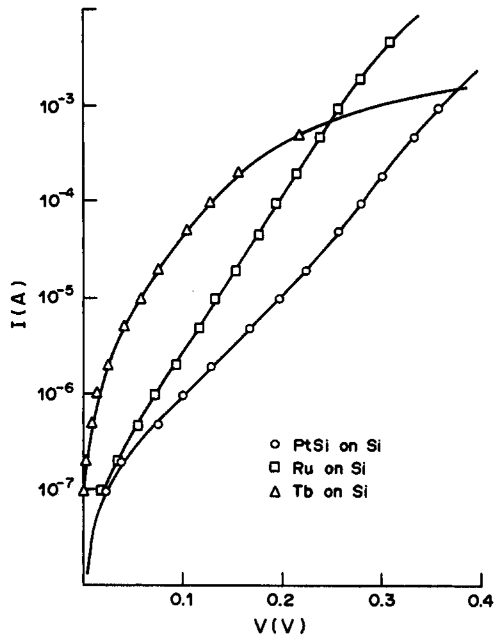

Fig. 2. A typical fit of the experimental IV-data by the procedure described in the text.

The question of constants used in such determinations is not trivial and is actually an important matter.

4. RESULTS

We have measured the IV characteristics of several diodes, upon which the values of ϕ_B were determined as described above. As a reference, an independent determination of ϕ_B was carried out by means of photoelectric measurements. We will present here three typical and representative diodes:

1. Terbium on 15 Ω cm p-type silicon, prepared by evaporation.
2. Ruthenium on 8 Ω cm n-type silicon; prepared by evaporation.
3. Platinum silicide (PtSi) on 1 Ω cm n-type silicon; prepared by rf-sputtering.

We show in Fig. 1 the common IV approach and in Fig. 2, the graphs obtained according to the computer approach. The results are tabulated in Table 1. The values obtained for ϕ_B by our approach match clearly those obtained by independent photoelectric measurements. We have noticed that the agreement is often better for diodes on n-type silicon—Table 1 reveals this fact. The small difference encountered for diodes on p-type material might well be removed by the use of a different value for the Richardson constant; using $A_p^{++} = 19 \times 10^4$ (instead of $32 \times 10^4\,\mathrm{A\,m^{-2}\,K^{-2}}$) for the Terbium diode, the value for the barrier height determined from IV-measurement will match that obtained from photoelectric measurements (0.653 eV). We have discussed the determination of A^{++} in a previous article (Ref. [8]).

The n-values for the Terbium diode (1.070) is not high. The departure from unity is primarily due to the high series resistance; I_g, which is about four times less than I_s, does not contribute too much. The Ruthenium diode has quite a low n-value and so the results obtained for $\phi_B = 0.77$ eV the three methods match quite well. However, a good n-value does not explain the processes involved, our approach gives a better explanation of the mechanisms involved by separating the different components (I_s, I_g and R_s).

Concerning the PtSi diode (fabricated by sputtering), although there is a portion of the data that can be fitted with a straight line with a good correlation coefficient (see Fig. 1), the usual procedure leads to 0.770 eV, a result that is not consistent *per se* nor confirmed by photoelectric measurements (0.847 eV). The value of n (1.332) is quite far from unity, indicating that the measured data are disturbed by "damage centers" recombination (I_g is two orders of magnitude higher than I_s) in a region quite far from kT/q (actually around 0.3 V). Instead, if our procedure is used, the value obtained for ϕ_B closely matches the value determined from independent photoelectric measurements.

5. CONCLUSIONS

We have presented a procedure for the determination of the barrier height across a metal–semiconductor interface without the use of the "ideality" factor n. The values of n (Table 1) are explained by the physical model as caused by the contribution of recombination current and high series resistance. The discrepancy in the ϕ_B values determined by the common IV approach and those obtained from photoelectric measurements almost vanishes if the proposed procedure is used. Greater accuracy is obtained by this procedure because it is possible to fit the experimental points in a much wider range of applied voltages. The fact that it is possible to find values for I_s, I_g and R_s that really fit the data is taken as evidence for the validity of the approach used.

Table 1. The derived values of ϕ_B at 294 K

Diode	Area ($\mathrm{m^{-2}}$)	Common approach I_s(A)	ϕ_B(eV)	n	Our approach I_s(A)	ϕ_B(eV)	I_g(A)	R_s (ohm)	Photoelectric ϕ_B(eV)
Tb–Si p	1×10^{-5}	1.21×10^{-6}	0.663	1.070	1.045×10^{-6}	0.666	2.8×10^{-7}	120	0.653
Ru–Si n	7.069×10^{-6}	5.74×10^{-8}	0.763	1.039	4.15×10^{-8}	0.771	7.9×10^{-8}	2.6	0.771
PtSi–Si n	4×10^{-6}	2.45×10^{-8}	0.770	1.322	1.05×10^{-9}	0.850	1.49×10^{-7}	11.7	0.847

In this way, it is possible to measure diodes with high series resistance or large recombination currents which is very difficult in the common *IV* approach.

The case where a fit is impossible (over a reasonably wide range) could well be used to detect some anomalies such as inhomogeneity of the barrier across the surface of the sample, edge effects, etc.

The n-value is sometimes used in a production line to evaluate the spread within a batch of diodes. Although this gives the n-value some importance from the engineering point of view, it is preferable to concentrate on the values obtained for I_s, I_g and R_s rather than a discussion on the n-value itself, if it is dependent on temperature, why it is dependent on temperature, etc. Such a temperature dependence can, for instance, be explained in terms of the different temperature dependences of I_g and I_s, but a discussion of the "natural" parameters I_s, I_g and R_s is more fruitful.

Finally we point out that the present experimental procedure is not the only method of interpretation of measured I–V data that avoids the use of the ideality factor n. We have chosen a case often occurring in practice where the deviation of I–V characteristics from ideal thermionic emission is caused by generation–recombination current and/or by high series resistance. Of course there are many other effects (mentioned above) which can cause deviation from an ideal I–V characteristic. To choose the dominant influence requires some experimental experience.

Nowadays the wide use of powerful personal computers PC AT creates possibilities for simultaneously taking into account more physical effects which are responsible for the deviations of experimental data from ideal I–V characteristics. This permits analysis of Schottky diodes with greater accuracy without the use of the physically meaningless ideality factor n.

REFERENCES

1. E. H. Rhoderick, *Metal Semiconductor Contacts.* Clarendon Press, Oxford (1978).
2. J. M. Andrews and M. P. Lepselter, *Solid St. Electron.* **13,** 1011 (1970).
3. H. Norde, *Appl. Phys.* **50,** 7 (1979).
4. S. M. Sze, *Physics of Semiconductor Devices*, 2nd edn. Wiley, New York (1981).
5. F. A. Padovani and G. G. Sumner, *Solid-St. Electron.* **9,** 3744 (1966).
6. J. D. Levine, *Appl. Phys.* **42,** 3991 (1971).
7. A. N. Saxena, *Surface Sci.* **13,** 151 (1969).
8. J. de Sousa Pires, D. Donoval and P. A. Tove, *Solid St. Electron.* **10,** 989 (1982).