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Theoretical study on the behaviour of metal-*p*-*n*-Si Schottky barrier solar cell*

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Abstract. The performance of Au-*p*-*n*-Si Schottky barrier solar cell has been investigated theoretically following Li's work on GaAs. The behaviour of the barrier height as a function of carrier densities in the *n* and *p* regions and the *p* layer thickness is investigated. The photovoltaic cell characteristics are worked out and conditions for maximum efficiency obtained.

Keywords. Schottky diode; silicon; solar cell.

Several authors have investigated the performance of metal-semiconductor Schottky barrier solar cells theoretically as well as experimentally (Anderson *et al* 1974; Fossum 1976). In order to increase the barrier height of such solar cells, an interfacial insulating layer is often introduced (Fonash 1976; Card and Yang 1976; Fabre 1976). However, there is an optimum thickness of the insulating layer, beyond which there is a photocurrent suppression.

Shannon (1974, 1976) observed considerable improvement in MS Schottky barrier cell in the presence of a thin layer of opposite doping between the metal and the semiconductor. Vander Ziel (1977) proposed a model of metal-*p*-*n* Schottky diodes which was applied to GaAs solar cells by Li (1978). This structure has the advantage that the barrier height can be increased to a value nearly equal to the band gap of the semiconductor without photocurrent suppression. On similar lines, we have investigated the behaviour of metal-*p*-*n*-Si Schottky barrier solar cells.

In this model, the intermediate *p* layer is completely ionised. The band structure for such a configuration is shown in figure 1. The effective barrier height of this structure as seen by the electrons from the metal is

$$\Phi_{Bn} = \Phi_M - \chi_S + eV_m, \tag{1}$$

where Φ_M is the work function of the metal, χ_S the electron affinity of the semiconductor and V_m the potential height. Solving Poisson's equation under appropriate boundary conditions (Vander Ziel 1977) we get

$$V_m = [e/(2\epsilon\epsilon_0 N_a)]\ (N_a W_p - N_d W_n)^2. \tag{2}$$

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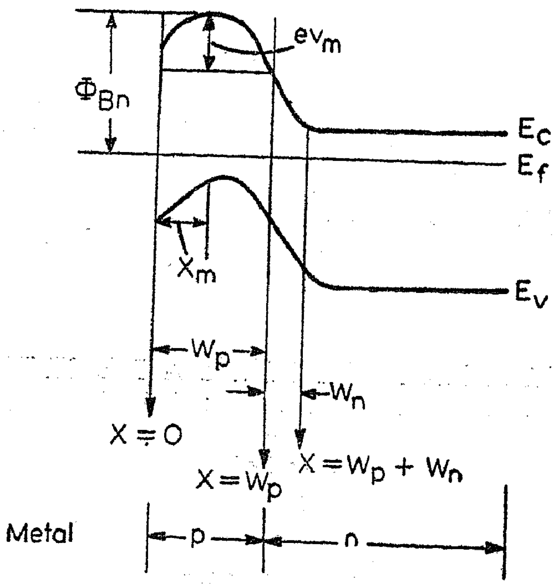

Figure 1. Schematic band diagram of metal-*p*-*n*-Si Solar cell.

The peak of the barrier occurs in the p layer at a distance

$$x_m = W_p - (N_d/N_a)\, W_n, \tag{3}$$

from the metal semiconductor junction, where N_a is the acceptor density, N_d the donor density, W_p the width of the p layer and W_n the width of the depletion layer in the n region, ϵ the dielectric constant of semiconductor, ϵ_0 the dielectric permittivity of free space and e the electronic charge.

For Schottky barrier on p substrate, the width of the depletion region

$$x_0 = \left[\frac{2\epsilon\epsilon_0}{e}\,\frac{(\Phi_p - \Phi_M)}{eN_a}\right]^{1/2}, \tag{4}$$

where $\Phi_p = E_g + \chi_S - kT \ln (N_v/N_a)$,

N_v being the effective density of states in the valence band and kT the thermal energy equal to 0·026 eV at room temperature.

The barrier height increases as x_m increases and is maximum when $x_m = x_0$ beyond which a flat band region appears. Using this condition and equations (1) and (2), we find the maximum value of the barrier height

$$(\Phi_{Bn})_{\max} = E_g - kT \ln (N_v/N_a), \tag{5}$$

which is less than the band gap E_g. Further, it can be seen that $(\Phi_{Bn})_{\max}$ is dependent upon N_a.

We have considered the Au-*p*-*n*-Si Schottky barrier solar cell to see the factors that would affect the photovoltaic performance. The values of various constants used are $\epsilon = 11$, $\chi_S = 4{\cdot}01$ eV, $E_g = 1{\cdot}1$ eV, $\Phi_{\mathrm{Au}} = 4{\cdot}8$ eV and $N_V = 1{\cdot}82 \times 10^{19}$ cm^{-3}.

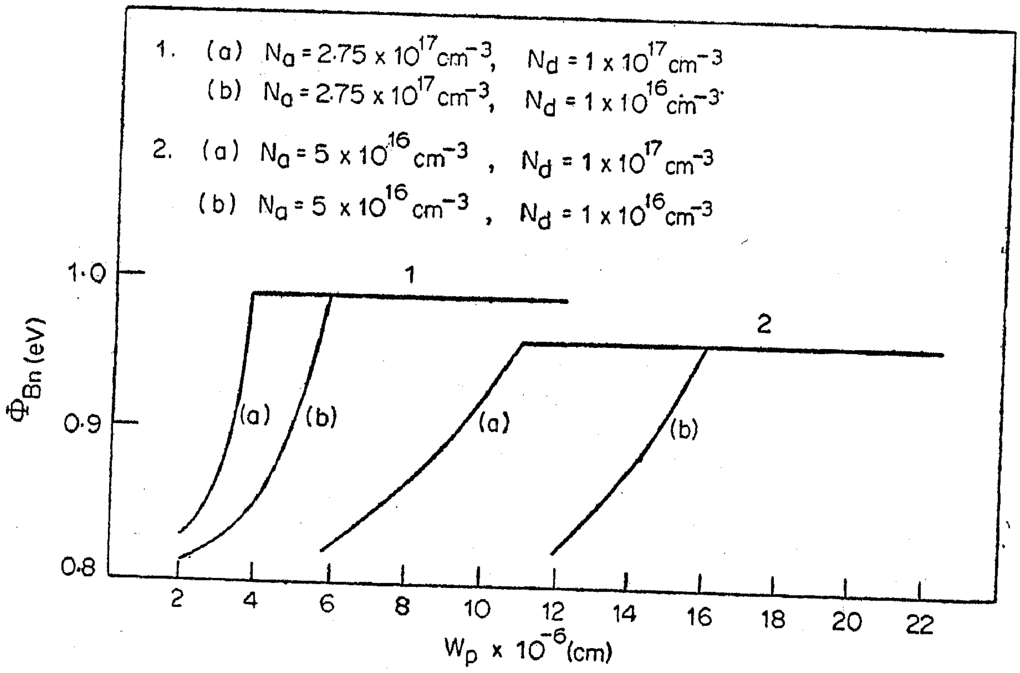

Figure 2. Barrier height Φ_{Bn} as a function of p layer thickness (W_p).

The values of N_a, N_d and W_p are systematically varied and the corresponding values of barrier height are found using (Vander Ziel 1977)

$$W_n = -W_p + \left[\frac{N_a + N_d}{N_d}W_p^2 + \frac{2\epsilon\epsilon_0}{e}\,\frac{(\Phi_M - \Phi_n)}{eN_d}\right]^{1/2} \qquad (6)$$

where Φ_n is the work function of n type semiconductor. For any given values of N_a and N_d, Φ_{Bn} increases as W_p increases (figure 2), till it reaches $(\Phi_{Bn})_{\max}$ [(see (5)]. The minimum value of W_p at which this maximum is obtained is called $(W_p)_{\text{opt}}$.

The $(\Phi_{Bn})_{\max}$ and the corresponding $(W_p)_{\text{opt}}$ values for different N_a and N_d are depicted in figure 3. To obtain a point corresponding to a given set of values of N_a and N_d the values of $(W_p)_{\text{opt}}$ and $(\Phi_{Bn})_{\max}$ are recorded and contours connecting constant values of $(W_p)_{\text{opt}}$ and $(\Phi_{Bn})_{\max}$ are drawn in figure 3. The constant $(\Phi_{Bn})_{\max}$ line is horizontal because it is a function of N_a but not of N_d. From this graph, one can readily find out the optimum value of W_p to use for any chosen N_a and N_d and the $(\Phi_{Bn})_{\max}$ that can be obtained. Alternatively, if W_p is fixed, one can read the optimum value of N_a to use and $(\Phi_{Bn})_{\max}$ that one would expect for any N_d. It is clear that for reasonable values of N_a and N_d (i.e. 10^{16}–10^{18} cm^{-3}), high $(\Phi_{Bn})_{\max}$ (approaching E_g) can be obtained only for sufficiently small values of W_p i.e. thin p layer region (~200Å).

It was claimed by Li (1978) that the maximum effective barrier height is equal to the band gap. Our calculations do not support this conclusion. The maximum effective barrier height turns out to be a function of N_a. This conclusion is significant in the optimisation of the solar cell parameters. Thus for a fixed value of N_a, the maximum

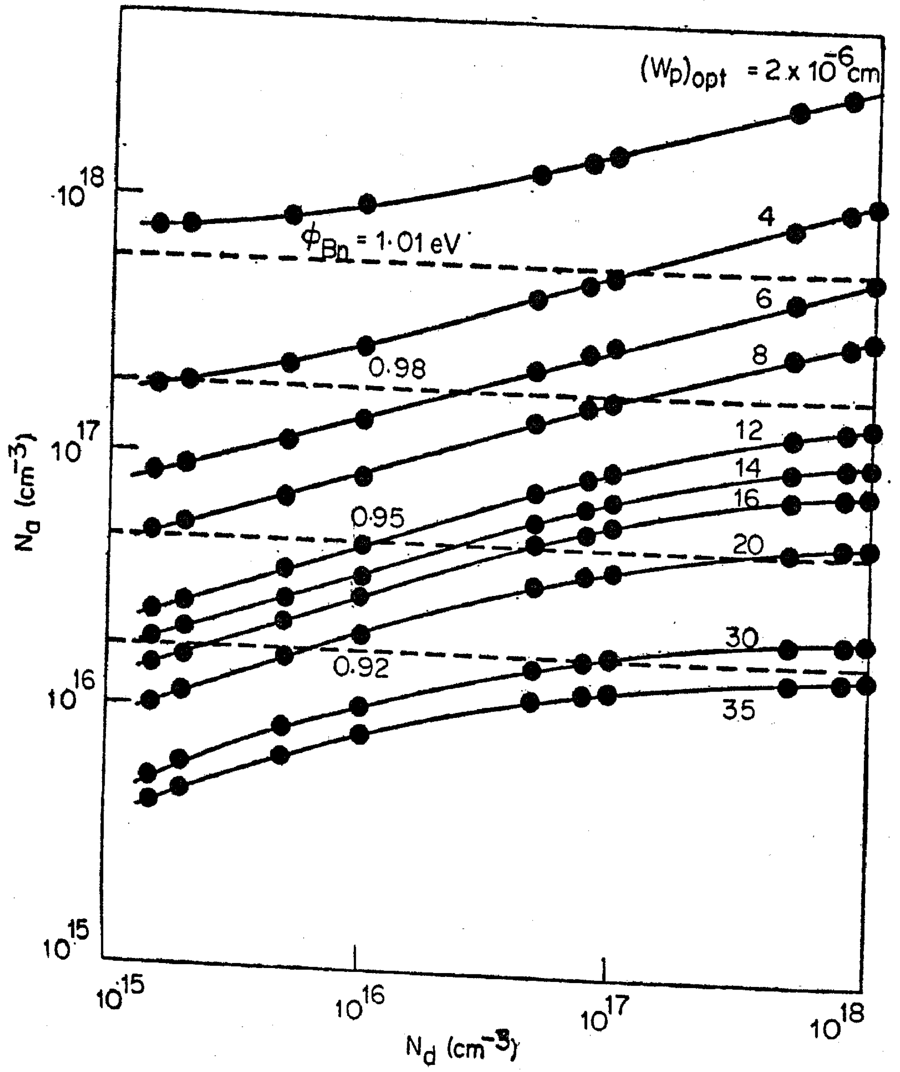

Figure 3. Φ_{Bn} and $(W_p)_{\rm opt}$ as a function of donor and acceptor densities (N_d, N_a).

effective barrier height is fixed, but depending upon the donor density, W_p has to be appropriately chosen. Figure 2 in Li's paper (1978) gives an erroneous impression because he has arbitrarily extended the $\Phi_{Bn}-N_a$ plots upto a maximum value equal to the energy gap.

To determine the photovoltaic performance of the cell the *I-V* characteristics are calculated using

$$I = I_0 \left\{ \exp \left[\frac{e\,(V - IR_s)}{kT} \right] - 1 \right\} - I_L, \tag{7}$$

where I_0 is the saturation current and I_L the photogenerated current of the cell including the grid effect. The total series resistance can be written as

$$R_S = R_b + R_{\rm diff} + R_{\rm front} + R_{\rm back} \tag{8}$$

where R_b=resistance of the base material; R_{diff}=resistance due to the diffused layer; R_{front}=resistance due to the front grid electrode including the Schottky metal effect and R_{back}=resistance due to the back electrode. The series resistance has been calculated for a finger-type grid pattern using the formulae given by Handy (1967) and taking the numerical values of 0·35 cm for the spacing between the grid lines and 0·01 cm for their width. Further,

$$R_b = \rho\,(t_1/A),$$

$$R_d = \bar{\rho}\cdot d,$$

and $$R_{\text{back}} = \rho_{\text{met}}\,(t_2/A)$$

where ρ is resistivity of base material, t_1 the thickness of the cell, d the thickness of the diffused layer and t_2 the thickness of the back contact. ρ_{met} is the resistivity of the metal used for Ohmic contact, $\bar{\rho}$ the resistivity of the diffused layer and A the area of the cell. (In this case t_1=250 μ, t_2=5000 Å and A=1 sq cm).

To simplify the calculations of photogenerated current, we neglect the effect of accumulation of photogenerated holes in the barrier regions, $x = x_m$. Under this assumption the following equation given by Li (1978) can be used

$$I_l\,(\lambda) = e\Phi_0\left[\exp\,(-\,\alpha x_m) - \frac{\exp\,(-\,\alpha W)}{1+\alpha L_p}\right], \qquad (9)$$

where $W = W_n + W_p - x_m$,

and Φ_0 is the photon flux density, α the absorption coefficient and L_p the minority carrier diffusion length in the n type base material.

Hence the total photocurrent under the entire AMO spectrum

$$I_L = \int_{\lambda_0\,=\,0\cdot3\,\mu}^{\lambda_g\,=\,1\cdot1\,\mu} I_l\,(\lambda)\,d\lambda \qquad (10)$$

Thus, using (7), (8) and (10), the open circuit voltage, short circuit current and the complete I-V characteristics have been obtained. The maximum power and hence the efficiency have been obtained from the I-V curve.

The values of $P_{\max}$ have been calculated for an optimum set of values of N_a, N_d and $(W_p)_{\text{opt}}$. For a given value of $(W_p)_{\text{opt}}$ say 2500, 2000, 1600, 1200, 800 or 200 Å), a set of points on the corresponding contour (figure 3) are chosen; the values of N_a, N_d and $(\Phi_{Bn})_{\max}$ at that point are read out and $P_{\max}$ calculated following the procedure mentioned above. The results are shown in table 1 and $P_{\max}$ is plotted as a function of N_d for different values of W_p in figure 4.

From the graph, it is clear that for a given N_d, the maximum power obtainable increases with decreasing W_p (increasing N_a). Further, there is a drop of $P_{\max}$ if N_d is increased beyond 10^{16} cm^{-3}. A good set of parameter appears to be N_a=7·7× 10^{17} cm^{-3},

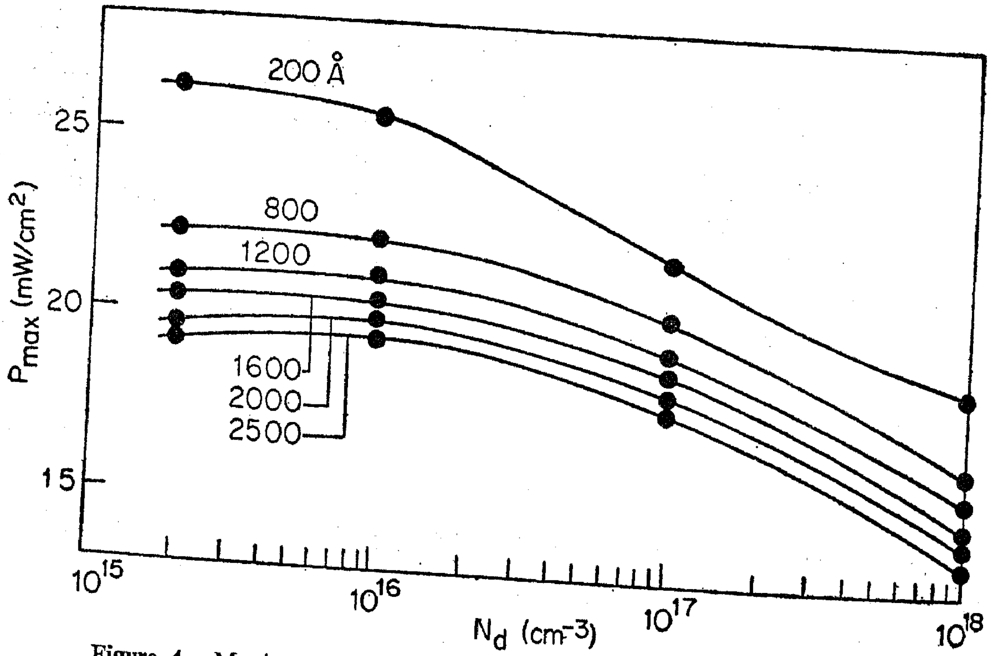

Figure 4. Maximum power as a function of donor density at different (W_p)opt.

Table 1. Au-*p*-*n*-Si Schottky barrier solar cell calculated under AMO illumination conditions.

N_d 10^{16} cm^{-3}	W_p 10^{-6} cm	N_a 10^{16} cm^{-3}	x_m 10^{-6} cm	$(\Phi_{Bn})_{max}$ eV	I_{sc} mA	V_{oc} Volts	P_{max} mW	η %
0·14	2	74·4	1·85	1·018	46·33	0·671	26·14	19·36
0·2	2	76·9	1·82	1·019	46·48	0·672	26·2	19·45
1	2	93·7	1·67	1·023	45·02	0·675	25·58	18·95
10	2	153·0	1·34	1·036	39·73	0·685	22·92	16·98
0·14	8	3·31	5·82	0·946	44·81	0·598	22·12	16·39
0·2	8	5·38	5·61	0·949	44·7	0·601	22·23	16·7
1	8	8·55	4·04	0·961	43·7	0·612	22·21	16·45
10	8	17·6	3·43	0·980	38·96	0·627	20·30	15·04
100	8	30·4	1·82	0·994	30·76	0·637	16·33	12·1
0·2	12	2·7	7·39	0·931	44·01	0·582	21·05	15·59
1	12	4·53	6·01	0·944	43·15	0·595	21·19	15·70
10	12	9·2	4·50	0·963	38·41	0·611	19·39	14·36
100	12	14	3·77	0·974	30·36	0·616	15·52	11·5
0·2	16	1·69	8·85	0·919	43·5	0·571	20·36	15·08
1	16	2·91	7·17	0·933	42·72	0·584	20·54	15·21
10	16	5·66	5·49	0·950	38·13	0·593	18·8	13·93
100	16	7·86	4·8	0·959	30·00	0·601	14·88	11·02
0·2	20	1·19	10·10	0·909	43·08	0·560	19·70	14·59
1	20	2·06	8·20	0·924	42·35	0·575	19·96	14·80
10	20	3·81	6·53	0·939	37·79	0·586	18·22	13·5
100	20	4·95	5·80	0·947	29·61	0·598	14·34	10·62
0·2	25	0·84	11·46	0·900	42·66	0·551	19·17	14·2
1	25	1·45	9·115	0·915	41·94	0·565	19·39	14·36
10	25	2·52	7·619	0·929	37·40	0·576	17·69	13·10
100	25	3·09	6·97	0·934	29·40	0·578	13·99	10·36

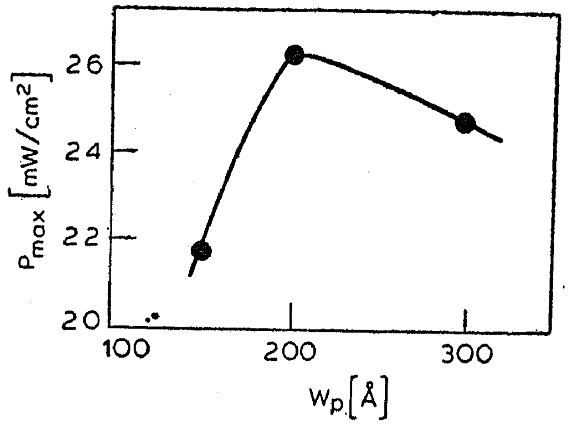

Figure 5. Maximum power as a function of p layer thickness W_p.

$N_d = 2\times10^{15}$ cm^{-3}, $(W_p)_{opt} = 200$ Å, which gives $(\Phi_{Bn})_{max} = 1{\cdot}02$ eV and the $P_{max} = 26{\cdot}25$ mw/cm² and hence the efficiency, $\eta = 19{\cdot}5\%$.

It thus appears feasible to increase the barrier height and the conversion efficiency of the Schottky solar cell by choosing proper N_d, N_a and W_p.

Also, to see the effect of experimental fluctuations in W_p around the chosen $(W_p)_{opt}$ value, we have calculated P_{max} at various values of W_p keeping N_a and N_d fixed as shown in figure 5. It is seen that the fall is steeper for $W_p < (W_p)_{opt}$ than $W_p > (W_p)_{opt}$. It is therefore desirable to design the cell by keeping the mean W_p at a value higher than $(W_p)_{opt}$.

Fabrication of experimental cells on these lines is in progress.

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