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ANALYTICAL ESTIMATE OF OPEN-CIRCUIT VOLTAGE OF A SCHOTTKY-BARRIER SOLAR CELL UNDER HIGH LEVEL INJECTION

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The open-circuit voltage developed across a Schottky-Barrier (SB) solar cell was theoretically modeled to estimate it under high level injection conditions. An Open-circuit voltage (V_{oc}) of 0.709 *V was obtained for specific metal/n*-Si *SB solar cell. A substantial increase of* 42.6 % *in V_{oc} was noticed while comparing our result with that previously calculated in low level injection conditions. Four different metals suitable for making Schottky contact with n-Si were investigated and calculated the variation of V_{oc} with different values of doping concentrations in the semiconductor. The effect of surface recombination velocities (SRV) of charge carriers on V_{oc} was also estimated at such high level injections.*

Keywords: *SCHOTTKY BARRIER SOLAR CELL, HIGH LEVEL INJECTION, OPEN CIRCUIT VOLTAGE, OHMIC CONTACT, SURFACE RECOMBINATION VELOCITY.*

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1. INTRODUCTION

A Schottky-Barrier (SB) formed by a metal/*n*-(*p*-) type semiconductor, that refers to the contact of a metal of higher (or lower) work function with the semiconductor of lower (or higher) work function [1] has long been considered as the simplest photovoltaic devices of all. The doping concentration of semiconductor in case of SB is low, that is less than the density of states in the conduction or valence band. A great amount of research has been taken place by several groups to theoretically estimate [2-5] and also experimentally [6-18] observe their open circuit voltage (V_{oc}) and short circuit current (I_{sc}) under low level of injection, when the photo-generation rate is relatively small. Besides, it has also been observed that the SB solar cells are characterized with low I_{sc} values, for which its efficiency is relatively low. The I_{sc} can be improved by various device optimizations, such as, larger cell area, better generation rate or greater diffusion length of photo-generated carriers. Alternatively, an easier way of improving the efficiency of such SB cell is possible by enhancing the V_{oc}. In the present study, it has been established that, this enhancement is possible by introducing high level of injection.

In this work we have evaluated the performance of Schottky-barrier solar cell under high level injection condition and compared our results with low level injection conditions. High level injection in a semiconductor refers to the non-equilibrium condition where the excess charge carrier concentration is very large than the doping density (Δn, $\Delta p >> N_d$, n_i^2/N_d) and reverse is the case for low level injection condition. The open circuit voltage has been modeled by Dubey et al. [4] under low level injection condition and related consequences have been discussed therein. An effort has been made in our present study to model similar system at high level injection and hence, calculated the open circuit voltage under various conditions such as, different doping densities and surface recombination velocities. Finally, the results have been compared with the model result by Dubey et al. as well as among all variations in the high- and low- level injection. In our study the SB solar cell is realized by considering four metals, Rh, Pd, Ag, and W with n-Si as the semiconductor.

2. FORMULATION

The energy-band diagram of metal/n-type semiconductor SB solar cell is shown in Fig. 1. Schottky contact forms at $X = 0$ and Ohmic contact at $X = L$ position of the semiconductor. Here it is seen that the depletion region of width W forms due to Schottky contact.

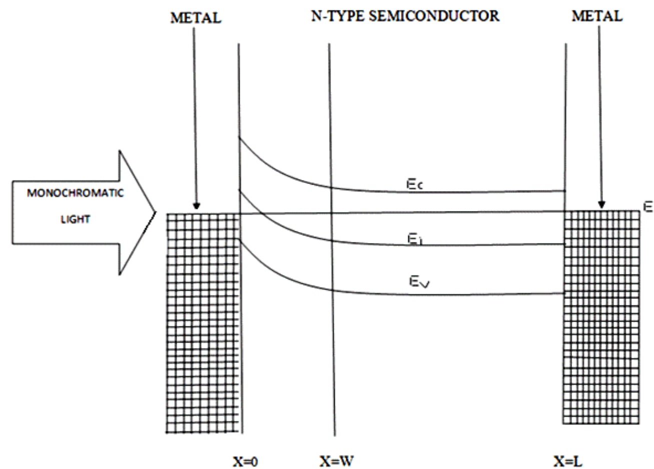

Fig. 1 *– Energy-Band diagram of a Schottky-barrier Solar cell*

2.1 Evaluation of open circuit voltage (V_{oc})

We have calculated the open-circuit voltage (V_{oc}) under illumination of monochromatic light at the interface of metal and n-type semiconductor SB solar cell. So the boundary condition is that total current (J_T) flowing in the cell must be zero that is the combination of drift and diffusion component of electrons and holes,

$$J_T = J_n(W) + J_p(W) \tag{1}$$

$$J_T = qn\mu_n E + qD_n \frac{dn}{dx} + qp\mu_p E - qD_p \frac{dp}{dx} \text{; Since } J_T = 0 \tag{2}$$

So,

$$qn\mu_n E + qp\mu_p E + qD_n \frac{dn}{dx} - qD_p \frac{dp}{dx} = 0 \tag{3}$$

Where n and p are the electron and hole concentrations, respectively. $\mu_{n,}$ D_n and $\mu_{p,}$ D_p are the mobility and diffusion coefficient of electrons and holes, respectively and E is the electric field. Now open circuit voltage V_{oc} is expressed as,

$$V_{oc} = V(L) - V(0) \tag{4}$$

$$= \left[V(L) - V(W)\right] + \left[V(W) - V(0)\right] \tag{5}$$

The above two brackets are evaluated in the following sections.

2.1.1 Depletion Region $(0 \le x \le W)$

We know in the depletion region, there exists built in electric field, E_b due to donor densities and electric field E_g due to generation of electron-hole pairs under monochromatic light illumination. So total electric field E express as,

$$E = E_b(x) + E_g(x) \tag{6}$$

$$n = n_0(x) + \Delta n(x) \tag{7}$$

$$p = p_0(x) + \Delta p(x) \tag{8}$$

Where $n_0(x)$, $p_0(x)$ are the equilibrium electron and hole densities and $\Delta n(x)$, $\Delta p(x)$ are the excess electron and hole densities. We are able to eliminate some terms in Equation (3), using Equation (6), (7) and (8)

$$\begin{aligned} q(n_0 + \Delta n)\mu_n E_g(x) + q(p_0 + \Delta p)\mu_p E_g(x) + q\Delta n\mu_n E_b(x) + \\ +q\Delta p\mu_p E_b(x) + qD_n \frac{d\Delta n}{dx} - qD_p \frac{d\Delta p}{dx} = 0 \end{aligned} \tag{9}$$

The expression for $E_g(x)$ can be evaluated from the above equation as,

$$\begin{aligned} E_g(x) = (qD_p \frac{d\Delta p}{dx} - qD_n \frac{d\Delta n}{dx})\left[(n_0 + \Delta n)\mu_n + (p_0 + \Delta p)\mu_p\right]^{-1} - \\ - \frac{(\Delta n\mu_n + \Delta p\mu_p E_b(x))}{(n_0 + \Delta n)\mu_n + (p_0 + \Delta p)\mu_p} \end{aligned} \tag{10}$$

We can eliminate Δn in Equation (10) using continuity equation. Continuity equation for electrons and holes can be read as,

$$\frac{1}{q}\frac{dJ_n}{dx} + G(x) - \frac{\Delta n}{\tau_n} = \frac{dJ_n}{dt} \tag{11}$$

and

$$-\frac{1}{q}\frac{dJ_p}{dx} + G(x) - \frac{\Delta p}{\tau_p} = \frac{dJ_p}{dt} \quad (12)$$

Where τ_n, τ_p are the electron and hole life times and J_n, J_p are the electron and hole current densities. In steady state, total current flow must be constant, therefore, total current is expressed as

$$J_T = J_n + J_p \quad (13)$$

$$\frac{dJ_T}{dt} = 0 \quad (14)$$

Using Equation (11)-(14) we found that,

$$\frac{\Delta n}{\tau_n} = \frac{\Delta p}{\tau_p} \quad (15)$$

Equation (15) is in match with the expression for space-charge neutrality assumption $\Delta n = \Delta p$. Substitution of Equation (15) in Equation (10) and integrating from 0 to W yields,

$$V(W) - V(0) = -\int_0^W E_g(x)dx = -\int_0^W \frac{\left(D_p - D_n\tau_n/\tau_p\right)d\Delta p/dx}{(n_0 + \Delta n)\mu_n + (p_0 + \Delta p)\mu_p}dx + \int_0^W \frac{\left(\frac{\tau_n}{\tau_p} + \mu_p\right)\Delta p E_b(x)}{\left(n_0 + \Delta p\frac{\tau_n}{\tau_p}\right)\mu_n + (p_0 + \Delta p)\mu_p}dx \quad (16)$$

Equation (16) gives the open circuit voltage developed across depletion region. Using depletion region approximation, $n_0(x), p_0(x) \ll \Delta n(x), \Delta p(x)$ equation (16) can be simplified. This approximation is reasonable because we are taking high level injection that is strong illumination.

$$V(W) - V(0) = -\Phi_S - \frac{D_p - D_n\tau_n/\tau_p}{\mu_n\tau_n/\tau_p + \mu_p}\log\left\{\frac{\Delta p(W)}{\Delta p(0)}\right\} \quad (17)$$

Where $\Phi_S = 0.5qN_dW^2/\varepsilon(s)$ is the surface potential, N_d is the donor density, and $\varepsilon(s)$ is the dielectric permittivity of the semiconductor.

2.1.2 Neutral region ($W \le x \le L$)

In neutral region, only the, electric field $E_g(x)$ associated with generation of electron-hole pairs with monochromatic light illumination exists. Therefore,

$$E = E_g(x) \tag{18}$$

$$n = N_d + \Delta n \tag{19}$$

$$p = n_i^2 / N_d + \Delta p \tag{20}$$

Where n_i is the intrinsic carrier concentration. Substituting equation (18), (19) and (20), in equation (9) and considering high level injection condition, we can take,

$$\Delta n, \Delta p \gg N_d \gg n_i^2 / N_d \tag{21}$$

So $E_g(x)$ can be written as,

$$E_g(x) = \frac{D_p - D_n \tau_n / \tau_p}{\Delta n \mu_n + \Delta p \mu_p} \frac{d\Delta p}{dx} \tag{22}$$

Integrating equation (22) using limit from W to L, we obtain the open circuit voltage developed across neutral region.

$$V(L) - V(W) = -\int_W^L E_g(x)dx = -\left\{ D_p - D_n \frac{\tau_n}{\tau_p} \int_W^L \frac{1}{\Delta n \mu_n + \Delta p \mu_p} d(\Delta p) \right\} =$$

$$= \frac{D_n \tau_n / \tau_p - D_p}{\mu_n \tau_n / \tau_p + \mu_p} \int_W^L \frac{1}{\Delta p} d(\Delta p) = \frac{D_n \tau_n / \tau_p - D_p}{\mu_n \tau_n / \tau_p + \mu_p} \left[\log\left\{\Delta P(L)\right\} - \log\left\{\Delta P(W)\right\} \right] \tag{23}$$

2.1.3 Total open circuit voltage

Substituting Equation (17) and (23) in Equation (5), we get an expression for total V_{oc} developed across a SB solar cell under high level injection condition,

$$V_{oc} = -\Phi_S + \frac{D_n \tau_n / \tau_p - D_p}{\mu_n \tau_n / \tau_p + \mu_p} \left[\log\left\{ \frac{\Delta P(L)}{\Delta P(0)} \right\} \right] \tag{24}$$

Here we cannot use the boundary condition $\Delta P(L) = 0$, at the plane $x = L$. Because depending on our consideration of high level injection, there exist some extra holes at the ohmic contact. Here in high level injection condition, ohmic contact provides a finite sink for excess holes instead of an infinite sink considered in low level injection conditions. For complete determination of V_{oc} we have to calculate $\Delta P(L)$ and $\Delta P(0)$.

2.2 Calculation of $\Delta P(L)$ and $\Delta P(0)$

Continuity equation is solved only for holes because we want to calculate only hole carrier concentration at $x = L$ and $x = 0$.

Continuity equation for hole is solved in depletion region and space charge region then matched at $X = W$ (junction). In steady state condition, the continuity equation for holes,

$$-\frac{1}{q}\frac{dj_p}{dx} + \varphi'\alpha\exp(-\alpha x) - \frac{\Delta P}{\tau_p} = 0 \tag{25}$$

Where
$$G(x) = \varphi\{1 - R(\lambda) - a(\lambda)\} f(\lambda)\alpha\exp(-\alpha x) \tag{26}$$

$$\varphi' = \varphi\{1 - R(\lambda) - a(\lambda)\} f(\lambda) \tag{27}$$

φ = no. of photons striking per unit area of the cell per unit time,
$R(\lambda)$ = Reflection coefficient from the metal surface,
$a(\lambda)$ = absorption in the thin metal film,
$f(\lambda)$ = probability that a photon will produce an electron-hole pair,
α = is the absorption coefficient of the semiconductor.

2.2.1 Depletion Region ($0 \le x \le W$).

We can approximate, $P_0 << \Delta P$ and considering only J_p (n-type semiconductor),

Therefore,
$$J_p = q\Delta P\mu_p E - qD_p\frac{d\Delta P}{dx} \tag{28}$$

The electric field in this case $E = E_b(x) + E_g(x)$ and boundary condition $J_T = 0$ and considering the approximation $n_0(x), p_0(x) \ll \Delta n(x), \Delta p(x)$, we solved equation (28),

$$E = \frac{A}{\Delta p}\frac{d\Delta P}{dx} \tag{29}$$

Where
$$A = \frac{D_p\tau_p - D_n\tau_n}{\mu_p\tau_p + \mu_n\tau_n} \tag{30}$$

Substituting equation (29) and (30), in equation (25),

$$D'_p\frac{d}{dx}\left\{\frac{d\Delta P}{dx}\right\} - \frac{\Delta P}{\tau(p)} + \varphi'\alpha\exp(-\alpha x) = 0 \tag{31}$$

Where
$$D'_p = D_p - \mu_p A$$

Solution of equation (31) is

$$\Delta P = C_1\exp\left(\frac{x}{L'_p}\right) + C_2\exp\left(\frac{-x}{L'_p}\right) - Q_1\exp(-\alpha x) \tag{32}$$

Where
$$L'^2_p = D'_p\tau_p \tag{33}$$

$$Q_1 = \frac{\varphi^{\tau_{p'}}\alpha}{\alpha^2 L_p'^2 - 1} \quad (34)$$

Where C_1 and C_2 are the constants of integration.

2.2.2 Neutral region ($W \le x \le L$)

Neglecting the drift current comparison to diffusion current and under high level of injection $n_0(x), p_0(x) \ll \Delta n(x), \Delta p(x)$. Therefore

$$J_p \cong -qD_p \frac{d\Delta P}{dx} \quad (35)$$

Substituting equation (35) in equation (25) yield

$$D_p \frac{d}{dx}\left\{\frac{d\Delta P}{dx}\right\} - \frac{\Delta P}{\tau(p)} + \varphi'\alpha \exp(-\alpha x) = 0 \quad (36)$$

The solution of equation (36) is given by,

$$\Delta P = C_3 \exp\left(\frac{x}{L_p}\right) + C_4 \exp\left(\frac{-x}{L_p}\right) - Q_2 \exp(-\alpha x) \quad (37)$$

Where

$$L_p^2 = D_p \tau_p \quad (38)$$

$$Q_2 = \frac{\varphi' \tau_p \alpha}{\alpha^2 L_p^2 - 1} \quad (39)$$

C_3 and C_4 are the constants of integration.

2.2.3 Evaluation of the constants of integration

The constants of integration C_1, C_2, C_3 and C_4 have been calculated by applying boundary conditions at $x = 0$ and $x = L$ and then matched in depletion region and neutral region,
The boundary conditions are,

$$J_p(x = 0) = -qS_p \Delta p(0) \quad (40)$$

Where S_p is surface recombination velocity, which is dependent on the interface state density, at surface $x = 0$. Using equation (28), (29) and (40), we get

$$qD_p' \frac{d\Delta P}{dx}\Big|_{x=0} = S_p \Delta p(0) \quad (41)$$

$$\Delta P(W)\, from\, left = \Delta P(W)\, from\, right \quad (42)$$

$$\left.\frac{d\Delta P}{dx}\right|_{x=W} from\ left = \left.\frac{d\Delta P}{dx}\right|_{x=W} from\ right \tag{43}$$

$$\Delta P(x) = (P_{n^0} - P_n^0)\exp(-\frac{x}{L_p}) \tag{44}$$

Where P_{n^0} is the concentration of hole in n-type semiconductor at $x = 0$.

P_n^0 is the concentration of hole in n-type semiconductor at thermal equilibrium. Using equations (41)-(44) in equations (32) and (37), constants of integration C_1, C_2, C_3 and C_4 are evaluated.

$$C_1 = \frac{C_3 \exp\left(\frac{W}{L_p}\right)\left(1+\frac{L'_p}{L_p}\right) + C_4 \exp\left(-\frac{W}{L_p}\right)\left(1-\frac{L'_p}{L_p}\right) + b_1 \exp(-\alpha W)(\alpha L'_p - 1)}{2\exp\left(W/L'_p\right)} \tag{45}$$

$$C_2 = \frac{C_3 \exp\left(\frac{W}{L_p}\right)\left(1-\frac{L'_p}{L_p}\right) + C_4 \exp\left(-\frac{W}{L_p}\right)\left(1-\frac{L'_p}{L_p}\right) - b_1 \exp(-\alpha W)(\alpha L'_p + 1)}{2\exp\left(-W/L'_p\right)} \tag{46}$$

$$C_3 = \frac{Q_2 \exp(-\alpha L)\exp\left(-W/L_p\right)Y + K\exp\left(-W/L_p\right)Y - 2b_1\exp\left(-L/L_p\right)}{\exp\left(L/L_p\right)\exp\left(-W/L_p\right)} \times$$
$$\times \frac{\exp(\alpha W) - Q_1(S_p+\alpha)\exp\left(-L/L_p\right)}{Y - \exp\left(W/L_p\right)X\exp\left(-L/L_p\right)} \tag{47}$$

$$C_4 = \frac{2b_1 \exp\left(L/L_p\right)\exp(-\alpha W) + Q_1(S_p+\alpha)\exp\left(L/L_p\right)}{\exp\left(L/L_p\right)\exp\left(-\frac{W}{L_p}\right)Y - \exp\left(W/L_p\right)X\exp\left(-L/L_p\right)} -$$
$$- \frac{Q_2\exp(-\alpha L)\exp\left(W/L_p\right)X - K\exp\left(W/L_p\right)X}{\exp\left(L/L_p\right)\exp\left(-W/L_p\right)Y - \exp\left(W/L_p\right)X\exp\left(-L/L_p\right)} \tag{48}$$

Where

$$X = \frac{S_p - D'_p/L'_p}{2\exp\left(W/L'_p\right)}\left(1 + L'_p/L_p\right) + \frac{S_p + D'_p/L'_p}{2\exp\left(-W/L'_p\right)}\left(1 - L'_p/L_p\right) \tag{49}$$

$$Y = \frac{S_p - D'_p/L'_p}{2\exp\left(W/L'_p\right)}\left(1 - L'_p/L_p\right) + \frac{S_p + D'_p/L'_p}{2\exp\left(-W/L'_p\right)}\left(1 + L'_p/L_p\right) \tag{50}$$

$$K = (P_{n^0} - P_n^0)\exp\left(-L/L_p\right) \tag{51}$$

$$b_1 = Q_2 - Q_1 \tag{52}$$

Thus $\Delta P(L)$ and $\Delta P(0)$ is given by equation (32) and (37) as,

$$\Delta P(L) = C_3 \exp\left(L/L_p\right) + C_4 \exp\left(-L/L_p\right) - Q_2 \exp(-\alpha L) \tag{53}$$

$$\Delta P(0) = C_1 + C_2 - Q_1 \tag{54}$$

Now open circuit voltage for the SB solar cell can be calculated from equation (24). The expression for V_{oc} calculated by Dubey et al. for low level injection condition is given by

$$V_{oc} = -\Phi_s + \frac{D_n \tau_n/\tau_p - D_p}{\mu_n \tau_n/\tau_p - \mu_p} \log\left\{\frac{\Delta P(W)}{\Delta P(0)}\right\} - \frac{D_n \tau_n/\tau_p - D_p}{\mu_n N_d} \Delta P(W) \tag{55}$$

The terms are already explained for high level injection condition.

3. RESULTS AND DISCUSSION

The numerical value of the open circuit voltage can be calculated using the expressions (24), (45), (46), (47) and (48) with a given set of parameters. The calculated open circuit voltage cannot be compared with the experimental data available so far, unless a detailed knowledge of reflection coefficient, $R(\lambda)$ and absorption coefficient, $\alpha(\lambda)$ as a function of incident light wavelength, λ are known. Due to this fact, all subsequent results are only numerical and relative. No attempt has therefore been made to compare them with any experimental results. By ignoring any reflection loss that may occur at higher wavelength ($\lambda > 1$ μm) or possible impact ionization to occur at lower wavelengths ($\lambda < 0.4$ μm), we found $V_{oc} = 0.71$ V for Rh/n-type Si SB solar cell with $N_d = 10^{14}$ cm^{-3}, $\alpha = 10^4$ cm^{-1} and $\phi = 2 \times 10^{17}$ cm^{-2}sec^{-1}, if the surface recombination is negligible. There is a substantial increase of 42.6 % in V_{oc} for high level injection condition (HLI) as compared to low level injection (LLI) condition invoke by Dubey et al.

As the surface states at the metal semiconductor interface would play a significant role in real devices, we have evaluated V_{oc} as a function of surface recombination velocity (SRV), S_p for a fixed value of doping density and four chosen metals Pd, Rh, W and Ag in relevance of their work functions. The V_{oc} is found to be highest for Pd/n-Si and lowest for Ag/n-Si SB solar cells at HLI. A general trend of lowering in V_{oc} is found with increase of SRV, as expected. It is also observed that, the lowering is substantial in the SRV range, $0 < S_p \leq 1000$ cm/s for both levels of injection (Fig. 2a for HLI and Fig. 2b for the LLI). This is important to note that, the effect of SRV in the range $0 < S_p \leq 10000$ cm/s is a lowering in V_{oc} by 20 % for HLI and 27 % for LLI in case of Pd/*n*-Si. This change is 45 % and 97 % for HLI and LLI, respectively, in case of Ag/n-Si. The less change in V_{oc} with SRV in the Pd/*n*-Si may be attributed to the catalytic property associated to Pd, with greater chance to neutralize surface states originated from impurity gases and is subject to experimental verification. Calculated result shows that, Pd would be a better choice for SB solar cell with n-Si.

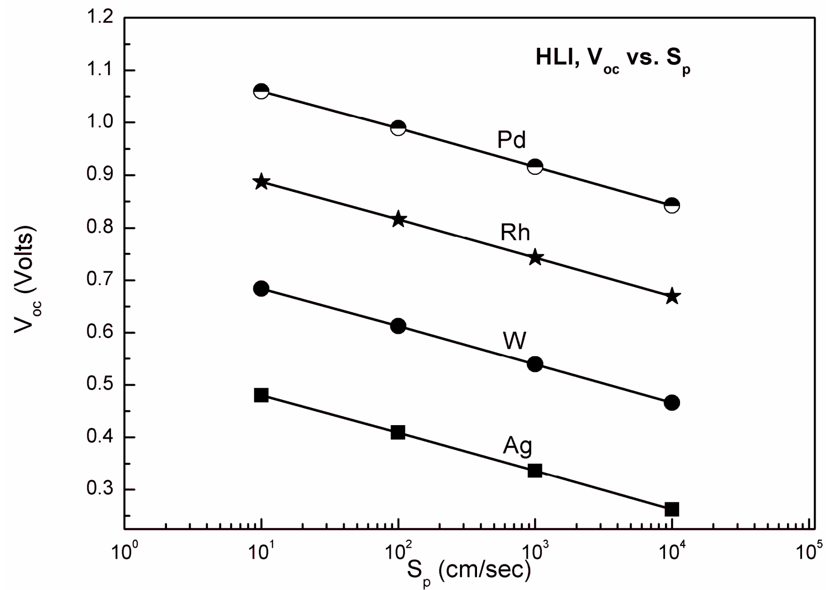

Fig. 2a *– Calculated variation of V_{oc} with S_p under high level of injection*

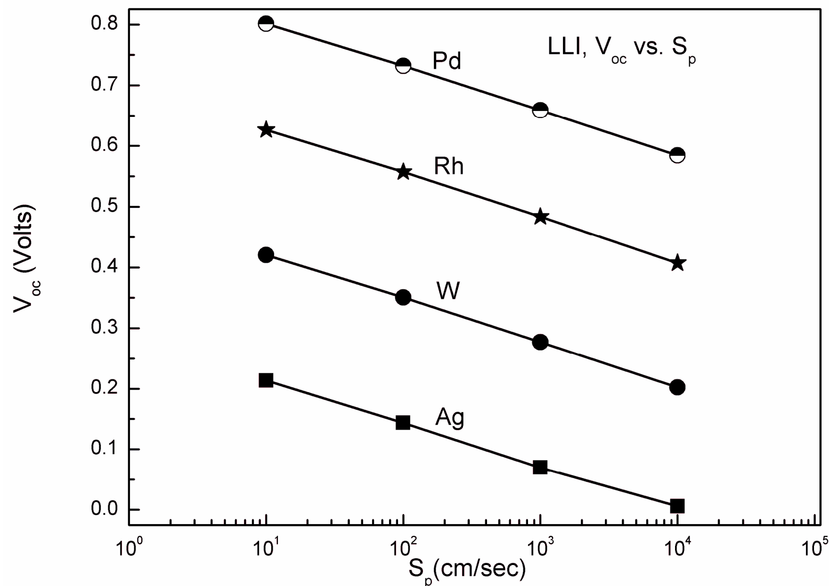

Fig. 2b *– Calculated variation of V_{oc} with S_p under low level of injection*

The effect of doping density, N_d of n-Si on V_{oc} of the SB solar cells is calculated for different concentration of donor atoms and found to be linear relationships at lower and higher levels of doping concentrations. Fig. 3a and 3b shows the variation of V_{oc} with N_d in the range, $10^{14} \leq N_d \leq 10^{17}$ cm^{-3} for a defect free surface, with $S_p = 1$ cm/s for HLI and LLI cases, respectively.

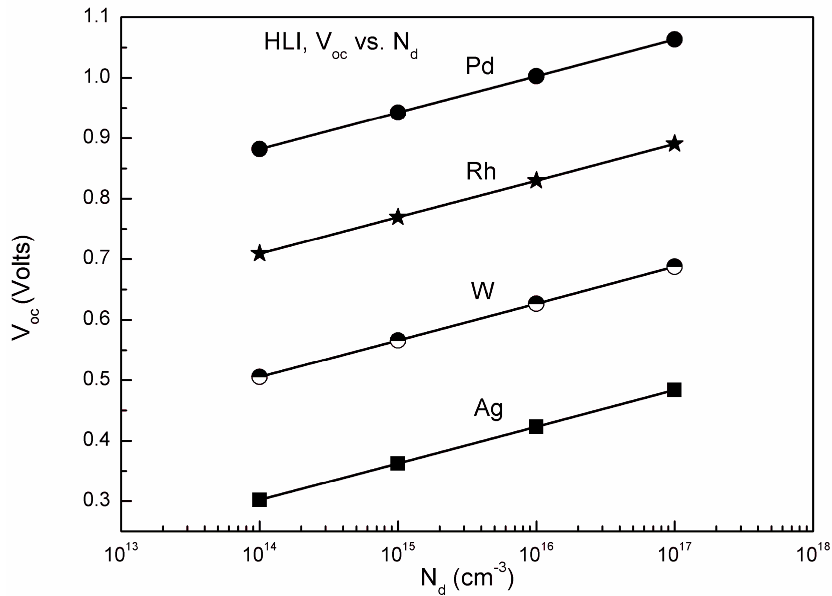

Fig. 3a *– Variation of V_{oc} with doping density of n-type Si under high level of injection*

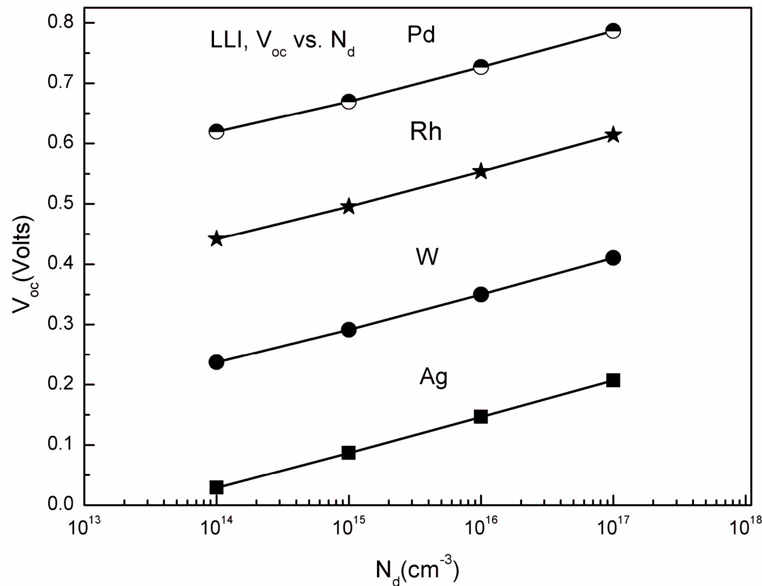

Fig. 3b *– Variation of V_{oc} with doping density of n-type Si under low level of injection*

The positive change in V_{oc} with doping density is found to be noticeably lower in case of Pd/n-Si (17 % under HLI and 21 % under LLI) as compared to much higher in case of Ag/n-Si (37 % under HLI and 90 % under LLI). The variation of V_{oc} with N_d usually stems from the current-voltage relationship of a Schottky barrier junction,

$$V_{oc} = \varphi_B + \ln\left(\frac{j_{sc}}{A^{**}T^2}\right) \quad (56)$$

where φ_B, j_{sc}, A^{**} and T are the Schottky barrier height, short circuit current of the device, the effective Richardson constant and temperature of the semiconductor, respectively. In Equation (56), j_{sc} is affected by the doping density, primarily because of the reduction in the field region. In other word, the bulk current in the device is affected by two mechanisms: (I) the movement of bulk region close to interface of metal and semiconductor with increasing doping density, causing the bulk current to increase and (II) a reduction in diffusion length causing the reduction in the bulk current. A counter balance of mechanisms (I) and (II) would then determine, whether the increase in N_d is reflected as an increase or decrease in V_{oc}. The second process might have been the significant one in the Pd/n-Si, where a lower change in V_{oc} is noticed as compared to the Ag/n-Si, where the first process would dominate.

4. CONCLUSION

We have investigated the variation of open circuit voltage with surface recombination velocity and doping density for both high and low level injection conditions in model Schottky barrier solar cells with different choice metals. We have noticed that there is an increase of 42.6 % in open circuit voltage of a metal/n-Si Schottky-barrier solar cell under high level injection condition compared to low level injection condition with surface recombination velocity (SRV) 1 cm/sec and doping concentration 10^{14} cm^{-3}. Pd has been found to be good choice in terms of lower surface recombination property when used with n-Si. The concentration of donor atoms in n-Si would play an important role at high and low level injections, which shows that, the donor concentration should preferably be lower to get higher V_{oc}. The above study can be extended further to check the effect of minority carrier life time (or diffusion length), the semiconductor thickness and also model the current in the device more appropriate when used as concentrator PV device using Schottky-barrier effect.

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