A MODEL ON THE EFFECT OF INJECTION LEVELS OVER THE OPEN-CIRCUIT VOLTAGE OF SCHOTTKY BARRIER SOLAR CELLS

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Abstract

The open-circuit voltage, V_{oc} developed across a Schottky-barrier (SB) solar cell has been modeled and calculated under low and high level injection conditions. The model predicted an increase of 42% in V_{oc} in a metal/n-Si Schottky-barrier solar cell under high level injection condition, as compared to the low level injection condition while the SB interface does not essentially contribute to large surface recombination velocity and a moderate doping concentration is maintained. The metal, Pd has been found to be a better choice in terms of making SB interface with n-Si. The concentration of donor atoms in n-Si has been found to play an important role at both types of injection and the donor concentration should preferably be kept at lower value ($<10^{16}$ cm^{-3}) to get higher V_{oc}. The effect of thickness on V_{oc} has been found in both the direct and indirect band gap semiconductors at high level injection condition only. A more pronounced reduction in the V_{oc} has been found for lower work function metals in use.

Keywords: Schottky barrier; Solar cells; Low level injection; High level injection.

I. INTRODUCTION

A Schottky-barrier is formed by a metal/n- (p-) type semiconductor refers to the contact of a metal of higher (lower) work function with the semiconductor of lower (higher) work function. By the built-in electric field generated at the junction, the contact may be exploited as photovoltaic device, namely the Schottky barrier solar cells (SBSC). A great amount of research efforts on SBSCs using inorganic semiconductors were made in the mid-seventies to eighties in order to understand the effect of various factors governing their efficiency, for example, in Cr/p-Si` (8% efficient)[1], Au/p-GaAs (6.56% efficient) [2], Al/ p-InP (14.5% efficient) [3], Pd/ a-Si [4] to cite few such studies. Of late, there has been a renewed interest in the SBSC using organic semiconductors like, copper pthalocyanine (CuPc) for its low cost, easy fabrication technique and application on light-weight and/or flexible plastic substrates [5-14]. The organic solar cells are often characterized with low short circuit current density (J_{sc}), which has been attributed to small exciton diffusion length, which is of the order of a few nm. However, SBSCs made of CuPc prepared by thermal evaporation [7, 8] have shown large open circuit voltage (V_{oc}). In a recent study, electrodeposited [15] CuPc based SBSC has been reported to have V_{oc}, in the range 400 - 1100 mV over varied thickness of the CuPc layer. They also accounted for different routes of the metallic layer deposition. A great amount of research is on to improve their J_{sc}, however, it would be much easier to embark upon an enhancement of their V_{oc}. One of the easier methods to do this is using the SBSC with concentrated solar radiations with proper heat removal arrangement, unless the method has an adverse effect on the chemical stability of the active layer. At high intensity, the semiconductor is in general on high-level of injection of carriers.

The purpose of the present study is to establish a model of highly injected n-type semiconductor in general, making Schottky contact with a standard metal. The present model has not considered a detailed representation of molecular energy levels, in case the semiconductor is an organic one. However, a focus is made on the high injection condition irrespective of the type of semiconductor. A high level injection in a semiconductor refers to the non-equilibrium condition where the excess charge carrier concentration is sufficiently large compared to the donor or acceptor doping density (i.e., $\Delta n, \Delta p \gg N_d$ or N_a, respectively) and reverse is the case for low level injection condition.

The approach is an extension of a previously worked out model by Dubey and Paranjape [16], where a low injection condition was considered to establish an analytical form of the V_{oc} of a Metal (Schottky)/n-Semiconductor/Metal (Ohmic) system in presence of monochromatic light. Our model for V_{oc} under both high and low level injections is described in Section 2. The dependence of V_{oc} on various factors, such as, surface recombination at the metal-semiconductor interface, Schottky barrier height, density of doping and semiconductor film thickness have been calculated and discussed. In Section 3, all boundary conditions and the injection conditions have been taken care of. In our study the SBSC is realized by considering different metals and semiconductors. Our model results at low level injection condition have also been discussed with that reported by Dubey *et al.* [16].

II. OPEN CIRCUIT VOLTAGE: THE MODEL

The energy-band diagram of metal/n-type semiconductor SBSC is shown in Fig.1. Schottky contact forms at x=0 and Ohmic contact at x=L position of the semiconductor. A depletion region of width, W forms near the Schottky contact.
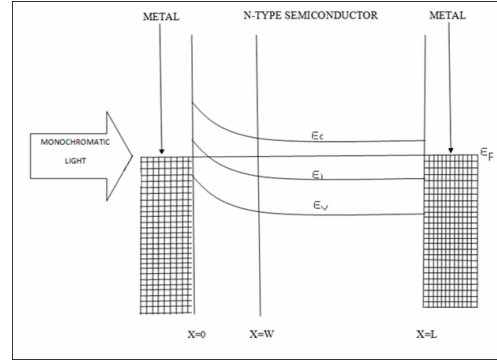

Figure. 1. Energy-Band diagram of a Metal/n-semiconductor Schottky barrier Solar cell

The open circuit voltage (V_{oc}) under illumination of monochromatic light at the interface of metal and n-type semiconductor SBSC is considered for the model. So the boundary condition is that the total current density (J_T) i.e. that is combination of drift and diffusion current component of electrons and holes flowing in the cell must be zero.

$$J_T = J_n + J_p \tag{1}$$

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

Since $J_T = 0$, $\tag{2}$

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

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

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

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

The potential difference, $V(W) - V(0)$, represents that developed within the depletion region, whereas, $V(L) - V(W)$, corresponds to that in the neutral region. These two open circuit potentials (OCP) would be evaluated in the following subsections, 2.1 and 2.2, respectively.

II.1 OCP in the Depletion region ($0 \leq x \leq W$)

Within 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 the total electric field, E can be expressed as,

$$E = E_b(x) + E_g(x) \qquad (6)$$

The carrier densities at non-equilibrium can be expressed as,

$$n = n_0(x) + \Delta n(x) \qquad (7)$$

$$p = p_0(x) + \Delta p(x) \qquad (8)$$

Where $n_0(x)$ and $p_0(x)$ are the equilibrium electron and hole densities, respectively. The $\Delta n(x)$ and $\Delta p(x)$ are the excess electron and hole densities. Substituting Eq. (6), (7) and (8) in Eq. (3), some terms are eliminated and we obtained,

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

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

$$E_g(x) = (D_p \frac{d\Delta p}{dx} - D_n \frac{d\Delta n}{dx})[(n_0 + \Delta n)\mu_n + (p_0 + \Delta p)\mu_p]^{-1} - \frac{(\Delta n \mu_n + \Delta p \mu_p)E_b(x)}{(n_0 + \Delta n)\mu_n + (p_0 + \Delta p)\mu_p} \qquad (10)$$

Here Δn can be eliminated from Eq. (10) using continuity equation for electrons and holes,

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

and

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

Where τ_n, τ_p are the electron and hole life times and J_n, J_p are the electron and hole current densities,

respectively. In steady state, total current density must be constant. Therefore, $\frac{d[J_n + J_p]}{dt} = 0 \qquad (13)$

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

Using Eq. (11)-(14) we obtain,

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

Eq. (15) corresponds to the expression for space-charge neutrality assumption, $\Delta n = \Delta p$.

Substitution of Eq. (15) in Eq. (10) and integrating from 0 to W yields,

$$V(W) - V(0) = -\int_0^W E_g(x)\, dx$$

$$= -\int_0^W \frac{\{D_p - D_n (\tau_n/\tau_p)\}\, d\Delta p/dx}{((n_0 + \Delta p\frac{\tau_n}{\tau_p})\mu_n + (p_0 + \Delta p)\mu_p)}\, dx$$

$$+\int_0^W \frac{((\frac{\tau_n}{\tau_p})\mu_n + \mu_p)\Delta p\, E_b(x)}{(n_0 + \Delta p\frac{\tau_n}{\tau_p})\mu_n + (p_0 + \Delta p)\mu_p}\, dx \qquad (16)$$

Eq. (16) gives the open circuit voltage developed across the depletion region.

Eq. (16) can be simplified further using depletion region approximation, $n_0(x), p_0(x) \ll \Delta n(x), \Delta p(x)$. This approximation is reasonable because a high level injection is satisfied under strong illumination and we obtain,

$$V(W) - V(0) = -\Phi s - \frac{\{D_p - D_n (\tau_n/\tau_p)\}}{(\frac{\tau_n}{\tau_p}\mu_n + \mu_p)} \log\frac{\Delta P(W)}{\Delta P(0)} \qquad (17)$$

Where $\Phi s = \frac{1}{2}\frac{qN_d W^2}{\varepsilon(s)}$ is the surface potential, N_d is the donor density and $\varepsilon(s)$ is the dielectric permittivity of the semiconductor.

II.2. OCP in the Neutral region ($W \leq x \leq L$)

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

Therefore,
$$E = E_g(x) \qquad (18)$$

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

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

Where n_i is the intrinsic carrier concentration.

Substituting Eq. (15), (18), (19) and (20), in Eq. (9) and considering high level injection condition,

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

It gives

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

Integrating Eq. (22) over the range, $W \le x \le L$, the open circuit voltage developed across the neutral region can be obtained as,

$$V(L) - V(W) = \int_W^L E_g(x)\,dx$$

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

$$= \left[\frac{D_n\left(\frac{\tau_n}{\tau_p}\right) - D_p}{\mu_n\frac{\tau_n}{\tau_p} + \mu_p}\right] \int_W^L \frac{1}{\Delta p}\,d(\Delta p)$$

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

II.3. The open circuit voltage

Substituting Eq. (17) and (23) in Eq. (5), an expression for total V_{oc} developed across the device under high level injection condition may be obtained as,

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

Here we can't 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. In high level injection, Ohmic contact provides a finite sink for excess holes instead of an infinite sink that would hold in case of low level injection.

For complete determination of V_{oc}, the quantities $\Delta p(L)$ and $\Delta p(0)$ should be evaluated separately.

II.3.1 Evaluation of $\Delta p(L)$ and $\Delta p(0)$

The continuity equation can be used only for holes to evaluate hole carrier concentration at x=L and x=0. This equation for hole is solved in the depletion region and neutral region separately, then matched at X=W (at the junction). In steady state condition, the continuity equation for holes may be written as,

$$-\frac{1}{q}\frac{dJ_p}{dx} + G(x) - \frac{\Delta p}{\tau_p} = 0 \tag{25}$$

Where, in the above equation, G(x) represents the generation rate for holes and this can be expressed as,

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

With a wavelength dependent pre-factor, φ' which is independent of the absorption coefficient, (λ) of the semiconductor layer and distance, x can be expressed as,

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

Here, φ indicates the flux of photons striking the interface, $R(\lambda)$ is the reflection coefficient of the metal surface, $a(\lambda)$ is absorptance of thin metallic layer and $f(\lambda)$ is the probability that a photon will produce an electron-hole pair.

II.3.1.1 Excess hole concentration in depletion region ($0 \le x \le W$):

We can approximate, $p_o \ll \Delta p$ and considering only the hole current, J_p, to obtain,

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

The net electric field in this case is given by, E= $E_b(x) + E_g(x)$. Using boundary condition, $J_T = 0$ and

considering the approximation, $n_o(x)$, $p_o(x) \ll \Delta n(x), \Delta p(x)$, E can be written as,

$$E = \frac{A}{\Delta p} \frac{d\Delta P}{dx} \qquad (29)$$

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

Substituting Eq. (28), (29) and (30), in Eq. (25), we obtain,

$$D_p' \frac{d}{dx} \left\{ \frac{d\Delta p}{dx} \right\} - \frac{\Delta p}{\tau_p} + \varphi' \alpha \exp(-\alpha x) = 0 \qquad (31)$$

Where $D_p' = D_p - \mu_p A$, a general solution of Eq. (31), may be written as,

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

$$(32)$$

Where, $L_p'^2 = D_p' \tau_p \qquad (33)$

$$Q_1 = \frac{\varphi' \tau_p \alpha}{\alpha^2 L_p'^2 - 1} \qquad (34)$$

Where C_1 and C_2 are the constants of integration still to be determined under proper boundary condition.

II.3.1.2 Excess hole concentration in neutral region (W$\leq x \leq$ L):

Neglecting the drift current in comparison to diffusion current in this region under high level of injection, the hole current can be written as,

$$J_P \cong -qD_p \frac{d\Delta P}{dx} \qquad (35)$$

Substituting Eq. (35) in Eq. (25),

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

A general solution of Eq. (36) may be written as,

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

$$(37)$$

Where, $L_p^2 = D_p \tau_p \qquad (38)$

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

C_3 and C_4 are the constants of integration still to be determined.

II.3.1.3 Evaluation of the constants C_1, C_2, C_3 and C_4:

The constants of integration, C_1, C_2, C_3 and C_4 are to evaluated by applying the boundary conditions at x=0 and x=L which further are matched in the depletion and the neutral region.

First boundary condition: $J_p(x=0) = -q S_p \Delta p(0)$

$$(40)$$

Where S_p is surface recombination velocity of holes, which is dependent on the interface state density at surface, x=0.

Using Eq. (28) and (29) in (40),

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

Second boundary condition reads:

$$\Delta p(W)_{\text{(depletion region)}} = \Delta p(W)_{\text{(neutral region)}} \qquad (42)$$

and third:

$$\frac{d\Delta p}{dx} \Big|_{x=w \text{ (depletion region)}} = \frac{d\Delta p}{dx} \Big|_{x=w \text{ (neutral region)}} \qquad (43)$$

We may consider the expression for excess minority carrier concentration, $\Delta p(x)$ above its equilibrium value at any point x from the semiconductor surface provided the minority hole diffusion length is L_p, as given below

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

where, $P_{n\circ}$ is the concentration of hole in n-type semiconductor at x=0, P_n^0 concentration of hole in n-type semiconductor at thermal equilibrium.

Using Equations, (41) - (44), (32) and (37), the constants of integration C_1, C_2, C_3 and C_4 are evaluated as,

$C_1 =$

$$\frac{C_3 \exp\left(\frac{W}{L_p}\right)\left(1+\frac{L_p'}{L_p}\right) + C_4 \exp\left(-\frac{W}{L_p}\right) \cdot \left(1-\frac{L_p'}{L_p}\right) + b_1 \exp(-\alpha W) \cdot (\alpha L_p'-1)}{2 \cdot \exp\left(\frac{W}{L_p}\right)}$$

(45)

$C_2 =$

$$\frac{C_3 \exp\left(\frac{W}{L_p}\right)\left(1-\frac{L_p'}{L_p}\right) + C_4 \exp\left(-\frac{W}{L_p}\right) \cdot \left(1+\frac{L_p'}{L_p}\right) - b_1 \exp(-\alpha W) \cdot (\alpha L_p'+1)}{2 \cdot \exp\left(-\frac{W}{L_p}\right)}$$

(46)

$C_3 =$

$$\frac{Q_2 \exp(-\alpha L)\exp\left(-\frac{W}{L_p}\right) \cdot Y + K \cdot \exp\left(-\frac{W}{L_p}\right) \cdot Y}{\exp\left(\frac{L}{L_p}\right) \cdot \exp\left(-\frac{W}{L_p}\right) \cdot Y - \exp\left(\frac{W}{L_p}\right) \cdot X \cdot \exp\left(-\frac{L}{L_p}\right)} -$$

$$\frac{2 \cdot b_1 \cdot \exp\left(-\frac{L}{L_p}\right) \cdot \exp(\alpha W) - Q_1 (S_p + \alpha) \cdot \exp\left(-\frac{L}{L_p}\right)}{\exp\left(\frac{L}{L_p}\right) \cdot \exp\left(-\frac{W}{L_p}\right) \cdot Y - \exp\left(\frac{W}{L_p}\right) X \cdot \exp\left(-\frac{L}{L_p}\right)}$$

(47)

$C_4 =$

$$\frac{2 \cdot b_1 \cdot \exp\left(\frac{L}{L_p}\right) \cdot \exp(-\alpha W) + Q_1 (S_p + \alpha) \cdot \exp\left(\frac{L}{L_p}\right)}{\exp\left(\frac{L}{L_p}\right) \cdot \exp\left(-\frac{W}{L_p}\right) \cdot Y - \exp\left(\frac{W}{L_p}\right) X \cdot \exp\left(-\frac{L}{L_p}\right)} -$$

$$\frac{Q_2 \exp(-\alpha L)\exp\left(\frac{W}{L_p}\right) X - K \cdot \exp\left(\frac{W}{L_p}\right) X}{\exp\left(\frac{L}{L_p}\right) \cdot \exp\left(-\frac{W}{L_p}\right) \cdot Y - \exp\left(\frac{W}{L_p}\right) X \cdot \exp\left(-\frac{L}{L_p}\right)}$$

(48)

where,

$$X = \frac{S_p - \frac{D_p'}{L_p'}}{2 \cdot \exp\left(\frac{W}{L_p}\right)} \left(1+\frac{L_p'}{L_p}\right) + \frac{S_p + \frac{D_p'}{L_p'}}{2 \cdot \exp\left(-\frac{W}{L_p}\right)} \left(1-\frac{L_p'}{L_p}\right)$$ (49)

$$Y = \frac{S_p - \frac{D_p'}{L_p'}}{2 \cdot \exp\left(\frac{W}{L_p}\right)} \left(1-\frac{L_p'}{L_p}\right) + \frac{S_p + \frac{D_p'}{L_p'}}{2 \cdot \exp\left(-\frac{W}{L_p}\right)} \left(1+\frac{L_p'}{L_p}\right)$$

(50)

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

$b_1 = Q_2 - Q_1$ (52)

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

$$\Delta p(0) = C_1 + C_2 - Q_1$$ (53)

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

(54)

Now, the open circuit voltage for the SBSC under high level injection can be calculated from Eq. (24), which can be expressed as,

$$V_{OC} = -\Phi_S + \frac{D_n \left(\frac{\tau_n}{\tau_p}\right) - D_p}{\mu_n \left(\frac{\tau_n}{\tau_p}\right) + \mu_p} [\log$$

$$\left\{\frac{(C_3 \exp\left(\frac{L}{L_p}\right) + C_4 \exp\left(\frac{-L}{L_p}\right) - Q_2 \exp(-\alpha L)}{(C_1 + C_2 - Q_1)}\right\}]$$

(55)

Here C_1, C_2, C_3 and C_4 are the constants of integration defined in Eqs. (45) – (48) and the coefficients Q_1 and Q_2 are defined by Eq. (34) and (39), respectively.

Under low level injection condition, the open circuit voltage, V_{oc} can be considered according to the model by Dubey et $al.$ [16]. By considering the expression for $\Delta p(x)$, at $x=W$ this model gives the open circuit voltage at low level injection as,

$$V_{OC} = -\Phi_S + \frac{D_n\left(\frac{\tau_n}{\tau_p}\right) - D_p}{\mu_n\left(\frac{\tau_n}{\tau_p}\right) + \mu_p}$$

$$\log\left\{\frac{\Delta P(W)}{\Delta P(0)}\right\} - \frac{D_n \frac{\tau_n}{\tau_p} - D_p}{\mu_n N_d} \Delta P(W)$$

(56)

In all our subsequent calculations, open circuit voltages have been calculated both for high and low level injection conditions using Eq. (55) and (56), respectively.

III. RESULTS AND DISCUSSION

The effect of carrier recombination on and near the surface plays a significant role in the Schottky barrier interface when the semiconductor is either of high absorption coefficients or the surface recombination velocity is large [17]. Similar condition prevails in case there is a higher injection of carriers that leads to a higher rate of recombination at surface or interface. The dependence of the open circuit voltage (V_{oc}) on the barrier metal work function (ϕ_m) is discussed in Sec. 3.1. The above model is applied to predict also the change in open circuit voltage when the surface recombination velocity (S_p) of electrons/holes at the Schottky barrier interface changes is discussed therein. The effects of semiconductor doping density (N_d) as well as the metal/semiconductor barrier height ($\emptyset_{Bn}$) over V_{oc} are discussed in Sec. 3.2. In

Sec. 3.3 the effect of device thickness (L) has been discussed.

The numerical value of the open circuit voltage can be calculated using the Eqs. (55) with a given set of parameters at high level injections. At low level injection, Eq. (56) can be used to calculate the same. One must note that, the V_{oc} could not be compared with the experimental data available so far, unless a detailed knowledge of reflection coefficient, $R(\lambda)$ and absorption coefficient, $\alpha(\lambda)$ were known. Due to this fact, all subsequent results presented 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 ($\lambda > 1\mu m$) or possible impact ionization to occur at lower wavelengths ($\lambda < 0.4\mu m$), corresponding values of V_{oc} were calculated for the SBSCs at $\lambda = 550$ nm monochromatic light, choosing metals with their work functions and semiconductors with their useful properties at room temperature as listed in table-1. In order to envisage the effect of S_p, N_d, and L, these parameters were varied in the range $100 \leq S_p \leq 10^6$ cm/s, $10^{14} \leq N_d \leq 10^{17}$ cm^{-3}, $200 \leq L \leq 1000$ μm for M/n-Si as well as M/n-Ge and $20 \leq L \leq 100$ μm for M/n-GaAs SBSCs. The photon flux was considered to be $\phi' = 2 \times 10^{17}$cm^{-2}s^{-1} for either cases of the high (HLI) and low level (LLI) injection condition. These two conditions were considered exclusively in terms of the magnitudes of the excess minority carrier concentrations with respect to the base doping concentrations.

III.1 Effect of barrier metal work function and surface recombination at the metal/semiconductor interface:

Fig. 2 shows the calculated V_{oc} as a function of metal work functions, ϕ_m under HLI condition mentioned as above. As expected, the V_{oc} is found to increase in accordance with the built in potential, which should increase for the selected semiconductors with the barrier metal work functions in the range 4.26 - 5.12 eV. The surface states at the metal semiconductor interface would play a significant role in real devices and therefore we have evaluated V_{oc} as a function of surface recombination velocity (SRV), S_p for a fixed value of doping density and all chosen metals. The calculated results at both injection levels are shown in Fig. 3 for M/n-Si and M/n-GaAs, respectively, for a base doping concentration, $N_d = 10^{14}$ cm^{-3} in all cases.
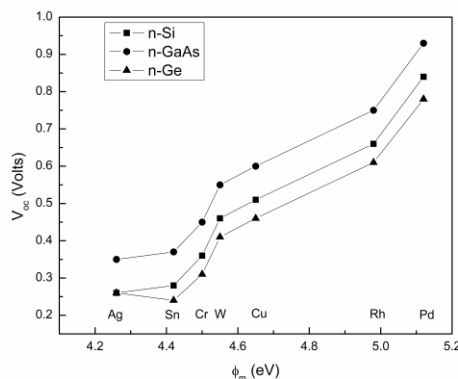

Figure 2: Variation of the open circuit voltage with metal work functions calculated under the high level injection by a monochromatic source at $\lambda = 550$ nm with different semiconductors at T = 300K. A surface recombination velocity, 100 cm/s is assumed at the metal-semiconductor interface

The V_{oc} is found to be highest for Pd as barrier metal and lowest for Ag with all selected semiconductors making the SBSC at both injection levels. A general trend of lowering in V_{oc} is found with increasing SRV, as expected.

Table -1:
Parameters selected for chosen Metals and Semiconductors

Metals:	Work function in eV (By ref.[18])
Ag	4.26
Sn	4.42
Cr	4.5
W	4.55
Cu	4.65
Rh	4.98
Pd	5.12

Semiconductors: (By ref. [19])	Electron Affinity (eV)	Room Temperature Band Gap (eV)	Absorption Coefficient at $\lambda = 550$ nm (cm^{-1})
n-Si	4.05	1.12	10^4
n-Ge	4.13	0.66	10^4
n-GaAs	4.07	1.42	10^4

It is also observed that, the lowering is substantial in the SRV range, $100 < S_p \leq 10^5$ cm/s for low injection, whereas, the V_{oc} lowering in same order is observed until an SRV of approximately 2×10^5 cm/s while a high injection prevails. This is important to notice that, the effect of SRV in the range $100 < S_p \leq 10^6$ 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 96% for HLI and LLI, respectively, in case of Ag/n-Si. A lesser 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 molecules and is subject to experimental verification. The calculated model results show that, Pd would be a better choice for SBSCs with both direct and indirect band gap semiconductors in use. Moreover, the GaAs would offer a higher Voc if HLI can be maintained and a relative compromise with the surface recombination would be promising.

10^{14} cm^{-3} in n-Si; (c) and (d) correspond to the n-GaAs for low and high injection levels, respectively.
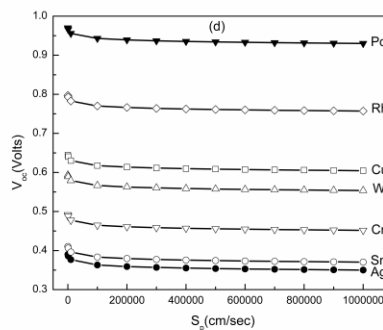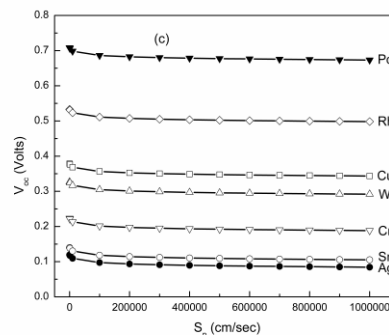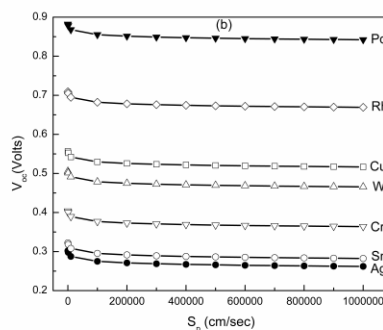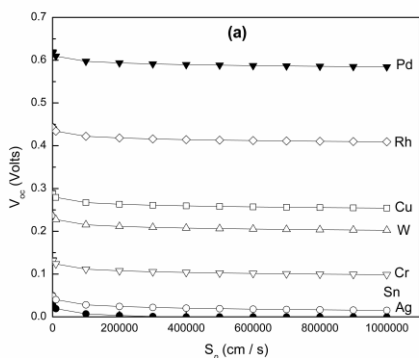

Figure 3: Calculated variation of open circuit voltage with surface recombination velocities for (a) low level and (b) high level injections for base doping concentration, $N_d =$

III.2 Effect of doping and Schottky barrier height at the interface on V_{oc}:

The effect of doping density, N_d of n-Si on V_{oc} of the SBSC is calculated for different concentration of donor atoms and they are found to be linear at lower and higher levels of doping concentrations. Fig. 4 (a) & (b) shows the variation of V_{oc} with N_d in the range, $10^{14} \leq N_d \leq 10^{17}$ cm^{-3} for a virtually defect free surface (with S_p = 100 cm/s) for HLI and LLI cases, respectively. 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 change in case of Ag/n-Si (37% under HLI and 90% under LLI). The variation of V_{oc} with N_d can be expressed from the current-voltage relationship of a Schottky barrier junction [19],

$$V_{oc} = \varphi_B + \ln\left(\frac{j_{sc}}{A^{**}T^2}\right) \qquad (57)$$

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 Eq. (57), 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 depletion boundary in the 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 probably 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.

Figure 5 shows corresponding results for n-GaAs system. Here, the doping density would play a crucial role unlike that in the n-Si systems.
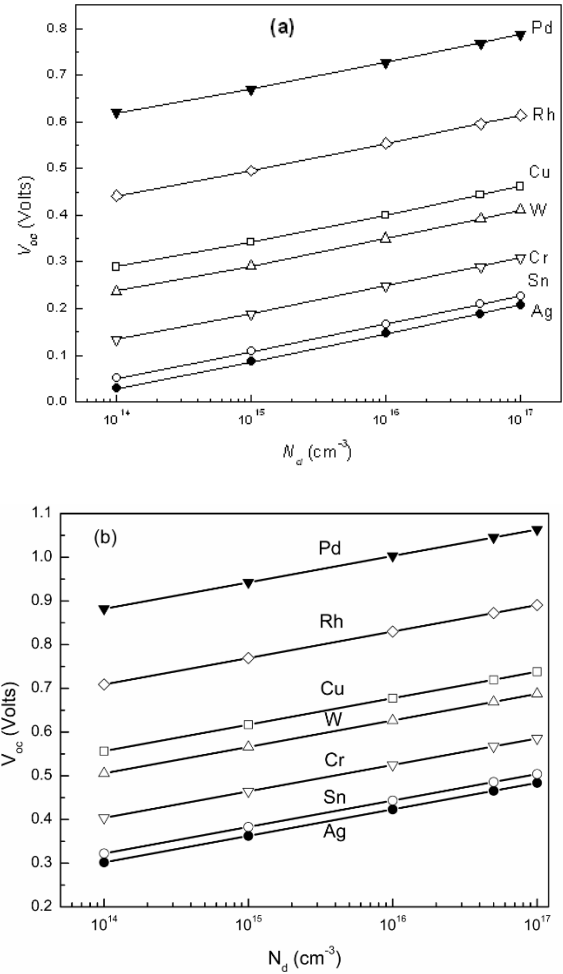

Figure 4: Calculated variation of open circuit voltage with base doping concentration for nearly defect free interfaces of metals and the n-Si under (a) low and (b) high injections.

The '*Mott transition*' behavior [20, 21] that essentially attributes to the effect of high doping concentration on the loss of semiconducting properties and an eventual transition to a metallic regime would be more prominent in GaAs systems than in the Silicon. By the simple model on this Mott criterion [21], this criticality can be expressed in terms of effective Bohr radius of the randomly distributed ionizing donors as,

$$a_B^* N_{crit}^{1/3} \approx 0.24 \qquad (58)$$

Here, N_{crit} is the critical donor concentration of the n-doped semiconductor above which it would behave as a metal. The effective Bohr radius of the Hydrogenic donor, a_B^*, that can be estimated in its ground state in terms of the Hydrogen Bohr

radius, $a_B = 0.53$ Å, the relative permittivity of the semiconductor, ε_r, the effective mass of the electrons, m_e^* and electron rest mass, m_0 as,

$$a_B^* = \frac{\varepsilon_r}{m_e^*/m_0} a_B \tag{59}$$
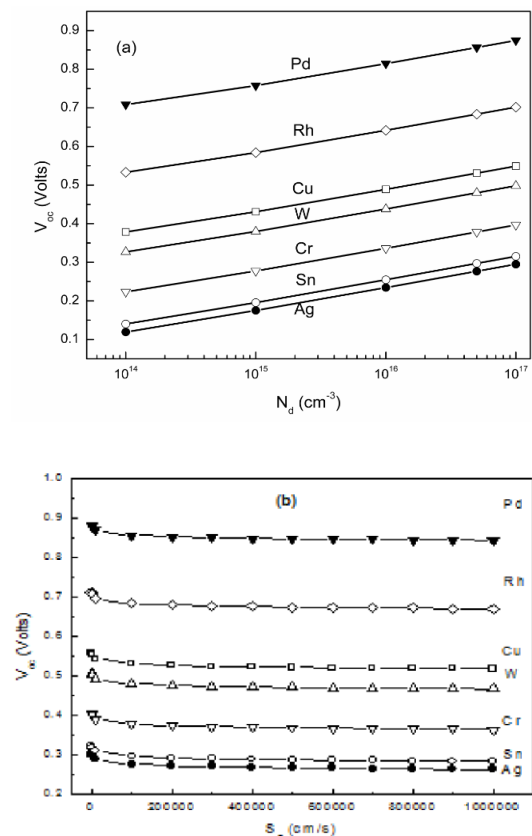

Figure 5: Calculated variation of open circuit voltage with base doping concentration for nearly defect free interfaces of metals and the n-GaAs under (a) low and (b) high injections.

As an example, for the hydrogenic donors in GaAs, with $\varepsilon_r = 13.1$ and $m_e^* = 0.067 m_0$, the critical doping concentration can be estimated as, $N_{crit} = 1.2 \times 10^{16}$ cm^{-3}. Consequently, for all $N_d > N_{crit}$, the n-GaAs should undergo a insulator-metal transition. A similar exercise in case of n-Si would result $N_{crit} \sim 10^{17}$ cm^{-3} or above. For this reason, the SBSCs using M/n-GaAs should take into consideration of doping concentration below 10^{16} cm^{-3} in order to produce substantial V_{oc}. Although, the present model does not consider this Mott criterion in calculating V_{oc}, its monotonic increase with increasing N_d above the

critical donor concentration should be ruled out with the above consideration.

III.3 Effect of the semiconductor thickness on V_{oc}:

In order to validate the requirement of further reduction of cost per unit power produced by a PV device, the semiconductor thickness should be reduced. However, it is also necessary to check the effect of thickness reduction on the performance of an SBSC.
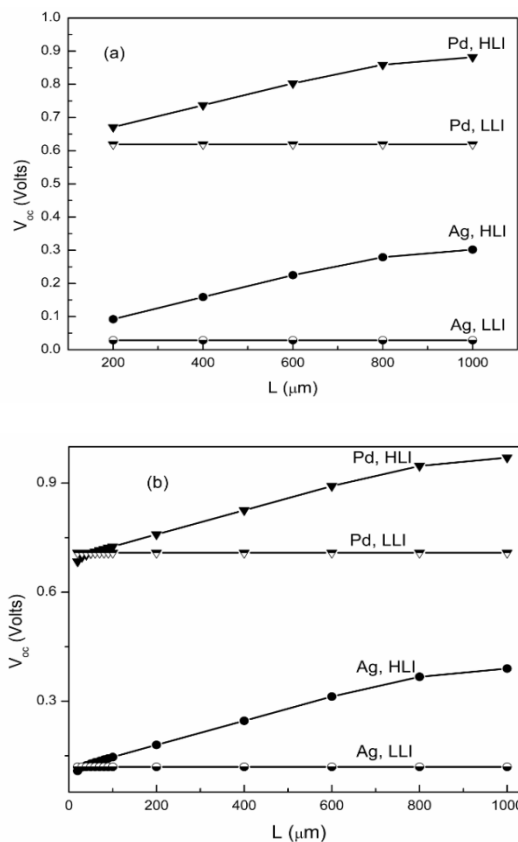

Figure 6: Variation of open circuit voltage with semiconductor thickness in case of (a) M/n-Si and (b) M/n-GaAs SBSCs of maximum thickness, 1mm with 'M' as Pd and Ag. Here LLI and HLI represents the low and high level injection conditions, respectively.

Fig 6a and b show the calculated effect of thickness on the V_{oc} both at low and high level of injection conditions in M/n-Si and M/n-GaAs SBSCs, respectively. In the above calculation it has also

assumed that, the minority carrier properties are not deteriorated over the lowering of thickness.

The open circuit voltage does not show any variation on cell length reduction at LLI, as the model here does not include the length term in its final expression (Eq. 56). Thus it may be predictable for n-Si, which is although an indirect band gap material, the reduction in cell thickness at LLI would not affect its efficiency, provided the short circuit current is maintained constant. On the other hand, at HLI, over a reduction of length in n-Si and n-GaAs from 800 μm to 200 μm, the V_{oc} is reduced by 21 % and 19 %, respectively for 'M' as Pd. The reductions in V_{oc} for the two semiconductors are 67 % and 51 %, respectively for 'M' as Ag. This clearly shows, while maintaining the high level injection condition in an indirect band gap semiconductor (*e.g.* n-Si, here), the V_{oc} reduction is more pronounced if lower work function metals are forming the Schottky barrier.

IV. CONCLUSION

We have investigated the variation of open circuit voltage with surface recombination velocity, doping density and semiconductor thickness for both high and low level injection conditions in a model Schottky-barrier solar cells with different choice metals. We have noticed that there is an increase of 42.6% in open circuit voltage as per the model of a metal/n-Si Schottky-barrier solar cell under high level injection condition, compared to the low level injection condition with negligible surface recombination velocities and moderate doping concentrations. Pd has been found to be good choice in terms of lower surface recombination property when used with either n-Si or n-GaAs. The concentration of donor atoms in n-Si would play an important role at high and low level injections, which shows that, a higher donor concentrations would give a V_{oc}, however, that should be lower than the critical value which would correspond to the transition of the semiconducting behavior into the metallic one. The effect of thickness is in line with the choice of direct/indirect band gap at high injection condition only. For lower work function metals, the reduction in the V_{oc} is more pronounced. The above study can be extended further to check the effect of minority carrier life time (or diffusion length) and the current

in the device which would be more appropriate for the Schottky-barrier solar cells used as concentrator PV devices.

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