Do solar cells need a built-in potential?

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The title issue has been a traditional, may be even ritual, controversy at QUANTSOL (and not only there) starting more than 20 years ago. In retrospect, this dispute might be viewed as one between chemists and electrical engineers. Since the solar cell is an electro-chemical device, i.e., electrochemical and electrical potentials play a role. (i) The chemist's view based on thermodynamics is that the nonequilibrium between the electro-chemical potentials of electrons and holes is the origin of the action of a photovoltaic device. The photocurrent is then enabled by the different selectivity of the two contacts to the solar cell absorber [1]. (ii) The electrical engineer's view based on Maxwell's equations is that whenever in a device a voltage appears there must be a capacitive element that accommodates the electrical charge to build up this voltage [2]. In order to avoid an electrical potential that is opposed to the intended flow of charge carriers a built-in potential in the right direction is desirable. The fact that both statements are completely correct did little in mitigating the controversy [3], which might be expressed as 'selective contacts vs. built-in potential'.

A final settlement could be enabled by a quantitative definition of the (zero bias) selectivity Σ_0 by Brendel and Peibst [4]

$$\Sigma_0 := \frac{kT/q}{R_c J_0} \quad (1)$$

where R_c denotes the contact resistance (in units Ωcm^2) and J_0 the saturation current density, and kT/q the thermal voltage.

Figure 1 illustrates a band diagram of a generic solar cell with an intrinsic absorber material with a band gap energy $E_g = 1.4 \text{ eV}$ and a thickness d_a of 1 µm and two undoped contacts of thickness thickness $d_c = 25 \text{ nm}$. The built-in potential V_{bi} is defined by the work function difference of the two metallic contacts. The two contact materials have a band gap energy of 1.7 eV arranged by a valence band offset $\Delta E_V = 0.3 \text{ eV}$ for the

electron contact on the left and a conduction band offset $\Delta E_{\rm C}=0.3$ eV for the hole contact on the right.

Recombination losses at the contact interfaces are given by interface recombination as well as by contact recombination, i.e. by respective minority carriers flowing to the metallic contact [5]. The band offsets in Fig. 1 are designed to prevent the latter loss. The saturation current density associated with interface recombination of holes at the electron contacts depends on the built-in potential via

$$J_0 = qS_p N_V \exp\left(-\frac{E_g + qV_{bi}}{2kT}\frac{1}{\dot{j}}\right)$$
(2)

where S_p is the hole recombination velocity and N_V the effective density of states in the valence band. For contact recombination we find analogously

$$J_0 = q \frac{D_p}{d_c} N_V \exp\left(-\frac{E_g + qV_{bi} + 2\Delta E_V}{2kT}\right) \frac{1}{j}$$
(3)

where D_p denotes the diffusion constant of holes in the electron contact. For electron recombination at the hole contact (r.h.s. in Fig. 1) hold analogous equations.

Resistive losses at the contact arise because of the limited conductivity of the contact layer. For the electrons at the electron contact we have $R_c = d_c/(qn_c\mu_n)$ with μ_n as the conductivity and n_c as the concentration of electrons in the electron contact. Since the latter is controlled by the Fermi level position at the contact interface, we have

$$R_c = \frac{d_c}{q\mu_n N_C} \exp\left(\frac{E_g - qV_{bi}}{2kT}\right) \frac{1}{\dot{f}}.$$
 (4)

where $N_{\rm C}$ is the effective density of states in the conduction band.

Finally we set Eqs. (2) and (3) into Eq. (1) to find

$$\Sigma_0 = \frac{kT/q}{d_c} \frac{\mu_n N_C}{S_p N_V} \exp\left(\frac{qV_{bi}}{kT}\right).$$
 (5)

In an analogous way we find from combining Eqs. (1),(2),(4)

$$\Sigma_0 = \frac{\mu_n N_C}{\mu_p N_V} \exp\left(\frac{q V_{bi} + \Delta E_V}{kT}\right)_{j}.$$
 (6)

Thus, in both cases the selectivity depends exponentially on the built-in voltage.

The final result, given by Eqs. (5) and (6), nicely demonstrates how the dispute 'selective contacts vs. built-in potential' is to be solved. In principle, a 'perfectly selective' contact, i.e.

 $\Sigma_0^{(\mathbb{R})} \infty$, can be achieved by a proper choice of the parameters in the prefactors of Eq. (5) and (6), e.g. by putting the respective majority carrier mobility to infinity, or the minority carrier mobility or the recombination velocity to zero. Thus, the purity of the thermodynamic argument [1,5] is preserved.

However, the possibility to control the contact selectivity via the built-in voltage is practically much more attractive, because this quantity enters exponentially in Eqs. (5) and (6). Furthermore, the built-in voltage in many cases is reasonably well controlled by doping of the contact layers or by a proper choice of work functions of the contact materials. This is why any solar cell of significant efficiency possesses a built-in potential.

It is important to stress that our arguments do *not* rely on carrier separation in the bulk of the absorber material via the built-in field (the derivative of the built-in potential). This argument is only valid if the carrier mobilities in the absorber are below a critical threshold [6]. It is rather that the built-in potential is the most important quantity that minimizes majority and minority carrier related losses at the contacts. Thus, again both opponents from the initial debate are right in their specific way. However, the present results show that the controversy is pointless: The built-in voltage is *determining the contact selectivity* to a large extent. A proper design of selective contacts has to start with optimizing this quantity in order to minimize resistive and recombination losses at the same time.



Figure 1: Band diagram of a generic solar cell with an undoped absorber and two contact materials. Recombination losses of minority carriers (holes at the electron contact to the left, electrons at the hole contact to the right) are given by interface or contact recombination. Resistive losses occur because of the finite conductivity of the respective majority carriers.

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