

Perspective

Fundamentals of solar cell physics revisited: Common pitfalls when reporting calculated and measured photocurrent density, open-circuit voltage, and efficiency of solar cells

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ABSTRACT

Very often, articles are found in the international literature reporting solar cells (single junction) with efficiencies above the Shockley-Queisser limit. In other similar papers, the short-circuit current density (J_{sc}) of solar cells are also reported with values that are above the maximum that a single absorber semiconductor can provide (without multiple-exciton generation), under the solar spectrum. For example, it will be easy to find both experimental and simulation reports for CdTe solar cells with J_{sc} values above 40 mA/cm², under the AM1.5 solar spectrum. Unfortunately, in a pattern of perpetuating unsound analysis, recent articles with such parameter values cite old erroneous articles to justify their results. This fact reveals that some of the solar cell's basic physics fundamentals have been forgotten or are not known by many researchers in the field. In this work, some of the solar cell physics basic concepts that establish limits for the efficiency, the short-circuit current density, the open-circuit voltage and even the fill factor for solar cells are reviewed. All these parameter limits will be shown as a function of the active semiconductor bandgap for single junction cells under the AM1.5 solar spectrum. Finally, it is explained what experimental and theoretical errors are typically made, causing the erroneous report of cell parameters, when the fundamental limits are not considered.



Dr. Morales-Acevedo's pioneering work contributed to establishing a strong solar cell and photovoltaic research community in Mexico with international academic recognition. He has done research on different kinds of solar cells such as Silicon, and CdTe and CuInGaSe₂ thin film cells. Recently he has focused his work on Metal Organic Halide Perovskite thin film solar cells. Much of his investigation has been devoted to understanding the physical limits and optimizing cell designs by simulating their behavior, but he also has done experimental work collaborating with other groups in Mexico for making and characterizing solar cell devices. He is currently a full Professor at Centro de Investigación y de Estudios Avanzados del IPN (CINVESTAV, in Mexico) and Emeritus Fellow of the Mexican

Scientific Research System (SNI). He has directed 30 M.Sc. and Ph.D. theses. He is Associate Editor for both Solar Energy Journal and Journal of Electronic Materials. He has edited one book on Solar Cell and Photovoltaic Research Perspectives (2013) and is the author of another solar cell popularization book in Spanish (1996). Currently, he is co-editing another book on new solar cells beyond Silicon.

1. Introduction

Solar cells are expected to be an important source of electrical energy in the following years, avoiding the emission of green-house gases to the earth's atmosphere, and helping in this way to solve the possible earth's climatic crisis in this century. Solar cells have been made on many different semiconductor materials, and now research in new materials for developing photovoltaic cells which are more competitive in price and efficiency is being done. For any of these materials, the most important parameter is the bandgap (E_g) because it determines the minimum energy for the incident photons to be absorbed by the material. Absorbed photons generate electron-hole pairs which are then collected at the solar cell junction. Some of the photo-generated electron-hole pairs will be lost by recombination. In this process, the inverse phenomenon occurs, and some electron-hole pairs recombine emitting photons.

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In addition to this minimum radiative recombination, in a real cell there will be non-radiative recombination, increasing the cell's energy loss. Understanding how to reduce this non-radiative recombination in real cells is the basis for improving them. In the limit, for an ideal cell, the non-radiative recombination is assumed to be zero, so that the limiting recombination is owed to the radiative recombination which exists by the thermal interaction of a solar cell with the surroundings, as will be explained below. These concepts and principles establish the limits for the conversion efficiency of any solar cell. Surpassing these limits would be equivalent to violate the thermodynamics laws for thermal machines.

Unfortunately, despite these fundamental basic physics concepts, it is possible to find journal articles (see for example [1–6]), where conventional solar cells are reported with parameters well above these limits. Then, this work intends to review those basic concepts and limits and try to explain the possible source of error for such experimental and theoretical reports, so that such errors are not repeated in future publications.

2. On the limits for the photo-current density, open-circuit voltage, and efficiency of solar cells

For ideal solar cells, the limiting efficiency occurs when all the absorbed photons generate electron-hole pairs that are fully collected, generating a photo-current, and in such a way that the carrier recombination rate is limited by the radiative recombination required for the cell to be in quasi-equilibrium with the surroundings at the cell's temperature T .

2.1. Ideal photo-generated current density

When the cell is illuminated (by sunlight), it will generate a photo-current. Ideally, all the photo-generated carriers (one electron-hole pair per absorbed photon) will be collected to produce the cell's photo-current. Therefore, assuming no optical losses (no reflectance) and 100% carrier collection probability, the maximum photo-current density (J_L) will be:

$$J_{L_{ideal}} = q \int_{E_g}^{\infty} N_0(E) dE \quad (1)$$

where $N_0(E)$ is the photon flux density from the solar spectrum (global AM 1.5) and q is the electron's charge magnitude. Photons with energy E smaller than the absorber's bandgap E_g do not produce electron-hole pairs. Then, as E_g becomes larger, the ideal photocurrent density will become smaller. In other words, a silicon cell will have a larger ideal photocurrent density than a CdTe solar cell, because in silicon more photons from the solar spectrum will have enough energy to be absorbed. This fact is expressed in equation (1) by the lower limit in the integral, which is just counting the photons (in the unit area each unit of time) absorbed by the respective semiconductor with bandgap E_g . This is a very simple expression that can be calculated very quickly, without using any solar cell simulator.

2.2. Radiative recombination losses

In thermal equilibrium, the absorbed energy flux should be equal to the cell's emitted energy flux (detailed balance principle). Hence, in equilibrium with the surroundings, the cell will emit photons at a rate equal to the rate of photons absorbed from the surroundings:

$$\varphi_{em,0}(E) = \varphi_{abs}(E) = a(E) \varphi_{bb}(E) \quad (2)$$

where $a(E)$ is the cell absorbance of photons with energy E and φ_{bb} is the flux of photons with energy E due to the surroundings, at temperature T . Ideally, φ_{bb} will have the blackbody energy spectrum at temperature T . For very thin cells, the total absorbance will vary as a function of the

absorber thickness because some photons from the surroundings will not be absorbed. However, for cells thick enough, the ideal absorbance $a(E) = 1$ for $E > E_g$ and $a(E) = 0$ for $E < E_g$ since these photons will not have enough energy to be absorbed by the material. Then, in the ideal case:

$$\begin{aligned} \varphi_{em,0}(E) &= \varphi_{abs}(E) = \varphi_{bb}(E) & \text{for } E > E_g \\ \varphi_{em,0}(E) &= 0 & \text{for } E < E_g \end{aligned} \quad (3)$$

The emitted photons from the cell should be generated by the radiative recombination of electrons (at the conduction band) and holes (at the valence band) in the absorber material. Hence, in equilibrium there will be absorbed photons, producing electron-hole pairs which will recombine at the same rate than the absorption rate, so that the thermodynamic equilibrium is achieved at a given ambient temperature.

When a voltage V is applied to the cell (in dark conditions), it will become out of equilibrium, and we expect the electron and hole concentration to increase, causing an exponential (in the Boltzmann approximation) enhancement of the radiative recombination rate:

$$\varphi_{em}(E) = \varphi_{em,0}(E) \exp\left(\frac{qV}{kT}\right) = \varphi_{bb}(E) \exp\left(\frac{V}{V_T}\right) \quad (4)$$

in which V_T is the thermal potential (kT/q) at temperature T , and k is the Boltzmann constant. Hence, when there is no other recombination process, the net recombination current density when a voltage V is applied becomes:

$$J_{rad}(V) = J_{0,rad} \left[\exp\left(\frac{V}{V_T}\right) - 1 \right] \quad (5)$$

Then, considering the blackbody spectrum at temperature T , the saturation current density is limited by the radiative recombination, so that $J_{0,rad}$ can be written as

$$J_{0,rad} = \left(\frac{2\pi q}{h^3 c^2} \right) \int_{E_g}^{\infty} \frac{E^2}{\exp\left(\frac{E}{kT}\right) - 1} dE \quad (6)$$

where h is the Planck's constant and c is the light velocity in vacuum. In real cells, in addition to this current due to radiative recombination there will be non-radiative recombination processes, causing an additional dark current and the reduction of the cell's open-circuit voltage.

2.3. Current – Voltage characteristics of ideal solar cells

We have now the ideal model for a solar cell, the total current density for a given applied voltage V is:

$$J(V) = J_{L_{ideal}} - J_{0,rad} \left[\exp\left(\frac{V}{V_T}\right) - 1 \right] \quad (7)$$

Then, the ideal open-circuit voltage will be:

$$V_{oc_{ideal}} = V_T \ln \left[\left(\frac{J_{L_{ideal}}}{J_{0,rad}} \right) + 1 \right] \quad (8)$$

The upper-limit conversion efficiency (η_{limit}) can be estimated using:

$$\eta_{limit} = \left(\frac{J_{L_{ideal}} V_{oc_{ideal}}}{P_{in}} \right) FF_{ideal} \quad (9)$$

where P_{in} is the total incident power from the sun radiation (100 mW/cm² for the AM 1.5 global solar spectrum), and the ideal fill factor FF_{ideal} in eq. (9) is:

$$FF_{ideal} = P_{max} / (J_{L_{ideal}} V_{oc_{ideal}}) \quad (10)$$

in which P_{max} is the maximum power density obtained from the $P(V) = V \times J(V)$ curve.

Our own notation has been used for the above set of equations, but all of them are based on the Shockley and Queisser model [7]. This model establishes the upper limits for each of the important parameters

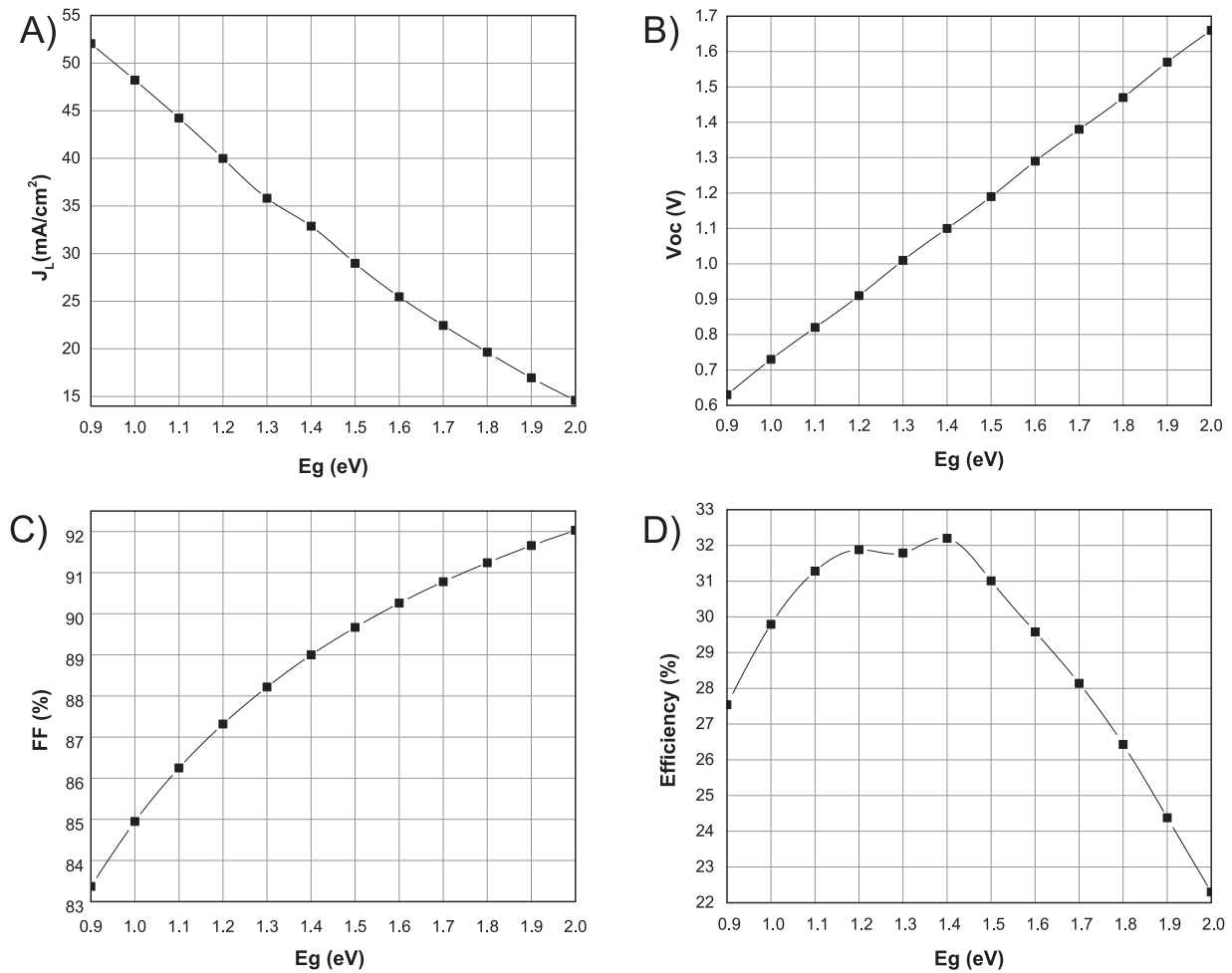


Fig. 1. Ideal (upper limit) single junction solar cell parameters as a function of the absorber bandgap (E_g), under the global AM1.5 solar spectrum (normalized to 100 mW/cm²). A) Photo-current density J_{Lideal} (mA/cm²). B) Open-circuit voltage $V_{ocideal}$ (Volts). C) Fill factor FF_{ideal} (%), and D) Efficiency η_{limit} (%).

in solar cells.

2.4. The efficiency limits for semiconductors with different energy bandgaps

Using the above set of equations, calculations were made for materials with bandgap energies in the range between 0.9 eV and 2 eV, under the AM1.5 global solar spectrum (normalized to 100 mW/cm²) at room temperature (300 K). The ideal efficiency (η_{limit}) as a function of the absorber bandgap is shown in Fig. 1. Notice that the maximum ideal efficiency is around 32.2% for a bandgap around 1.4 eV. Therefore, either experimental or theoretical efficiencies for single absorber solar cells cannot be much higher than this value (32%–33%). Similar considerations can be followed for determining the upper limits for multi-junction solar cells, but here we shall limit our discussion to single absorber solar cells.

In Fig. 1, the ideal photo-current density (J_{Lideal}), open-circuit voltage ($V_{ocideal}$) and fill factor (FF_{ideal}) are also shown. Notice for example that for a silicon solar cell ($E_g = 1.1$ eV), J_{Lideal} would be around 44 mA/cm², while for a CdTe cell ($E_g = 1.5$ eV), J_{Lideal} would be approximately 29 mA/cm², under the global AM1.5 solar spectrum (100 mW/cm²). Unfortunately, some articles, both theoretical and experimental, report values above 40 mA/cm², for CdTe solar cells, and values above the ideal for cells made with other absorbers. This kind of articles are then used to justify new reports, in an unending string of wrong reports. This is why it is important to establish the upper-limits for the efficiency, the photo-current density, the open-circuit voltage, and the fill factor (FF). These

limits for V_{oc} and FF are also shown, as a function of the absorber bandgap, in Fig. 1.

3. Pitfalls when reporting calculated and measured photocurrent density, open-circuit voltage, and efficiency of solar cells

3.1. Experimental errors

It is frequent to find in the literature experimental reports for different solar cells with parameter values above the ideal limits shown in the preceding section (see for example [1,2,5]). The most common error when characterizing a solar cell is in the determination of the short-circuit current density (J_{sc}). Errors for experimental V_{oc} are small because typically these voltages are of the order of mV which can be measured by modern instruments without much error. Similarly, from an I - V curve under illumination, the FF can be determined from the $P(V) = I \times V$ curve, as the ratio given by eq. (10) can also be estimated with relative accuracy.

However, the short-circuit photo-current density (J_{sc}) is determined from the measured total short-circuit current (I_{sc}) and then divided by the effective area (A) of the cell ($J_{sc} = I_{sc}/A$). This process usually leads to several error sources. Depending upon the area for the device, I_{sc} will be small for a small cell area, so that the measured I_{sc} can be inaccurate. This is a consequence that in order to report high cell efficiencies, avoiding series and shunt resistance effects and non-uniformity problems associated to large areas, the cells are usually made with small

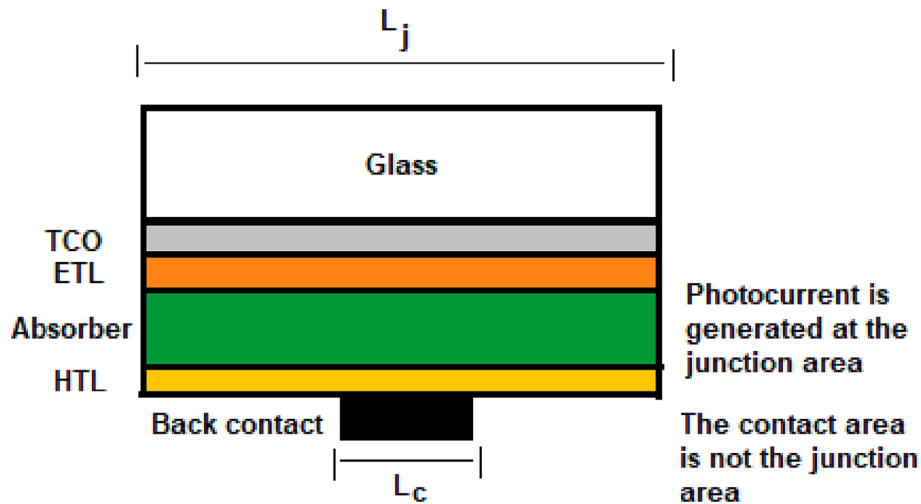


Fig. 2. Schematic of a typical thin film solar cell cross section. TCO is a transparent conducting oxide. ETL is an electron transport layer. HTL is a hole transport layer. The active cell material is the absorber with bandgap E_g . The junction area is the (ETL/absorber/HTL) effective area. Usually, the back contact has a different area than the junction area. As an example, in the case shown here, for a square cell, the area ratio (junction/contact) in this case would be $(L_j/L_c)^2$.

areas, of the order of $1 \text{ mm}^2 = 10^{-2} \text{ cm}^2$, or even less. This means that the measured I_{sc} could be of the order of 100–400 μA , which are susceptible of measurement errors as high as 10% or more, particularly when calibrating the sun simulator used for this measurement. Another error source is the simulated solar spectrum, which typically does not provide the real AM1.5 solar spectrum. However, the most important error comes when delimiting the effective area. The real effective area of a cell of such dimensions ($1 \text{ mm} \times 1 \text{ mm}$) is not correct because it depends upon the different processes followed for making the cells, and many times the deposited area for thin films are larger than the assumed areas (for example when using masks with a certain area). But the most relevant error comes from the lack of understanding of how a solar cell device works. Typically, for thin film cells, J_{sc} is determined dividing the short-circuit current I_{sc} by the area of the contact at the back of the cell, as shown in Fig. 2. This implies again that the physics of the cell is misunderstood: the photocurrent is generated at the junction and not at the contact, so that the relevant area is the real junction area, not the contact area. Then, if the measured I_{sc} is divided by the back contact area, having a larger junction area, the value of J_{sc} will be overestimated with a similar overestimation of the cell efficiency. This overestimation sometimes can be as high as 100%. And even when the cell area is well defined (by laser scribing or any other technique) the contact area is usually smaller than the junction area. In summary, the effective cell area must be measured with care, avoiding the use of the back contact area to determine the photo-current density.

3.2. Theoretical errors

Theoretical efficiencies and cell parameters above those shown in Fig. 1 have also been reported for single absorber junction devices (for example [3,4]). Unfortunately, these publications are used by some experimentalists for justifying their own wrong results. Different tools have been used, for example SCAPS, AMPS, COMSOL, etc., and even computer programs developed by the authors themselves for solving the transport and continuity equations in solar cells. The most common error is due to the authors missing the carrier radiative recombination in the absorber material. The radiative recombination rate corresponds to the minimum recombination mechanism in a solar cell (causing a minimum saturation current density $J_{0,rad}$ expressed by equation (6), as explained above.

For conventional cells with low efficiencies, the radiative recombination is very low compared with the non-radiative recombination and typically it is not considered in cell modelling. However, as the non-

radiative recombination is reduced, giving increased bulk lifetimes and reduced surface recombination velocities, the radiative recombination must be included. For example, perovskite solar cells have reached the record efficiency levels ($>25\%$) where an important part of the total recombination is the radiative recombination contribution. Therefore, including this contribution is important for having a good model for perovskite solar cells [8] and for other high efficiency cells. When the model does not include the radiative recombination and the assumed non-radiative recombination rate becomes lower than the limiting radiative recombination, the result will be an erroneous efficiency above the upper limit shown in Fig. 1. Therefore, researchers should be careful to not neglect the bulk radiative recombination in the solar cell absorber when doing calculations.

Similarly, equation (1) is a simple equation for $J_{L_{ideal}}$ that can be evaluated very easily since it corresponds to adding all the photons (per unit area and per second) from the solar spectrum being absorbed by the solar cell. Photons with less energy than the bandgap E_g of the absorber will not contribute to the photo-current density. Unfortunately, again, some theoretical papers report J_L values above those shown in Fig. 1 [3,4]. Clearly, their calculations, usually made with the help of a solar cell simulator, are wrong. A real cell, with finite electrical and optical losses with respect to the ideal cell (Fig. 1), should always have an even smaller photo-current density.

In summary, equations (1), (5), and (6) give the ideal cell J - V curve (7) and determine the ideal upper limit parameters ($J_{L_{ideal}}$, $V_{oc_{ideal}}$ and FF_{ideal}) for a cell with a specific absorber bandgap (E_g). Researchers should always verify that their results (either experimental or theoretical) do not violate the ideal cell parameters shown in Fig. 1. If their experimental results are confirmed to be above these values, an unexpected effect should be looked for the materials used in the solar cells. For example, assume that there is a cell where the confirmed experimental J_{sc} is above $J_{L_{ideal}}$ in equation (1), then it will be possible to speculate that the absorber generates more than one electron-hole pair for each absorbed photon with energy at least twice the absorber bandgap E_g . Under some circumstances this may happen by means of the phenomenon called Multiple Exciton Generation, already observed in different materials [9]. However, this is not a common effect, and in general, the maximum photocurrent density is the one shown in Fig. 1.

4. Conclusions

A solar cell is an energy converter (light radiation to electrical energy). The solar cell conversion efficiency is then a very important

parameter. As for any other energy conversion device, the thermodynamic limit is the Carnot efficiency (below 100%), but the maximum solar cell conversion efficiency is even below this thermodynamical limit as has been well established by Shockley and Queisser [7], based on the solar cell physics. Similarly, the upper limits for other important parameters such as J_L , V_{oc} and FF can be calculated easily, as has been shown above. However, many wrong articles have been published with experimental or theoretical results which violate these upper limits. In this work, I have reviewed and re-written the ideal cell model with which the upper-limit values for J_L , V_{oc} , FF and efficiency can be calculated. I also have explained common reasons for obtaining erroneous values, both experimental and theoretical, which are above the ideal upper limits for these parameters. It is expected that this will help other researchers understand the fundamental cell physics, avoiding future reports with results that violate the ideal solar cell limits.

Declaration of Competing Interest

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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