One-dimensional analytical model for photovoltaic cells based on wide gap semiconductors

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One-dimensional analytical model suitable for large scale cells under illumination has been developed. The model is based on two main assumptions. The first one is that in the case of wide gap semiconductors the concentration of the free dark carriers related to the non-equilibrium (generated) carriers can be neglected. This assumption simplifies the transport equations. In the second one, we assume an mean value (E_{gc}) of the electrical field across the i-layer in accordance with the relationship ($E_{gc}w = \int_0^w E_{gx}dx$) were E_{gx} is the field created by light generated charges, w is the thickness of the i-layer of the cell. These assumptions allow us to transform the system from continuity and transport equations in a first order differential equation that simplify the solution of the system.

The experimental solar cell characteristics are fitted using the finite number of fundamental parameters, namely the electron and hole diffusion lengths (l_n ands l_p, respectively), the light intensity (L_0) and light absorption coefficient (α). If we know the values of L_0 and α, we can derive from the fitted curve the l_p value with satisfactory accuracy. The value of l_n influences more weakly on the I-V dependence. A simple formula for optimal thickness of the i-layer of the cell is derived.

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1. Introduction

In last few years the interest in thin-film solar cells has increased due to possibility for large scale production and cost reductions. Amorphous silicon and its alloys are promising materials for that. Microcrystalline silicon (mc-Si:H) modules and micromorph tandem (a-Si:H/mc-Si:H) modules are already well established [1,2]. A single junction amorphous silicon solar cell shows conversion efficiency of about 12 % [3]. Initial efficiency of 14.7% has been achieved for 1 cm^2 a-Si/interlayer/poly-Si stacked cell by optimizing the deposition conditions including an interlayer [4].

A large number of solar cell structures use different semiconductor materials. Usually solar cells are based on amorphous silicon p^+-i-n^+ structures. The p^+ and n^+ layers provide the built-in potential in the i-layer of the cell. The p^+ and n^+ layers are highly doped, with increased density of localized gap states and due to that a strong recombination of the light generated carriers occurs in these layers. We assume that only non-equilibrium (light generated) carriers create photocurrent. The processes in the i-layer and in the boundary regions (i/p^+ and i/n^+) of the illuminated cell determinate its basic parameters. Several models are developed in order to understand the physical nature of the solar cells. We suppose that the first developed theoretical model for crystalline silicon solar cell was reported in [5]. In order to develop further the technology, numerical simulation of devices can be used. Several software packages for this kind of simulations have been developed, e.g. SCAPS, AFORS-HET and AMPS [6-8]. While these are slightly different in their respective approaches to simulations, they are all very competent software. Silvaco TCAD offers complete and well integrated simulation software for all aspects of solar cell technology [9]. Each of these programs needs a proper physical model and too many known parameters, such as gap state density distribution, cross capture section of these states, life time of the non-equilibrium carriers, electron and hole mobilities etc.

In this paper we consider a simple one-dimensional theoretical model. One-dimensional simulations are adequate for large area solar cells. We consider cells based on wide gap semiconductors, for which the density of the light-generated non-equilibrium carriers is much more than the density of free dark carriers. Also we consider light genered electrical field as a parameter. These assumptions allow us to derive a relatively simple formula with finite number of parameters to simulate cell's I-V characteristic with satisfactory accuracy.

2. Physical model

As an example, we consider an amorphous silicon p^+-i-n^+ structure. Under illumination the electrons and holes

are generated and recombine as couples and, thus their generation and recombination rates are equals.

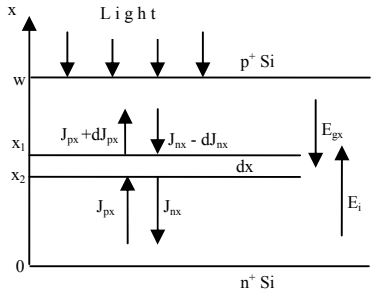

Fig. 1. Scheme of cross section a solar cell under illumination (p^+-side).

For such structure, under illumination the continuity equations are [10]:

$$\frac{dJ_{nx}}{dx} = -qL_0\alpha e^{-\alpha(w-x)} + q\frac{n_x}{\tau_n} \qquad (1)$$

$$\frac{dJ_{px}}{dx} = qL_0\alpha e^{-\alpha(w-x)} - q\frac{p_x}{\tau_p} \qquad (2)$$

where J_{nx} and J_{px} are electron and hole current densities, respectively, α is the light absorption coefficient; L_0 is the light intensity at x = w; n_x and p_x are electron and hole distribution across the i-layer and w is the thickness of the layer. Here we use a simplified model for recombination rate assuming that the recombination rate for electrons and holes is an arbitrary process at which the concentration of the traps is much larger than the concentrations of the generated carriers. In addition during long time illumination an effect of light induced defect creation exists at which the efficiency of the cells decreases**.** In the case of position sensitive detectors the diffusion length of the collected electrons and holes, in lateral (along the no illuminated n+-layer for electrons or along the no illuminated p+ layer for holes) direction is about two orders longer. For example lateral electron diffusion length in crystalline silicon can reach 1cm [11] while across the silicon depletion region it is about 200μm.

For each dx layer, the condition for steady state needs the $\frac{dJ_{px}}{dx} = -\frac{dJ_{nx}}{dx}$ relationship to be fulfilled. In order to simplify our consideration, we assume that the quantum efficiency of the photons is equal to unit (g = 1). In accordance with the above consideration, from eq. (1) and eq. (2) follows:

$$\frac{d}{dx}\left(J_{nx} + J_{px}\right) = 0 \qquad J_{nx} + J_{px} = J_g \qquad (3)$$

The light-generated current density (J_g) is a sum from electron and hole current densities and it is a constant across the i-layer. The electrons and holes are generated and recombine as couples. Their generation rates (G_n and G_p) are equal. Their recombination rates also are equal: $q\frac{p_x}{\tau_p} = q\frac{n_x}{\tau_n}$. From the last relationships follows:

$$n_x = cp_x \qquad (4)$$

were $c = \frac{\tau_n}{\tau_p}$ .For wide gap semiconductors at relatively strong light illumination, when the concentration of the generated (non-equilibrium) carriers is much larger than the concentration of the free dark carriers we can neglect the concentration of the free dark carriers in the transport equations. An intrinsic electric field $E_i = V_{bi}/w$ exists in i-silicon layer due to the energy difference (qV_{bi}) between the Fermi levels of p+ and n+ layers of the cell. At open circuit mode (J_g = 0, $U_g = U_{oc}$) at relatively high intensity illumination of the cell, do not band bending and $V_{bi} \approx U_{oc}$. J_g and U_g are the light generated current and voltage at $x = w$. The transport equations in this case are:

$$q\frac{kT}{q}\mu_n c\frac{dp_x}{dx} + q\mu_n E_x c p_x = J_{nx} \qquad (5)$$

$$-q\frac{kT}{q}\mu_p\frac{dp_x}{dx} + q\mu_p E_x p_x = J_{px} \qquad (6)$$

were $E_x = E_i - E_{gx}$ is the field which acts on the light generate carriers and separates the electrons from the holes. E_{gx} is the field created from non-equilibrium light generated carriers. It is directed opposite to the E_i field. The mobility of the electrons and holes are denoted with μ_n and μ_p, respectively. From eq. 5 and eq.6 follows:

$$\frac{dp_x}{dx} = -\frac{q}{kT}\frac{\left(\mu_n c + \mu_p\right)}{\left(\mu_n c - \mu_p\right)}E_x p_x + \frac{q}{kT}\frac{1}{\left(\mu_n c - \mu_p\right)}\frac{J_g}{q} \qquad (7)$$

Substituting 7 in 6 we obtain:

$$p_x = \frac{1}{2\mu_n c}\frac{J_g}{q}\frac{1}{E_x} + \frac{\mu_n c - \mu_p}{2\mu_n c\mu_p}\frac{J_{px}}{q}\frac{1}{E_x} \qquad (8)$$

Substituting 8 in 2 and taking into account that $c = \frac{\tau_n}{\tau_p}$ we obtain a differential equation relative J_{px}

$$\frac{dJ_{px}}{dx}+\frac{kT}{2q}\frac{l_n^2-l_p^2}{l_p^2}\frac{1}{l_n^2}\frac{1}{E_x}J_{px}-qL_0\alpha e^{-\alpha(w-x)}+\frac{kT}{2q}\frac{1}{l_n^2}\frac{l_n^2-l_p^2}{l_p^2}\frac{l_p^2}{l_n^2-l_p^2}J_g\frac{1}{E_x}=0$$

In the above equation the electrical field E_x is accepted as a parameter. This allows us to reduce system from continuity and transport equations to one linear first order differential equation. If we know the distribution of the charges in depth of the i-region, the electrical field E_x can be determined. The measurement of the density of states for electron and holes and their capture cross sections in injection mode is not the same as in generation mode because in generation mode the states in forbidden gap act as recombination centers. The captured charge in this (generation) mode is much smaller than in injection mode that complicates too much the determination of the light generated E_{gx} field.

The above equation can be written in the kind:

$$\frac{dJ_{px}}{dx}+C\frac{1}{E_x}J_{px}-qL_0\alpha e^{-\alpha(w-x)}+C\frac{l_p^2}{l_n^2-l_p^2}J_g\frac{1}{E_x}=0 \quad (9)$$

Analogically for electron current (J_{nx}) it is obtained the following equation:

$$\frac{dJ_{nx}}{dx}+C\frac{1}{E_x}J_{nx}+qL_0\alpha e^{-\alpha(w-x)}-C\frac{l_n^2}{l_n^2-l_p^2}\frac{1}{E_x}J_g=0 \quad (10)$$

where $l_n=\sqrt{\frac{kT}{q}\mu_n\tau_n}$, $l_p=\sqrt{\frac{kT}{q}\mu_p\tau_p}$ are the diffusion lengths of the electron and holes, respectively, and C is a constant $\left(C=\frac{1}{2}\frac{kT}{q}\frac{1}{l_p^2}\frac{l_n^2-l_p^2}{l_n^2}\right)$.

The general solution of eq. 9 at boundary conditions $J_{px}(x=w)=J_g$ and $J_{px}(x=0)=0$ is:

$$J_g=-qL_0\alpha e^{-\alpha w}e^{-C\int_0^w\frac{dx}{E_x}}\int_0^w e^{\alpha x}e^{C\int_0^x\frac{1}{E_y}dy}+\frac{l_n^2}{l_n^2-l_p^2}J_g\left(1-e^{-C\int_0^w\frac{dx}{E_x}}\right) \quad (11)$$

If we know the distribution of the captured charges in the i-layer (respectively the E_x field) the eq. 9 can be solved. We assume a mean value (E_{gc}) in the $(0,w)$ interval of the light generated field across the i-layer in accordance with the relationship: $-E_{gc}w=-\int_0^w E_{gx}dx=U_g$.

The E_{gx} fields has one important property-all E_{gx} fields have to satisfy one relationship: $-\int_0^w E_{gx}dx=U_g$ were U_g is an experimental value This is a reason to use mean electrical field. Then $E_x=E_c=E_i-E_{gc}=\frac{U_{oc}-U_g}{w}$. This assumption is an approximation. If the deviation of the electrical field are small relatively to the value of the intrinsic electrical field it can be used. Many authors use different commercial programs (some of them are noted in the introduction) which use density of the traps and their capture cross section for electrons and holes as parameters to calculate fixed charge and respectively the deviation of the electrical field in the i-region. These parameters can be measured separately only in injection mode, while in generation mode (under illumination) the traps act as recombination centers. Then the density of the captured charge in these traps is much smaller than the concentration of light generated carriers. Due to higher mobility of the electrons than the holes a bulk positive charge in the i-region is created, which screens the intrinsic electrical field in the i-region.

In this way, we substitute the real distribution of the electrical field across the i-layer with a constant electrical field. This model describes an ideal cell relative to the electrical field in the i-layer. The comparison of the I-V dependences under illumination of an ideal solar cell with the experimental one can help us to understand the processes in the cell. Model with constant electrical field is considered in [12], but from the other point of view.

In the case of a constant electrical field across the i-layer the general solution of eq. 11 at boundary conditions $J_{px}(x = 0) = 0$ and $J_{px}(x = w) = J_g$ is:

$$J_g=\frac{qL_0\alpha}{C\frac{1}{E_c}+\alpha}\times\frac{1-e^{-\left(C\frac{1}{E_c}+\alpha\right)w}}{\frac{l_n^2}{l_n^2-l_p^2}-\frac{l_p^2}{l_n^2-l_p^2}e^{-C\frac{1}{E_c}w}} \quad (12)$$

were $C=\frac{1}{2}\frac{kT}{q}\frac{1}{l_p^2}\frac{l_n^2-l_p^2}{l_n^2}$ and $E_c=\frac{U_{oc}-U_g}{w}$.

Equation 12 as matter of fact describes an I-V dependence of a p-i-n structure under illumination using three intrinsic parameters (α, l_p and l_n) of the i-layer. The parameter α is an average value of the light absorption coefficient. The parameters L_0 and α can be determined preliminary by independent measurements.

3. Calculation (Simulation)

In Fig.2 is shown the simulated I-V dependences in accordance with eq. 12 at $L_0 = 1.\ 10^{17} cm^{-2}.s^{-1}$, $\alpha = 1.10^5$ cm^{-1}, w = 200 nm l_n = 300 nm and at different values of hole diffusion length: l_p = 50, 100, 200 and 250 nm.

It can be seen that the value of the hole diffusion length influence mainly on the fill factor respectively on the efficiency of the cell. The electron diffusion length (l_n) much more weakly influence on the J_g value and on the fill factor of the cell because the value of the constant C is determined mainly from l_p value. The light intensity (L_0) and light absorption coefficient (α) influence strongly on the value of short circuit current (J_{sc}).The values of L_0 and α can be determined preliminary by independent measurements. In this way, in accordance with equation 12, the current I_g is determined mainly from the diffusion lengths of the holes and electrons which depend directly on the lifetimes of the electrons and holes i.e. from the density of the states in the forbidden gap of the i-region

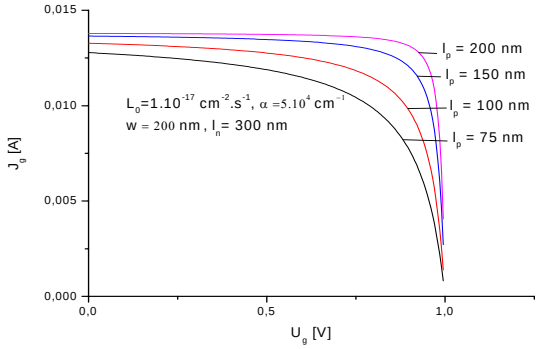

Fig. 2. Simulated I-V dependences at $L_0 = 10^{17}$ $cm^{-2}.s^{-1}$, $\alpha = 5.10^4$ cm^{-1}, w = 200 nm and l_n = 300 nmfor different values of hole diffusion length: l_p = 50, 100, 150 and 200 nm.

On Fig. 3a and Fig. 3b are shown the experimental [after 13] I-V dependences of an a-Si:H and a-Si:Ge:H based solar cells under illumination (dashed line) and fitted ones. The fitted parameters are described in the figures. To determine more accuracy electron and hole diffusion lengths it is need to know the values of L_0 and α from other (independent) measurements. For ambipolar diffusion length (which is closer to the diffusion length of the holes than to electron one) in [14] is obtained value 80 nm. In [15] for microcrystalline silicon is obtained 150 nm ambipolar diffusion length which is close to the value determined form Fig. 3 (a).

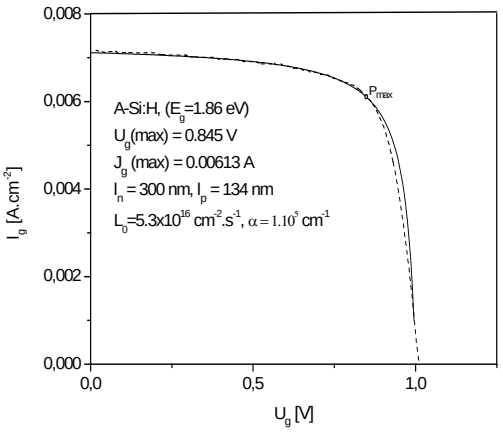

Fig. 3 (a). Dashed line: experimental I-V dependences [after 13] of a-Si:H (E_g = 1.86 eV) based solar cells under illumination, solid line fitted one at light intensity $L_0 = 5.3x10^{16}$ $cm^{-2}.s^{-1}$, light absorption coefficient $\alpha = 1.10^5$ cm^{-1}, electron and hole diffusion lengths 300 nm and 134 nm, respectively.

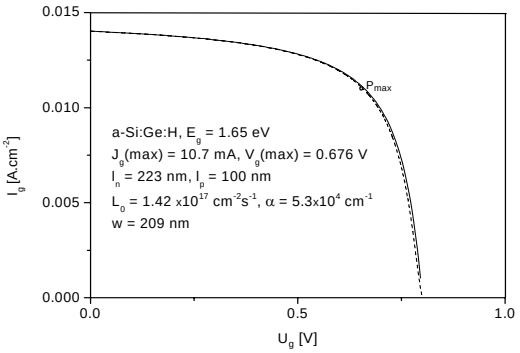

Fig.3 (b). Dashed line: experimental I-V dependences [after 13] of a-Si:Ge:H (E_g = 1.65 eV), solid line fitted one at light intensity $L_0 = 9.76x10^{16}$ $cm^{-}2.s^{-1}$, light absorption coefficient $\alpha = 5.10^4$ cm^{-1}, electron and hole diffusion lengths 223 nm and 100 nm, respectively.

The deviation of the fitted dependence in Fig.3a (for a-Si:H (E_g = 1.86 eV) based solar cells) from the experimental one for $U_g > U_g$(max) can be explained with increased recombination rate, respectively with a decreasing of the life time of the holes due to diminishing of the E_c field, which is responsible for separation of the both kinds of carriers.

If we decrease smoothly hole diffusion length (l_p) from 134 nm to 114 nm when U_g increase from U_g(max) to U_{oc} we can reach very good coincidence between experimental and fitted curves.(see Fig. 4) Therefore the lifetime of the carriers depends on the E_c electric field, which separates the both kind of carriers. For this cell it is pronounced when E_c becomes sufficiently small. In this case if E_c is smaller than 2.5×10^3 $V.cm^{-1}$.

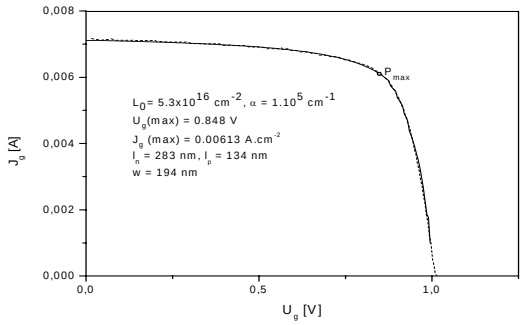

Fig. 4. Experimental I-V dependences [after 13] of an a-Si:H (E_g = 1.86 eV) based solar cell under illumination (dashed line), and fitted one (solid line) when l_p decreases smoothly from 134 nm up to 114 nm. The other parameters are the same as for Fig. 3.

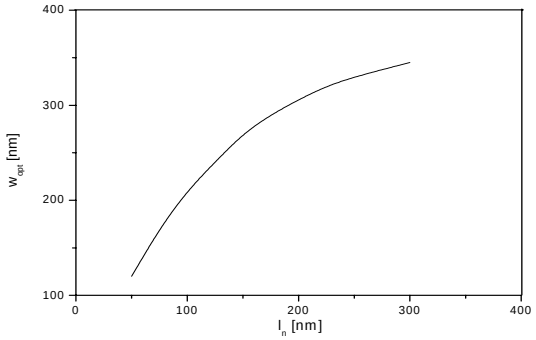

Fig. 5. Dependence of the optimal thickness of a-Si:H based cell on electron diffusion length at the same parameters as in Fig. 3 (a).

In the case of a-Si:Ge:H (E_g = 1.65 eV**),** based solar the coincidence between fitted and experimental I-V characteristics is better. Perhaps the difference between concentrations of the generated carriers when the cell is in open circuit mode and in short circuit mode is smaller due to smaller light absorption coefficient and higher conductivity of the a-Si:Ge:H than the a-Si:H. In this case the dependence of the lifetime of the both kind of the carriers on the working mode is weak.

4. Optimal thickness

In the case of p-side illumination, the condition $\frac{dJ_{nx}}{dx}(x=0)=0$ at which the generation rate of the electrons becomes equal to the recombination rate can be used to find the i-layer optimal thickness (w_{opt}). At $x = 0$ the hole current (J_{nx}) is equals to J_g, that is the second condition. Tacking into account these conditions eq. 9 leads to the follow transcendental equation for the optimal thickness of the i-layer:

$$\frac{e^{-\alpha w_{opt}}}{w_{opt}} = \frac{kT}{2q}\frac{1}{qL_0\alpha}\frac{1}{l_n^2}\frac{1}{U_{oc}-U_g(\max)}J_g(\max) \quad (13)$$

In accordance with eq. 13 the optimal thickness depends on generation rate ($qL_0\alpha$), electron diffusion length (l_n) and from working mode (J_g, U_g). Using above relationship, the optimal thickness (w_{opt}) for the maximum power point mode (J_g=6.13 mA, U_g = 0.85 V) at L_0 = 5.3x10^{16} cm^{-2}.s^{-1}, α = 1.10^5 cm^{-1} and l_n = 283 nm is 340 nm winch is thicker than the real one (194 nm). In Fig. 5 is given the dependence of the optimal thickness on the electron diffusion length.

5. Conclusion

One-dimensional analytical model is developed by assuming a mean (constant) electrical field across the i-layer and by neglecting the concentration of the free dark carriers relative to concentration of non-equilibrium (generated) carriers that is valid for wide bandgap semiconductors. Accepting light electrical field (E_x) as a parameter we have a possibility to reduce the system from continuity and transport differential equations to one first order differential equation. A relatively simple formula with finite number of parameters is derived to simulate experimental I-V characteristics of solar cells based on wide gap semiconductors. The model is successfully applied for a-Si:H, a-Si:Ge:H based cells and by fitting the simulated I-V characteristic to the experimental one the electron and hole diffusion lengths (l_n, l_p), the light absorption coefficient (α) and light intensity (L_0) are determined. To determine l_n and l_p with more accuracy it is needs to know L_0 and α from independent measurements. In accordance with this model the change of l_p value influences mainly on the value of the fill factor, respectively on the cell efficiency. The electron diffusion length (l_n) influence weakly on the J_g value and on the fill factor of the cell because the value of the constant C is determined mainly from l_p value.
On the base of the considered model a dependence of the optimal thickness of the i-layer on the electron diffusion length and light absorption coefficient, which are parameters of the i-layer, is derived. The optimal thickness depends also on generation rate ($qL_0\alpha$), and working mode (J_g, U_g) of the cell.

References

[1] B. Rech, T. Repmann, S. Wieder, M. Ruske, U. Stephan, Thin Solid Films **502,** 300 (2006).
[2] B. Rech, T. Repmann, M. N. van den Donker, M. Berginski, T. Kilper, J. Hupkes, S. Calnan, H.Stiebig, S.Wieder, Thin Solid Films

511–512, 548 (2006).
[3] M. Yoshimi, T. Sasaki, T. Sawada, T. Suezaki, T. Meguro, T. Matsuda, K. Santo, K. Wadano, M. Ichikawa, A. Nakajimaand, K. Yamamoto, Conf. Record, 3rd World Conference on Photovoltaic Energy Conversion, p. 1566 (2003).
[4] K. Yamamoto, M. Yoshimi, Y. Tawada, S. Fukuda, T.Sawada, T. Meguro, H. Takata, T. Suezaki, Y. Koi, K.Hayashi, T. Suzuki, A. Nakajima, Technical Digest of the International 12th Photovoltaic Science and Engineering Conf., Jeju, Korea, p. 547 (2001).
[5] P. T. Landsberg, Solid-State Electronics, **18**(12) 1043 (1975).
[6] M. Burgelman, P. Nollet, S. Degrave, Thin Solid Films, **361–362,** 527 (2000).
[7] A. Froitzheim, R. Stangl, L. Elstner, M. Kriegel, W.Fuhs, Proceedings of the 3rd World Conference on Photovoltaic Energy Conversion, p. 279 (2003).
[8] http://www.ampsmodeling.org/
[9] http://www.silvaco.com
[10] S. M. Sze, Kwok K. Ng, Physics of Semiconductor Devices, 3rd edn, (John Wiley& Sons 2007) 732.
[11] S. S. Georgiev, D. Sueva, N. Nedev, Journal of Physics: Condensed Matter, **9(**23), 4995 (1997).
[12] K. Taretto, U. Rau, J. H. Werner, Appl. Phys. **A77** (2003) 865-867.
[13] A. Luque, St. Hegedus, Handbook of Photovoltaic Science and Engineering, (Wiley 2003) 545.
[14] Nowak M., Starczewska A.**,** J. Non-Cryst. Solids**,** **351**(16-17), 1382 (2005).
[15] M. Goerlitzer, N. Beck, P. Torres, J. Meier, N. Wyrsch and A. Shah, J. Appl. Phys., **80(**9), 5111 (1996).

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