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Effects of inhomogeneous grain size distribution in polycrystalline silicon solar cells

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Abstract

We investigate the effects of grain size inhomogeneity on the performance of thin film polycrystalline silicon solar cells with columnar grains. We focus on cells with an exponential distribution of the grain diameter, which approximates the grain size inhomogeneity in polycrystalline silicon films made via aluminum induced crystallization (AIC) with low temperature annealing. Through equivalent circuit simulation, we demonstrate that the size inhomogeneity will only play a role when intra grain defects, which is common in AIC cells, can be avoided. We further demonstrate that the inhomogeneity itself is not a dominant factor which limits the efficiency of these cells.

Keywords: Polycrystalline silicon solar cells, Effective diffusion length, Grain size distribution

1. Introduction

Amid the advancement and success of silicon based solar cell technology, thin film polycrystalline silicon solar cells are still in the process of maturing. Challenges in using polycrystalline material for solar cells mainly arise due to the fact that grain boundaries limit the effective diffusion length of the cell to a few micrometers, and hence also the usable cell thickness. The grain boundaries in silicon act as an

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effective non-radiative recombination center that cannot be properly passivated [1]. Furthermore, because silicon is a rather inefficient optical absorber, advanced light trapping methods are needed. Even so, the polycrystalline form of silicon is still an attractive solar cell material as it can be more economical than its monocrystalline counter-part [2]. In order to increase the useful cell thickness, fabrication technologies that produce larger grains are being continually investigated. A promising method is the metal induced crystallization technology, particularly with aluminum [2-6], followed by epitaxial thickening. This technology can achieve large grains with a relatively low annealing temperature, meaning less energy and thus less cost (around 400 ºC) [3-5]. However, the growth process leads to a large grain size variance [1-5]. This translates to variance in open circuit voltage (V_{oc}) of each individual grain with the smaller grains having lower V_{oc} [7]. The existence of these small grains can essentially hinder the solar cell performance. In addition, this method also introduces a significant number of nonradiative recombination centers in the form of intra-grain defects which can decrease the diffusion length substantially [1,5].

In this contribution, we investigate the effect of grain size inhomogeneity on the total cell efficiency by means of an equivalent circuit simulation. Solar cells with an exponential distribution of the grain diameter were used to approximate size distribution in AIC cells in which there are more smaller grains than larger grains. In Section 2 of this paper, we discuss the details of the equivalent circuit simulation, the single grain model, the figure of merit chosen, and the choice of the statistical distribution. In Section 3 we discuss the results from examining the contribution to the total power of each grain as a function of its size. Conclusions are presented in section 4.

2. Equivalent circuit simulation

In our system, we consider columnar grains with the same height equal to the cell thickness but different diameters. The simulated structure is depicted in Fig.1a. The current inside the grains is vertical; the lateral current, that collects the contribution of all grains only flows through the ITO and back contact layer. The effective medium approach formulated by Brendel and Rau was used to model charge carrier propagation in a system with grain boundaries [8]. In their approximation, the effect of grain boundaries can be lumped into a change in effective diffusion length which is described by

$$L_{eff,poly} = \frac{L_{mono}}{\sqrt{1+\dfrac{2S_{GB}L_{mono}^2}{D_n\, g}}} \tag{1}$$

Where S_{GB} is the grain boundary recombination velocity, D_n is the diffusion constant, g is the grain diameter, and $L_{eff,poly}$ is an effective diffusion length that should be used in the Shockley equation to calculate the I-V characteristics in the polycrystalline case. In this contribution, we take D_n = 20 cm^2/s, and S_{GB} = 10^4 cm/s, which is the typical value for polycrystalline silicon cells, and we will vary g and L_{mono}.

The L_{mono} in equation (1) is basically the effective diffusion length in the monocrystalline case where there are no grain boundaries. $L_{eff,poly}$ changes from 0 to L_{mono} as grain size changes from 0 to infinity. For silicon, provided there are no other defects in the cell, L_{mono} is around 100 µm. In previous work, Van Gestel et.al. [1] calculated a value L_{mono} = 1.5 µm in their polycrystalline cells, signifying a large amount of very efficient additional recombination centers in the cell.

Each grain is modeled as a current source and two diodes as depicted in Fig. 1b to account for recombination in the bulk and in the space charge region. The total current coming out of each grain will be modeled with

$$I = I_{01}\left[\exp\left(\frac{V}{n_1 kT}\right) - 1\right] + I_{02}\left[\exp\left(\frac{V}{n_2 kT}\right) - 1\right] - I_{sc} \qquad (2)$$

Where I is the total current coming out of a grain to the ITO layer, $I_{01}$and I_{02} are the saturation currents, n_1 and n_2 the ideality factors of the two diodes, used to model recombination in bulk and space charge regions respectively; V is the voltage, k is the Boltzmann constant, T is the temperature and I_{sc} is the short circuit current. The effective diffusion length $L_{eff,poly}$ affects the saturation currents by the relations mentioned in [9].

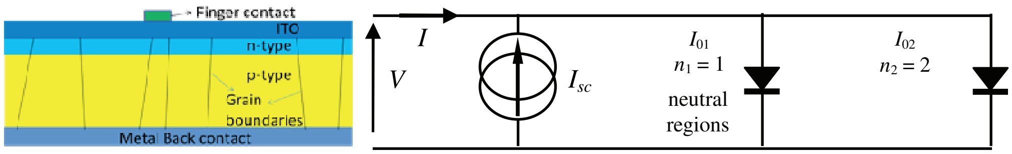

Fig. 1. (a) The modeled structure. (b) The equivalent circuit for each grain

Data on the grain structure, with distributions of the grain diameter, are commonly given in papers regarding Electron Back Scattering Diffraction (EBSD) measurements of polycrystalline cells [3]. We will model these experimental distributions by an exponential distribution, in which there are far more small grains than large grains. We will cut the exponential distribution at diameter value of 0.5 μm and 45 μm to mimic the situation typically found in cells made with low annealing temperature AIC. We assume that the grains are columnar, and connected in a 2-D parallel circuit. The outline of our model is: starting from a grain size distribution (Fig. 2a); continued by random placement of the grains in a 2-D structure with an own developed algorithm (Fig. 2b) followed by the determination of the electrical connection between the grains (Fig. 2c); attribution of solar cell properties to the individual grains by standard analytical models (Eqs. (2) and (1); ref. [9]); and solving of the 2-D network with a standard network solver (SPICE). Series resistances are placed at the grains' interconnections to account for the sheet resistance in the ITO layer.

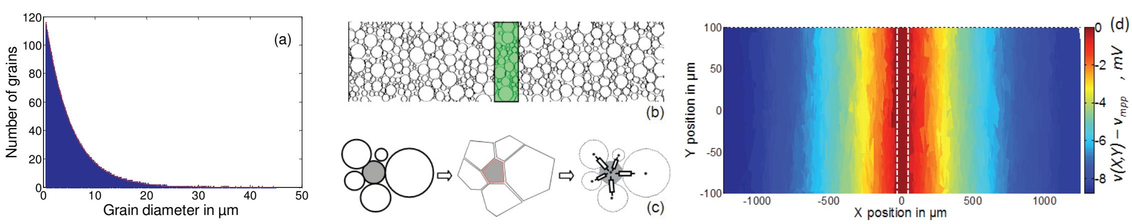

Fig. 2.(a) Example exponential grain diameter distribution, with average grain size g_{av} = 5 μm. (b) Placement of the grains in a 2500 μm × 200 μm unit cell; the green block in the cell picture is the top contact. (c) Electrical connections between grains in an 2D equivalent network. (d) Map of the local voltage $v(x,y)$ in the ITO layer of a polycrystalline cell, biased at maximum power voltage. The cell area is 2500 μm × 200 μm and the dashed lines indicate the position of the transparent finger contact.

We investigate here the power delivered by each grain to the ITO layer in order to find out to which extent the contribution of each grain is exploited in the total power generation, as it can be suspected that the smallest grains might consume some of the power generated by the larger grains, depending on the voltage bias. Therefore, we define a figure of merit that we call 'contribution strength' Cs as:

$$Cs(g) = \frac{\sum_{n=1}^{N(g)} P_n(g)}{P_{\max}} \qquad (3)$$

Here, P_n is the power delivered to the ITO layer by a specific grain n with diameter g, and $P_{\max}$ is the power that would be generated if the area made of N grains with diameter g were occupied by the largest grains available in the distribution. The summation goes through all the grains of that specific diameter g. Cs is a measure of the power generation efficiency of the area in the thin film cell, that is occupied by grains of diameter g as compared to the case if that same area is occupied with the largest grains in the cell. The Cs also gives us an idea of the local operation conditions of the grains, i.e. how the local voltage $v(x,y)$ is situated against the open circuit voltage v_{oc} and maximum power voltage v_{mpp} of a grain of size g.

We consider a thin film solar cell with finger contacts at 2.5 mm periodicity. The short circuit current used is 18 mA/cm^2 which is common in silicon thin film cells of 3 µm thickness. Here we consider the sheet resistivity of the ITO layer to be 70 Ω/sq common for current thin solar cells, the base doping density is taken to be 10^{16} cm^{-3}, and the emitter doping density is 10^{19} cm^{-3}. The contacts are considered to be perfect conductors. The width of the finger contacts simulated is 50 µm. In the model, the top contact is assumed to be transparent; we believe that this model simplification does not impact on the results significantly. To obtain a statistically meaningful description of the inhomogeneity effect, we need to consider how the current is flowing between grains, the metal contact placements and the size distribution itself. To understand how the current propagates, we show a voltage map of the ITO layer, in Fig. 2(d), taken from simulation of a cell with 2500 × 200 µm^2 area with a front finger contact in the middle, and biased at maximum power voltage (of the whole cell). From the voltage map in Fig. 2(d), we see that the voltage is only significantly varying in the horizontal direction, even though the nature of the grain connection is quite erratic. This horizontal voltage variation indicates that the current is mainly travelling horizontally therefore increasing the width of the cell(in the Y direction) mainly serves to increase the statistical sampling only. The Y width is kept at 200 µm for all our simulations discussed below. For the contacting method we are dealing with, it is sufficient to simulate a unit cell of one finger period width, without any additional boundary conditions due to symmetry arguments. The voltage drop over the unit cell is only a few mV, which is to be expected with such fairly low sheet resistance.

3. Results and Discussion

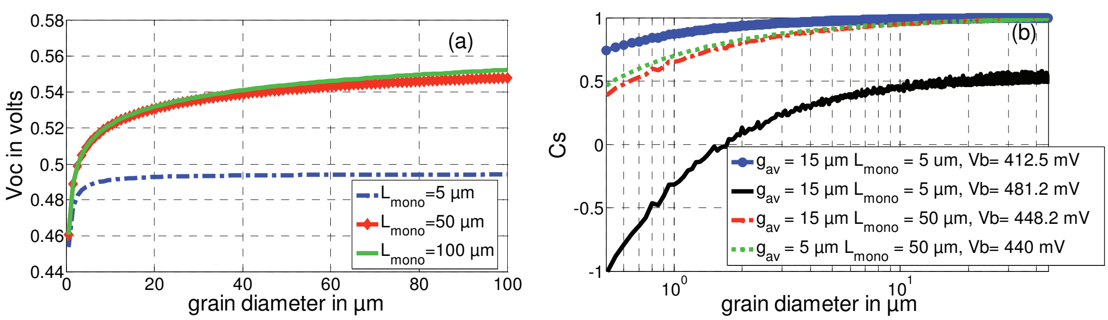

Fig. 3(a) Plot of open circuit voltage as a function of grain diameter for a single grain with different L_{mono}. There is only a small difference beyond L_{mono} of 50 µm for our case. (b) Plot of the contribution strength Cs for cells with exponential diameter distribution as a function of grain size g. For g_{av} =15 µm , V_{oc} = 498.3 mV when L_{mono} = 5 µm and V_{oc} =531.6 mV when L_{mono} =50 µm. For g_{av} =5 µm and L_{mono} = 50 µm, V_{oc} = 521.9 mV

The effect of grain size (the diameter g) on the performance of the solar cells is shown in Fig. 3(a), where we plot the open circuit voltage as a function of grain size for three different L_{mono} values. For a small L_{mono} value of 5 µm, there is hardly any improvement in V_{oc} for $g > 10$ µm. It is apparent that inhomogeneity effect will only be felt when L_{mono} is high which is when electrically active intra-grain defects are avoided. This is confirmed in Fig. 3(b) where we show Cs of a cell with exponential grain size distribution with average diameter g_{av} of 15 µm (shown in Fig. 4(a)) and also of 5 µm. The former distribution approximates the inhomogeneity in the size distribution found in AIC cells with lower annealing temperature [4]. The blue solid-circle curve in Fig. 3(b) shows Cs of a cell with $L_{mono} = 5$ µm at maximum power voltage V_{mpp}. We see that Cs depends rather weakly on grain size g. This indicates that the local voltage $v(x,y)$ felt by grains of different sizes is close to their individual maximum power voltage v_{mpp}. The black solid curve in Fig. 3(b) shows Cs calculated at a bias voltage V higher than V_{mpp}, but lower than V_{oc}. The smaller grains, having a negative Cs, are biased above their local open circuit voltage v_{oc}, and hence consume instead of generate power. Because of this, the open circuit voltage V_{oc} of the total cell will be lower than the v_{oc} of the largest grains in the cell. The red dash-dot curve in Fig 3(b) shows Cs at V_{mpp} of an identical cell but with L_{mono}= 50 µm. We see that Cs varies more significantly and only approaches $Cs = 1$ for larger grains. This indicates that the total cell is optimum when the bigger grains are optimum.

The reason why the larger grains have more importance can be seen by examining the area occupation of these grains. Fig. 4(b) shows the area occupied by grains of different size species from the distribution in Fig. 4(a). From Fig. 4(b), it seen that the cell area is dominantly occupied by grains larger than 20 µm, and thus the cell performance is mainly dictated by these larger grains. Therefore, the small grains are not very harmful. From this, it is seen that the statistics of grain occupation area is thus more relevant than the statistics of grain size population to predict the characteristics of a cell.

To see how effective the small grains are in inhibiting the performance of the total cell, we show the cumulative area occupation in Fig. 4(c). From the red dash-dot curve in Fig. 3(b), it is found that when L_{mono}= 50 µm and g_{av} = 15 µm, grains with $g < 10$ µm contribute less than 95% of the optimum. However, these suboptimal grains only occupy 6% of the total area (red square cumulative curve figure Fig. 4 (c)). The green dot curve in Fig. 3(b) shows Cs for a cell with exponential size distribution with $\underline{g_{av}}$ = 5 µm instead of 15 µm (Fig. 2(a)), but still with L_{mono}= 50 µm. It is apparent that there is a close similarity between the green dot Cs curve with the red dash-dot curve in trend and value. The maximum power voltage V_{mpp} is slightly lower for the $\underline{g_{av}}$ = 5 µm distribution (440 mV compared to 448.2 mV), illustrating a slightly larger influence of the smaller grains. This is apparent in Fig. 3(b) from the fact that the Cs of "$\underline{g_{av}}$ = 5 µm distribution" is slightly higher than that of "$\underline{g_{av}}$ = 15 µm distribution" for smaller grains. Combining the green dot Cs curve in Fig. 3(b) and the blue circle cumulative area curve in Fig. 4(c), it is found that 30% of the total area is contributing below 95% capability but only 4% of the total area is contributing below 90%. Note that this extreme size distribution is quite far from the ones obtained from AIC but even then, the small grains are not truly harmful.

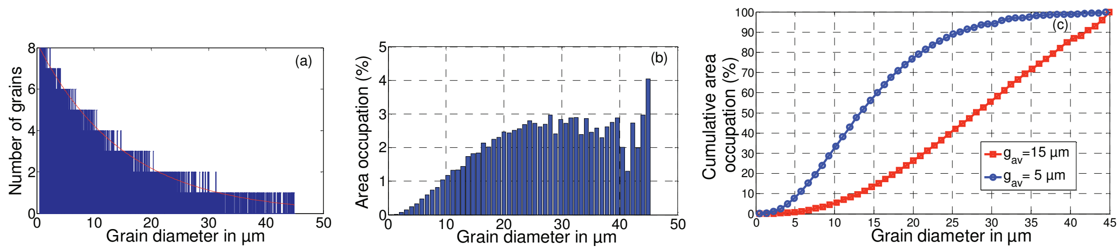

Fig. 4. (a) Plot of the exponential grain diameter distribution with cut off at 0.5 µm and 45 with $\underline{g_{av}}$ = 15 µm. (b) the area occupation percentage of different grain size species in (a). (c) The cumulative area occupation of the 2 different statistical distribution used.

4. Conclusions

Polycrystalline silicon solar cells with exponential grain diameter distribution have been investigated. The effect of grain size inhomogeneity will only be apparent when the cell is not hindered by intra-grain defects, that is with a fairly large intra-grain diffusion length L_{mono} of a few tens of a µm. In this case, our simulation results suggest that AIC poly-Si cells annealed at low temperature can still show a good efficiency despite the large grain size variation and the relatively many small grains present. This is because there is only a rather small variation in the solar cell characteristics of the individual grains (maximum power voltage and open circuit voltage), and also because the small grains still only cover a small fraction of the total area. Thus, grain size inhomogeneity in thin film polycrystalline silicon solar cells made by AIC is not the main limiting factor of their performance. The small grains can harm the cell performance severely only when their area occupation becomes comparable with the large grains.

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