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Cast silicon of varying purity for high efficiency PERC solar cells

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Abstract

In this work we investigate the effect of the bulk metal contamination level in cast silicon on the electrical performance of PERC (passivated emitter and rear cell) solar cells [1]. The bulk contamination is varied in two different ways. In the first approach, cast silicon crystallized with high purity silicon feedstock and reduced metal contamination from crucible and coating is used. Second, an extended gettering step is introduced in the PERC process flow. The interstitial iron concentration is taken as a measure of the bulk metal contamination of the investigated cells. Both the higher purity cast silicon and the gettering step significantly lower the interstitial iron concentration in the resulting PERC cells. This clear positive effect is also mirrored in solar cell parameters such as the open circuit voltage $U_{OC}$. In this experiment, the impact of gettering is larger than the effect which is reached by reducing the bulk metal concentration during the crystallization process. Device simulations show that most of the difference in $U_{OC}$ can be explained by the different interstitial iron levels while other recombination active defects might also be present.

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1. Motivation

The passivated emitter and rear solar cell (PERC, [1]) is one of the most promising new solar cell concepts which is currently transferred from lab scale into production. In this cell design the solar cell efficiency is less limited by surface recombination but rather by the bulk excess carrier lifetime. Thus the quality of the used silicon material plays a crucial role.

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One important parameter limiting the quality of cast silicon is the contamination of the material by transition metal impurities which are contained in silicon feedstock, industrial crucibles and silicon nitride coating materials. Within the long list of contaminants, iron is one of the most detrimental for the bulk excess carrier lifetime in p-type silicon. It is also often chosen as a representative for transition metal impurities because the interstitial iron concentration in silicon wafers and cells can be easily determined by lifetime measurements before and after iron-boron pair dissociation [2]. In this paper, we also focus on iron as a major representative of all impurities.

Both crucible and coating can contain iron in concentrations well above $1 \times 10^{17}$ at/cm$^3$ [3]. This can lead to total iron concentrations of more than $1 \times 10^{15}$ at/cm$^3$ in the edge regions of cast silicon by solid state diffusion during ingot cooling. Part of the iron can also be dissolved in the silicon melt and then lead to a contamination of the ingot center. Detailed simulations and measurements of this process can for example be found in the works of Schubert et al. [3].

The contamination of the cast silicon can thus be reduced by using purer resources: high purity crucibles and coatings [4] and high purity silicon feedstock [5].

The remaining metal contamination in cast silicon can be further reduced during the solar cell process. During emitter diffusion in p-type silicon, part of the metal contaminants get trapped in the highly phosphorous doped emitter layer. This process can be enhanced by introducing a high temperature step after diffusion [6,7] thereby further reducing the bulk contamination and increasing the excess carrier lifetime of the material.

In this work, we investigate the influence of both of these routes for bulk iron reduction on the PERC solar cell performance.

2. Experimental setup

Table 1 displays the different PERC solar cell groups investigated in this experiment. Cast silicon material with three different bulk contamination levels is used. The lower contamination levels are obtained by using high purity silicon feedstock and by reduced diffusion of metal contaminants from crucible and coating into the silicon ingot. As a measure of the bulk contamination, the total iron concentration $c_{Fe}$ is measured by glow discharge mass spectroscopy (GDMS). The three groups show a significant difference, $c_{Fe}$ is more than one order of magnitude smaller in group 3 as compared to group 1, where the iron contamination is in the range of $(1…4) \times 10^{14}$ at/cm$^3$. The used material was chosen from similar ingot positions and is thus comparable regarding other material parameters: the dislocation density is in the range of $(0.9…1.2) \times 10^4$ cm$^-2$, the carbon content is $(1…2) \times 10^{17}$ at/cm$^3$ and the oxygen content is $(2…3) \times 10^{17}$ at/cm$^3$.

Of each material, one batch is processed with the reference PERC process (all a-groups) [8], while a second batch is treated with an extended gettering step (all b-groups) by adding a high temperature step after diffusion. The cells (50-70 cells per group) are then measured on an IV tester. As a measure of the remaining bulk metal contamination after the cell process, the interstitial iron concentration $c_{Fei}$ is determined on 5-10 cells per group. This is done by measuring lifetime topograms at a constant injection rate before and after iron boron pair dissociation. The necessary illumination time for complete FeB dissociation is determined by illuminating the cells with a higher iron contamination level until the lifetime stays at a stable level. The median interstitial iron concentration of the cells is then obtained from the two lifetime maps according to the formulae given in [2]. The detection limit of this method is about $1 \times 10^{10}$ at/cm$^3$. Thus, we can only give an upper limit for groups with low iron contamination.

<table>
<thead>
<tr>
<th>group</th>
<th>initial bulk contamination level</th>
<th>bulk iron concentration $c_{Fe}$ relative to group 1</th>
<th>extended gettering step</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>high</td>
<td>1</td>
<td>no</td>
</tr>
<tr>
<td>1b</td>
<td>high</td>
<td>1</td>
<td>yes</td>
</tr>
<tr>
<td>2a</td>
<td>medium</td>
<td>0.6</td>
<td>no</td>
</tr>
<tr>
<td>2b</td>
<td>medium</td>
<td>0.6</td>
<td>yes</td>
</tr>
<tr>
<td>3a</td>
<td>low</td>
<td>0.09</td>
<td>no</td>
</tr>
<tr>
<td>3b</td>
<td>low</td>
<td>0.09</td>
<td>yes</td>
</tr>
</tbody>
</table>
3. Results and discussion

Figure 1 shows the interstitial iron concentration $c_{\text{Fe i}}$ of PERC cells produced from cast silicon material with three different bulk contamination levels. The blue boxes represent the standard PERC processed groups, the orange boxes are the groups which obtained an additional gettering step. It is clearly visible that the initial iron concentration of the cast silicon material determines the interstitial iron level in the PERC cell. Group 1 with the highest metal contamination level also has the largest interstitial iron concentration $c_{\text{Fe i}}$ after the cell process. Thus, after the reference process there is still a remarkable amount of iron left in the cell. When an optimized gettering procedure is used, $c_{\text{Fe i}}$ decreases significantly, it is then similar in all groups (orange boxes). However, group 3 with the cleanest bulk material already features a low $c_{\text{Fe i}}$ even without additional gettering step.

Since the open circuit voltage $U_{\text{OC}}$ of a solar cell depends strongly on the wafer quality, we choose this parameter to investigate the influence of the bulk iron contamination on the cell performance. Figure 2 shows $U_{\text{OC}}$ for PERC cells made from the different materials. As expected, in the groups which were processed with the reference cell process (blue boxes), the open circuit voltages increases with decreasing interstitial iron content. For the material used here, the spread is approximately 4 mV. Consequently, with the reference PERC cell process used here, the influence of the initial iron contamination is still visible on cell level.

When an extra gettering step is applied (orange boxes in Figure 2), all groups show an increased $U_{\text{OC}}$ compared to the reference process leading to similar values of 653 mV to 655 mV in all groups. The optimized gettering thus seems to be able to reduce metal contaminations equally well for the three material groups used here. However, due to the rather large spread of the obtained results it is hard to say whether group 3b still benefits from the lowest initial contamination level after the optimized gettering as it is suggested from the interstitial iron measurements in Figure 1. Further experiments need to be carried out in order to answer this question.

The increase in $U_{\text{OC}}$ obtained by extended gettering is larger (4-7 mV) than what is obtained by cleaner bulk material (4 mV). Obviously, the extended gettering should also act on other metal contaminations in the cell besides iron. So the extra gettering should also lower the concentration of other lifetime limiting defects. This leads to the expected higher open circuit voltages in the b-groups.
In order to evaluate our experimental data, we calculate open circuit voltages for the PERC cell design used here based on 2D Sentaurus Device simulations [9]. The state-of-the-art physical models described by P. Altermatt [10] are applied. We assume that the Shockley-Read-Hall bulk lifetime of the cast silicon material is limited to $\tau_0 = 500 \mu$s. This is a median value which we typically find in gettered lifetime samples of cast silicon with a low bulk contamination. Additionally, the effect of the FeB defect is simulated with the parameters according to Macdonald et al. [11]. We assume that in our measurements of $c_{Fei}$ all FeB pairs are dissociated and thus $c_{Fei}$ also gives the number of FeB pairs in the associated “dark state” which is simulated here.

Figure 3 shows the simulated dependence of $U_{OC}$ on the FeB pair concentration in the cell. For a FeB concentration above $10^{10}$ at/cm³, a decrease of $U_{OC}$ can be expected in our PERC cell design.

In Figure 2, the bars show the predicted $U_{OC}$ range for each group according to the respective measured interstitial iron content. It can be seen that the measured values of $U_{OC}$ correspond well to the values predicted from the interstitial iron level $c_{Fei}$. However, the model predicts a higher $U_{OC}$ for the cells in group 3a with very low iron contamination. A possible explanation is that our model does not accurately describe the effect of other defects which might become lifetime limiting when the iron contamination is negligible. In that case, the curve in Figure 2 would saturate at lower voltages for lower FeB pair concentrations.

For all groups with an extended gettering step, we performed the simulation with the measured range of $c_{Fei} = 1...5\cdot10^{10}$ at/cm³. The predicted value of $U_{OC}$ is then close to what is experimentally obtained for these cells. Hence, the optimized gettering seems to eliminate further lifetime limiting defects which might still be present in group 3a.
Fig. 3. Simulated dependence of the open circuit voltage $U_{\text{OC}}$ on the FeB pair concentration in the PERC cell bulk. For a concentration above $1 \times 10^{10}$ at/cm$^3$, a decay in cell performance can be expected.

4. Summary

In this work we investigate the effect of the bulk metal contamination level (with the focus on iron) in cast silicon on the electrical performance of PERC solar cells. Our results demonstrate that initial iron concentrations in cast silicon ranging from below $10^{13}$ at/cm$^3$ to more than $10^{14}$ at/cm$^3$ are mirrored in the open circuit voltage of the processed cell. The negative effect of an increased bulk metal contamination can be reduced by introducing an adapted cell process with extended gettering. 

Device simulations confirm that the differences in the open circuit voltage for the groups of low and medium material purity can be explained to a large extent by the FeB defect. Only when the iron concentration reaches very low values, other defects become dominant. The impact of these defects can be reduced by an optimized gettering procedure.

Our findings indicate that different strategies can be applied in order to obtain high quality cast silicon for high efficiency PERC solar cells. As a first option, the metal contamination can be reduced during crystallization by using high purity silicon feedstock and reducing the contamination of the cast silicon from crucible and coating. Alternatively or additionally, an extended gettering step can be used to further optimize the cell performance. In solar cell production it has to be evaluated which option is easier to implement. Extended gettering can lead to prolonged solar cell processing times and increased step costs. On the other hand, providing resources of high purity may lead to higher production costs of cast silicon. Either way, high quality silicon with high bulk excess carrier lifetime is absolutely necessary in order to fully exploit the PERC cell potential.

Acknowledgements

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[9] Sentaurus Synopsys, Mountain View, CA.