



Development of Novel Hydrogen Trapping Techniques for Breakthrough Si Casting and Wafering Technologies

Project results and lessons learnt

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Executive Summary

With silicon still a dominant cost of making solar cells, the focus of this project is to develop new techniques to heal defects that form in cheaper silicon wafers. New cheaper wafer sources such as cast quasi-mono (QM) and kerfless small-grain wafers offer the potential for significantly reduced solar cell cost, but generally have lower performance due to these defects that form during the silicon growth. Previously, testing typical advanced hydrogenation processes on such wafers was shown to be ineffective at healing these grown-in defects, likely due to the rapid dispersion of hydrogen throughout all the silicon. This project focuses on newly patented methods of controlling the hydrogen that utilise the defects to absorb more hydrogen into the silicon and trap it in the defected regions where it is needed the most. The project aims to improve the understanding of defects in these cheaper materials in order to optimise, develop and commercialise the new patented hydrogen trapping processes.

We have developed hydrogen trapping techniques that can enhance the quality of quasi-mono Si by over 70% compared to conventional hydrogenation processes. Somewhat surprisingly, we found that a hydrogen trapping processes alone provide better passivation (healing) of grown-in defects than combinations of hydrogen trapping and advanced hydrogenation processes. We found that some localised types of grown-in defects (certain dislocations in QM Si) do not respond well to the trapping processes applied, or any other process applied to date. Further investigation into these particular defects is required and they will ultimately need to be treated differently, or prevented from forming through optimised silicon growth techniques. These defects aside, the vast majority of grown-in defects respond very well to the hydrogen trapping techniques developed in this work.

The introduction of hydrogen into silicon is not always beneficial for silicon wafer quality. We recently found that having excess hydrogen in silicon can actually be a problem, as it can be released from less stable bonds under heat and light (the sun!) and interact with other species in the silicon to cause a degradation in wafer quality. It is therefore very important to also test and understand the stability of the wafers in this work as well as the stability after any processes that may control and move the hydrogen. We have shown that both quasi-mono and kerfless small-grain wafers are susceptible to degradation when hydrogen is introduced. This was expected as such degradation has been shown to form in all silicon wafer types on the market. We show that this can be minimised in both wafer types through processes to control the hydrogen. However, conditions to control the hydrogen for optimised trapping and improved wafer performance appear to be quite different from the conditions used for controlling the hydrogen to prevent degradation. As a result, although we demonstrate that trapping techniques greatly improve the quality of the lower cost silicon wafers, without also controlling any excess hydrogen, we find that the wafers suffer from subsequent degradation under light and heat. Further optimisation, and possibly a multi-step approach, is the ongoing focus of this work to ensure that effective hydrogen trapping can be achieved while also preventing any ensuing degradation to achieve maximum performance that is stable.

Finally, the transfer of hydrogen trapping processes from a wafer level to finished cell level has not been without complications. It seems that an optimised process time is required to prevent degradation of the solar cell's metal contacts (caused by hydrogen atoms accumulating at the metal- silicon interface). With further optimisation and development, the processes for controlling the hydrogen for trapping in defects and to prevent degradation and metal contact issues are likely to be well-suited to commercial implementation so that these cheaper wafers can be used in manufacturing without sacrificing electrical performance. Trapping processes applied to a full-size commercial quasi-mono solar cell in this work were able to achieve over 21% efficiency, in-line with commercial cells produced on more expensive wafers. The continued success of this project will enable the use of cheaper wafers sources in the high efficiency cell structures of the future through increased understanding of defects formed in cheaper wafer sources and development of commercial hydrogen trapping processes.

Project Overview

Project summary

The aim of the project is to develop new techniques for controlling hydrogen to maximise and trap it within defects in silicon wafers for enhanced passivation (healing), to enable cheaper wafers to be used as a direct replacement for more expensive silicon wafers in solar cells, while maintaining or even improving solar cell efficiencies.

In particular, the work has so far focused on three important components required for optimization and development of these techniques. The first is the investigation into the potential of the trapping techniques, which counterintuitively use hydrogen charge state control techniques in direct contrast and almost opposite to those typically used for hydrogenation. By maintaining the hydrogen in the majority charge state we have been able to target the silicon crystal defects with the hydrogen, drastically improving the electrical quality, specifically of the defected regions. The second component is studying and understanding the defects within the cheaper forms of silicon, particularly the localised regions that do not respond well to the trapping techniques tested so far. This is crucial for being able to develop optimised universal trapping processes that will work across all defect forms and all types of defected silicon. The third, and equally as important component, is testing and reducing the degradation of the silicon that occurs under the sun when excess hydrogen is in the silicon to ensure that cells are stable and reliable.

Evidence for project success to date can be seen in the fantastic progress in developing trapping techniques, which have led to over 70 % enhancement in quality of quasi-mono Si and a commercial cell with over 21 % efficiency with light-induced degradation of less than 1 %. All milestones for this stage of the project have been achieved as hoped, while we have also recognised the challenges still to be overcome throughout the rest of the project. Ongoing work will focus on understanding the localised defects that do not so far respond to trapping treatments, developing processes to optimise trapping while also minimising degradation, and development of commercial processes and prototypes for rapid deployment to manufacturers to enable immediate replacement of expensive wafer types with these new cheaper wafers.

Project scope

The aim in undertaking this project is to bring down the cost of solar power by enabling the use of cheaper silicon wafers without sacrificing solar cell efficiencies. Typically to achieve high efficiencies or to move to higher efficiency cell structures, it is thought that high quality silicon wafers are required, these are expensive and use massive amounts of time and energy to produce. Cheaper forms of silicon that are grown more quickly are prone to electrical defects that limit the performance. Advanced hydrogenation is a cheap and effective way of passivating many defects in silicon solar cells, however the electrical defects such as dislocations formed in cheaper wafers such as cast quasi-mono and kerfless wafers have not responded well to these previously developed processes. These established processes were designed to maximise the hydrogen movement all throughout the silicon, which means that the hydrogen easily escapes many of defects where it is needed for passivation. This project seeks to overcome this by developing new

techniques of controlling and trapping hydrogen within defected regions to specifically target and passivate harmful defects in cheaper wafer sources to enable their use in current and future high efficiency solar cell technologies with reduced cost.

The success already achieved in this regard, as well as the new insights and understanding gained have been a particularly important outcome for enabling the use of cheaper wafer sources given the dominance that the silicon wafers have in determining the cost of typical silicon solar cells. In addition, the successful reduction of degradation has demonstrated that cells produced on these wafers can be made to be stable and reliable.

The ongoing scope of this project will further develop valuable knowledge on the various types of defects and how they uniquely respond to different hydrogen control processes to enable the use of any type of cheap silicon no matter the defects within. The ultimate outcome will be a commercial process implemented in a prototype tool that effectively heals defected regions in various forms of cheap silicon and simultaneously prevents degradation so that current more expensive wafers can be directly replaced with cheaper wafers without sacrificing performance.

Outcomes

Important outcomes that satisfied aims of this project have been:

1. development of a new hydrogen trapping (HT) technology
2. significantly improved electrical quality of cheap wafer types
3. improved performance stability through elimination of light-induced defects (LID)
4. solar cell process optimisation for improved lifetime (wafer electrical quality) & stability in finished commercial cells achieving cell performance in-line with those produced on more expensive wafers, and with even greater stability
5. advancement of the Technology Readiness Level (TRL) from 3 towards TRL 4, and on-track to 5 by the end of the project with development of a commercial prototype tool.

For this stage of the project, things are progressing very well with all stage-1 planned milestones achieved. Many lessons have been learnt and specific strategies have been developed for moving forward to ensure generation of valuable knowledge regarding defects and hydrogen control, and for the ongoing success of the project and technology commercialisation.

There have been a few surprising results, which are discussed in more detail in the lessons learnt reports. Notably, it was expected that advanced hydrogenation techniques would be required to be used in conjunction with the new hydrogen trapping techniques. However, when optimised, trapping processes alone appear to be the most effective at passivating the vast majority of defects formed in quasi-mono wafers. Though it should be noted that some localised defects do not respond well to the trapping processes tested to date. Further analysis will be required to understand and eliminate the electrical impact of these defects. Additionally, although the degradation has been shown to be able to be reduced or eliminated, the processes used are different to those required for hydrogen trapping. Further optimisation, and possibly a multi-step approach will be required to ensure that effective hydrogen trapping can be achieved while also preventing any subsequent degradation in order to accomplish maximum performance that is also stable. Finally, the transfer of trapping processes from a wafer level to finished cell level has not been without complications. It

seems that an optimised process time is required to prevent degradation of the metal contacts occurring. As the hydrogen is moved throughout the silicon it can accumulate underneath the metal contacts, creating a high contact resistance which reduces the amount of electricity able to be extracted from the solar cell. Alternatively, a subsequent process to repair the contact resistance issues could be implemented or the trapping process applied prior to full cell formation, at a stage when the contacts have not been added and will therefore not be affected.

Transferability

Multiple conference and journal publications, a media article and public patent PCT related to this project have been published, as well as multiple presentations and plenaries at leading global conferences by the research team. We hold regular workshops to share confidential knowledge to the consortium of partners that are contracted to and currently licensing UNSW technologies. Frequent company visits to project partners are also carried out in order to further facilitate technology transfer and to ensure that the latest developments and optimised processes can be implemented as they are developed.

The hydrogen trapping technology developed in this project will be able to be applied to many (or all) forms of cheap silicon, not just those directly investigated within this work; and potentially even other semiconductor materials where the hydrogen can be similarly controlled due to similar energy configurations within the material. As a result, the knowledge gained will be very valuable and important to be shared widely. The design and development of a commercial prototype tool will be particularly important for incorporating the hydrogen trapping technology to enable rapid uptake of the technology and to make it available for use in any industry and by any company under license.

Conclusion and next steps

The new hydrogen trapping technology being developed in this project not only achieved all milestones and outcomes for this stage of the project, but more importantly demonstrated the potential for commercial solutions to passivate (or heal) defects grown in cheaper silicon wafers so that they may be used as direct replacements for more expensive wafers, even in high efficiency cells, bringing down the cost of solar cells without sacrificing performance.

By controlling the hydrogen in new ways that specifically target the defects and maximise the hydrogen where it is needed the most, we have been able to significantly enhance the electrical quality of the wafers by over 70%, over and above the benefits already provided by typical hydrogenation processes. We have also demonstrated that although the wafers are prone to degradation (as all silicon wafers are), we can effectively reduce this degradation for improved stability and reliability.

Many valuable lessons have already been learnt throughout the project to date, that will further direct the ongoing investigations and developments in this project, and which have been published and presented via various means, nationally and globally. While the vast majority of electrical defects formed during the growth of quasi-mono silicon (dislocations) respond very well to hydrogen trapping, some sporadic localised dislocated regions remain unaffected. Investigation into the properties of these defects will help provide insight into modified trapping processes which can then be used successfully on these defects, or to enable optimised growth techniques to prevent such defects from forming in the first place. It was also found that the hydrogen processes developed do

not themselves prevent or limit degradation, and that when applied to finished solar cells, contact resistance issues can arise if the conditions and time are not optimised accordingly. To solve both of these issues, the trapping processes will be further developed and may require a multi-step approach to passivate the defects prior to solving the degradation and/or contact resistance issues.

Trapping processes applied to a full-size commercial quasi-mono cell have already achieved over 21% stable efficiency, comparable to commercial cells produced on more expensive, less defected wafer types. With continued optimisation and development, the processes for controlling the hydrogen for trapping and to prevent degradation of wafer quality and the metal contacts are likely to be highly transferable to industry enabling these cheaper wafer types to be used in the manufacturing of high efficiency solar cells.

Lessons Learnt

Lessons Learnt Report: Hydrogen trapping can significantly improve the electrical performance of defected regions in quasi-mono silicon wafers and solar cells

Project Name: Development of novel hydrogen trapping techniques for breakthrough Si casting and wafering technologies

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Solar PV
State/Territory:	NSW

Key learning

Previously developed advanced hydrogenation techniques have been shown to be relatively ineffective at passivating defects that form when growing cheaper forms of silicon, likely due to the rapid dispersion of hydrogen throughout all of the silicon. New methods of controlling the hydrogen have been identified and patented, these methods utilise the defects to get more hydrogen into the silicon and trap it in the defected regions where it is needed the most. It was thought that a multi-step approach of hydrogen trapping followed by advanced hydrogenation would provide the best results, however, the trapping process alone surprisingly appears to provide the best results for passivating defects in cheaper silicon.

Implications for future projects

Much work is being done to optimise the trapping processes in this work in order to minimise harmful impacts of the defects grown into cheaper forms of silicon. This learning, that indicates trapping processes alone can provide the most benefit, points to a potentially simpler process required for passivating these defects that will likely be very well-suited to implementation into a future high-throughput commercial tool.

Knowledge gap

Where hydrogen is used to heal the defects in silicon, thorough testing and evaluation needs to be carried out to ensure that both the passivation is stable and that excess hydrogen does not remain loosely bound in the silicon in a way that can cause degradation. For the former, it will be useful from an academic perspective to better understand the nature of the defects and the ability of the hydrogen to passivate or fix such damage to ensure stable passivation. In both cases, it is important to test and ensure the wafers and cells are stable against all the operating conditions solar cells will

face when operating in the field. Both of these factors are already being considered with initial learnings discussed in the following lessons learnt reports.

Background

Objectives or project requirements

The aim of this part of the project was to investigate the potential of hydrogen trapping processes in contrast to or in addition to the previously developed advanced hydrogenation processes.

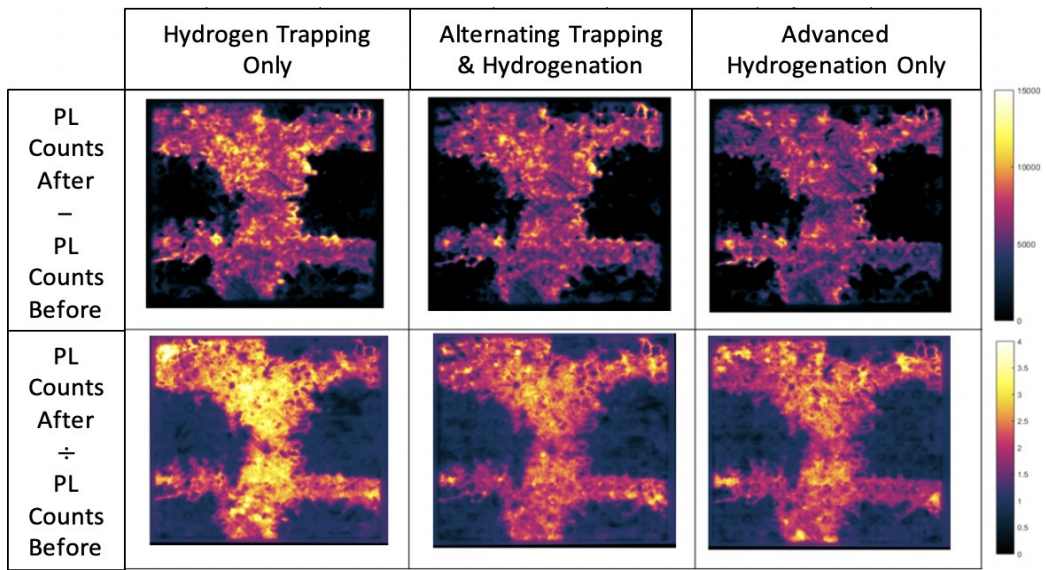
Process undertaken

Structured screening experiments were conducted to assess a wide parameter space for controlling the hydrogen in a variety of ways (including established advanced hydrogenation processes) in order to optimise trapping processes. Parameters tested consisted of a range of temperatures, illumination (wavelength) sources and illumination intensity conditions. We tested wafers from three different manufacturers of quasi-mono silicon and one set of small-grain kerfless wafers. Samples were characterised by multiple means, most notably by monitoring the average electrical carrier lifetimes (wafer electrical quality), and the use of photoluminescence (PL) images which provide spatially resolved localised information on wafer quality to assess the changes happening specifically in the defected regions.

Supporting information (optional)

Trapping processes were applied following typical commercial hydrogenation process using a belt furnace to distribute hydrogen throughout the bulk of the silicon. The conventional hydrogenation process resulted in a 40 % enhancement in electrical carrier lifetime (the electrical quality of a silicon wafer). The subsequent trapping processes designed to trap the hydrogen within the dislocations enabled a further >70 % lifetime enhancement on top of the already improved lifetime for a total improvement of ~140 %. The trapping processes have also been demonstrated to work on commercial cells, improving an already hydrogenated cell by 0.3% absolute to over 21% conversion efficiency.

The following figure shows example PL image subtractions and ratios demonstrating the difference in quality of very heavily defected silicon wafers before and after trapping and/or advanced hydrogenation. The images show that the trapping only process results in the largest improvements (the largest change in PL counts show up as brightest regions, and therefore largest quality improvements). Note here that the dark regions represent areas that did not change significantly in quality (as the images are ratios and subtractions of two separate PL images), and are actually the higher quality regions of the wafer.



Lessons Learnt Report: Some localised defects formed during the growth of quasi-mono silicon are unaffected by hydrogen trapping processes

Project Name: Development of novel hydrogen trapping techniques for breakthrough Si casting and wafering technologies

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Solar PV
State/Territory:	NSW

Key learning

The application of trapping processes designed to trap the hydrogen within the dislocations resulted in significant improvements to the vast majority of defected regions in quasi-mono silicon, enabling a >70% averaged lifetime enhancement (improvement in the wafer's electrical quality). However, some localised types of grown-in defects (certain dislocations in quasi mono) did not respond well to the trapping processes applied, or any other process applied to date, indicating that these particular defects have some different properties that need to be better understood.

Implications for future projects

Further investigation into these particular defects that do not respond to any existing processes is required to understand the properties that make them resistant to existing treatments. These defects will ultimately need to have new or additional processes developed to control the hydrogen in a way that can penetrate and passivate such defects. Alternatively, if a successful hydrogen control treatment is not identified, understanding these defects and how they form can help develop optimised growth techniques to prevent such defects from forming.

Knowledge gap

It is not yet clear what are the properties of these particularly localised defects that make them resistant to existing treatments as discussed in supporting information, ongoing investigation is underway.

Background

Objectives or project requirements

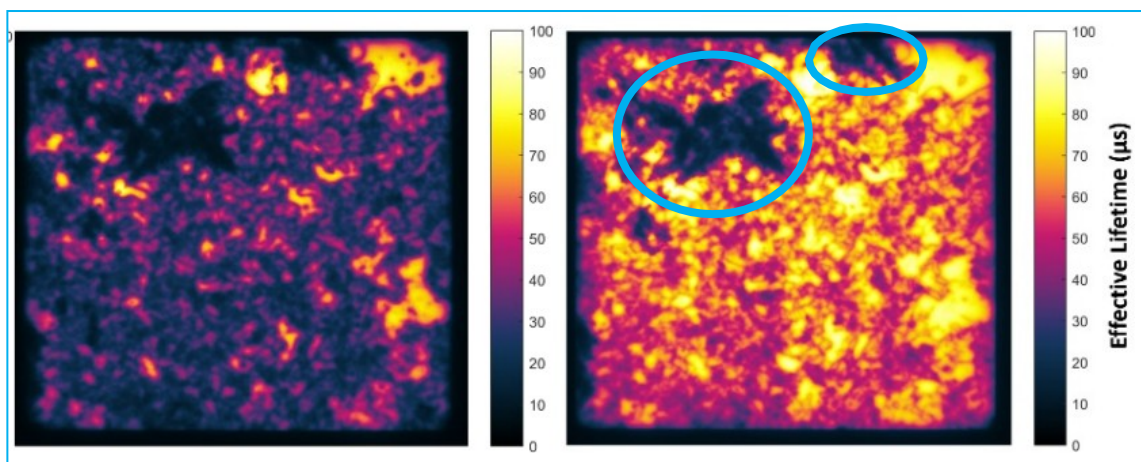
The aim of this part of the project was to develop hydrogen trapping processes to improve defected regions in cheap silicon wafers, and investigate varying behavioural responses and their respective defect properties.

Process undertaken

Hydrogen trapping processes were applied to quasi-mono silicon wafers and Photoluminescence (PL) images were taken of the wafers before and after processing. The PL images are essentially a map of wafer quality and therefore show spatially where the improvements occur on the wafer.

Supporting information (optional)

The PL images below shows the electrical quality of a quasi-mono wafer (brighter regions = higher quality) before (left) and after (right) a hydrogen trapping process. Significant improvement is obtained after hydrogen trapping over the vast majority of the wafer. Two regions (circled) are less responsive to the treatment. Work to characterise these defected regions and understand why they are not improved by hydrogen trapping is ongoing.



Lessons Learnt Report: The hydrogen trapping processes will need to control the hydrogen in a way that also prevents hydrogen-induced degradation

Project Name: Development of novel hydrogen trapping techniques for breakthrough Si casting and wafering technologies

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Solar PV
State/Territory:	NSW

Key learning

The processes developed for enhanced hydrogen trapping, are not effective for clearing out excess hydrogen that we now know can cause degradation. As a result, although we demonstrate that trapping techniques greatly improve the electrical quality (lifetime) and performance of the lower cost silicon wafers, without also controlling any excess hydrogen, we find that the wafers suffer from degradation under light and heat (hydrogen-induced degradation, commonly referred to as Light- and elevated Temperature-Induced Degradation or LeTID).

Implications for future projects

It is very important to test and understand the stability of the wafers as well as how this is impacted by any processes that control and move the hydrogen.

Knowledge gap

Further optimisation of the hydrogen trapping process is needed to determine if the defects can be passivated simultaneously with the clearing out of excess hydrogen, or potentially a two-step process will be required to ensure stable cells.

Background

Objectives or project requirements

This part of the project aims to investigate and solve degradation in silicon wafers to ensure stable and reliable solar cells.

Process undertaken

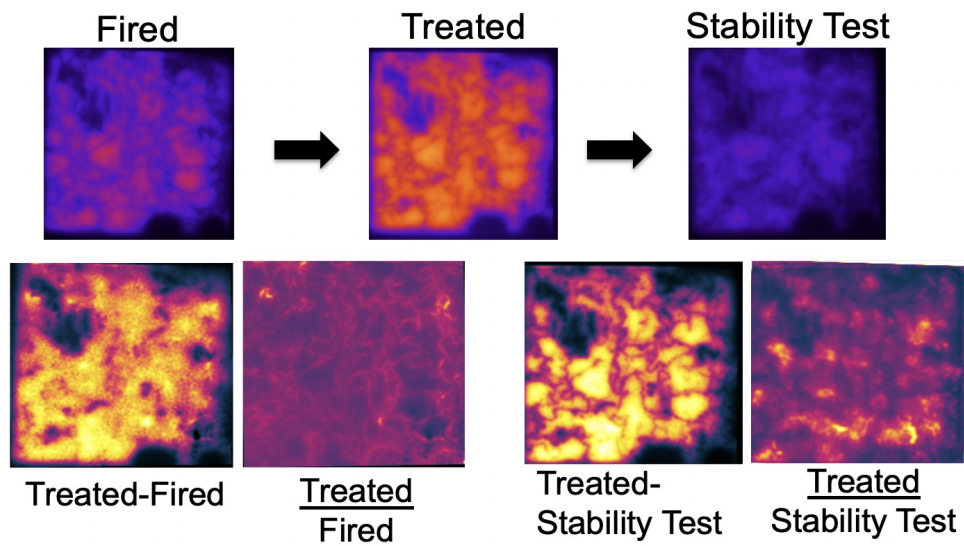
After application or modification of any process for controlling the hydrogen, samples are tested under typical stability testing conditions that simulate the light and heat that would be experienced under the sun.

Supporting information (optional)

In the figure below, the top three images show the PL images (localised silicon quality; brighter is better) after firing (a standard hydrogenation treatment), after a hydrogen trapping treatment ('treated') and after a stability test. The bottom images compare the local regions in the above PL images via subtraction (absolute changes) and division (relative changes).

The brighter colours in the PL images in the top row represent higher electrical quality, and it can be seen that the trapping treatment significantly increases the wafer quality. Without attempting to then clear out the excess hydrogen, after a stability test the samples degrade and actually end up poorer than they were prior to the trapping treatment.

Comparing the local regions in the images via subtraction (absolute changes) and division (relative changes) we can learn a lot more. The bottom row of the figure shows this analysis. In this case, the bright regions correspond to the largest changes in quality. The clear patterns of defects that appear brighter in the PL comparison of the treated sample divided by the fired sample, shows that the trapping treatments provides the largest relative improvements to the defects themselves. In contrast, the subtraction of the treated sample by the stability tested cell shows that the largest change and hence the degradation occurs in the silicon itself - between the defects. This is positive as it indicates the trapping process and passivation of defects are remaining stable. The stability can likely be solved by a second process separately developed to solve the degradation issue, and ideally with further development incorporated into the same process as the trapping.



The top three images show the PL images (localised silicon quality; brighter is better) after firing, after a hydrogen trapping treatment and after a stability test. The bottom images compare the local regions in the above PL images via subtraction (absolute changes) and division (relative changes).

Lessons Learnt Report: Hydrogen trapping processes can result in increased electrical resistance at the metal contacts when applied to solar cells

Project Name: Development of novel hydrogen trapping techniques for breakthrough Si casting and wafering technologies

Knowledge Category:	Technical
Knowledge Type:	Technology
Technology Type:	Solar PV
State/Territory:	NSW

Key learning

Processes developed on silicon wafers can have added complications when applied to finished solar cells produced on the same wafers. The hydrogen trapping processes developed in this project result in significant improvements to the silicon quality which appear as improved electrical carrier lifetime or implied open-circuit voltages on silicon wafers. When such processes are applied to cells, these lifetime improvements appear as improved open-circuit cell voltages, current collected, and also improved fill factor (FF; squareness of the current-voltage curve) as defects that otherwise cause junction recombination are passivated (healed). However, it has been found that the trapping processes when applied to cells can also harm the FF by causing high electrical resistance at the metal contacts (high contact resistance), likely by hydrogen accumulating at the interface between the metal and silicon, if the processes are not time optimised.

Implications for future projects

Processes may need to be optimised for different cell architectures, or wafer types, or an additional process introduced to heal any serious resistance issues introduced by hydrogen trapping processes applied to cells. Alternatively, if the trapping processes can be applied to the wafers prior to contact formation this issue can likely be alleviated. These options are currently being explored.

Knowledge gap

Further investigations are needed and are currently ongoing to better understand the mechanisms causing the contact resistance issues. In addition, the impact of different processes and treatment times on different wafers and cells are being investigated with the possibility of applying trapping processes prior to cell formation.

Background

Objectives or project requirements

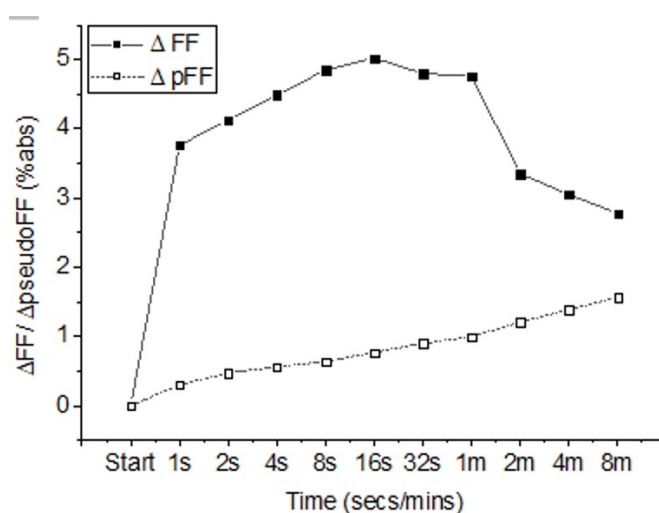
The aim of this part of the project is to apply the hydrogen trapping processes being developed to finished cells.

Process undertaken

Following the significant electrical carrier lifetime (wafer quality) enhancements on defected quasi-mono silicon wafers test structures, the same hydrogen trapping processes were applied to similarly defected quasi-mono solar cells. The performance of the cells was measured with increasing process application time,

Supporting information (optional)

The performance/efficiency of the quasi-mono cells were greatly enhanced by the hydrogen trapping processes; the open-circuit voltage and short-circuit current both improved significantly - not shown. The Fill Factor (FF) of a solar cell is a parameter related to the squareness of the current-voltage curve and it is directly proportional to efficiency (so the higher the better). It is affected by a number of factors including contact resistance and junction recombination. The pseudo-FF is the same as the FF but unaffected by contact resistance so a comparison can highlight contact resistance issues - as shown in the following figure. The pseudo-FF of the cells is greatly improved by the trapping processes as the hydrogen likely passivated/healed defects that were causing carrier recombination at the junction. However, the FF curve shows that after improving significantly due to the trapping processes, after an optimal time, it starts to drop significantly indicating contact resistance issues with increasing time.



Changes in quasi-mono cell Fill Factor (FF; affected by contact resistance) and pseudo-FF (unaffected by contact resistance) with increasing application time of hydrogen trapping processes shows that there is an optimal time of application before contact resistance problems can arise.

Lessons Learnt Report: China's new '531' policies can add increased complexity to legal/financial agreements, and require increased management and legal engagement

Project Name: *Development of novel hydrogen trapping techniques for breakthrough Si casting and wafering technologies*

Knowledge Category:	Financial
Knowledge Type:	Financial information
Technology Type:	Solar PV
State/Territory:	NSW

Key learning

The solar industry in China has faced major challenges since the Chinese government announced subsidy reductions for photovoltaic power generation on May 31 2018 (widely known as the '531' policy). This move led to the sudden contraction of China's PV market and had significant impact on the local solar industry. As a result, many companies are facing increased legal and financial restraints making contract and payment commitments extremely difficult. In addition, leadership changes at these companies can happen quite frequently, creating significant difficulty in negotiating contracts despite the enthusiasm of their research or technical team.

Implications for future projects

We are finding it increasingly important to have very engaged and ongoing discussions with all levels of management and legal teams for project success, in addition to the technical and research teams for technology development.

Knowledge gap

N/A

Background

Objectives or project requirements

All necessary partner agreements.

Process undertaken

The project team has made an increased number of trips to China to ensure engaged and ongoing discussions with all levels of management and the legal teams of each project partner.

Supporting information (optional)

N/A