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 Photoluminescence based defect imaging of a multicrystalline wafer (left to right: photoluminescence of an as-cut wafer, lifetime map, interstitial iron concentration).
Simulated (in the front) and measured (perspective view) interstitial iron concentration after solar cell processing.

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Silicon Photovoltaics – Characterization of Process Materials and Silicon Materials

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ANALYSIS AND SIMULATION OF IMPURITY DISTRIBUTIONS

In order to further increase the quality of their products, manufacturers of silicon wafers and cells are challenged to perform detailed analysis of the impurity distribution in their materials. Fraunhofer ISE provides customized Impurity Distribution Analysis services encompassing experimental results as well as detailed expert reports based on our unique methodology. Two analysis packages are available. Our Ingot Impurity Distribution Package is geared towards customers, wanting to investigate the impact of the crystallization process on the impurity distribution in specific ingot material. Our Solar Cell Impurity Distribution Package provides detailed information on the effects of the solar cell process - i. e. gettering and temperature treatments - on impurities and optimization potential. The analysis combines state-of-the-art measurements and simulations to assist manufacturers in optimizing their crystallization and cell processes with respect to material quality.

Ingot Impurity Distribution Analysis

This analysis package aims at identifying the dominant impurities in crystallized silicon, usually causing significant losses in solar cell efficiency. The most detrimental impurities in multicrystalline silicon are metals in meta-stable states e. g. interstitial iron (Fe_i). Wafers taken from different ingot heights are measured with newest methods, including photoluminescence based metastable defect imaging and inductively coupled plasma mass spectrometry (ICP-MS). The analysis is focussed on iron as a trace impurity, though other impurities can be examined as well.

The distribution of interstitial iron and iron precipitates is simulated two-dimensionally, taking into account segregation, backdiffusion, in-diffusion and precipitation. We especially analyse the edge of silicon bricks, which is affected by in-diffusion of impurities into the solidified silicon. The correlation of measurements and two-dimensional



simulations enables us to predict the distribution of impurities after optional process variations. The experimentally confirmed simulation results can then be used as input parameter for simulations concerning the optimization of the impurity distribution.

Ingot Impurity Distribution Analysis Package

- measurement of spatially-resolved charge carrier lifetime in different ingot heights of the edge-brick
- imaging of metastable defects
- determination of the fraction of charge carrier recombination via the investigated defects in different ingot regions
- ICP-MS measurement of the total impurity concentrations
- simulation of the impurity distribution in the center-block of iron and other important impurities
- simulation of the distribution of iron or other important impurities in regions influenced by in-diffusion from the crucible into the solidified silicon
- determination of contamination of the solidified silicon from crucible and coating
- determination of the concentration of investigated impurities in the melt
- report of results and conclusions

Optionally Available Analyses

- optimization of the cooling profile during the crystallization process regarding the dominant impurities in processed wafers
- local dislocation density mapping (etch pit density)
- light element analyses (FTIR)

Solar Cell Impurity Distribution Analysis

This analysis package aims at determining detrimental impurities and their distribution in processed wafers and solar cells. It encompasses simulation based process optimization to minimize solar cell efficiency losses caused by iron related defects.

Initially we determine the charge carrier lifetime and the metastable defects of interstitial iron and chromium before and after high temperature solar cell process steps. Then we use the results to determine the fraction of charge carrier recombination in different regions via these defects and thus their impact on the cell performance.

The analyses are supported by twodimensional simulations of the impurity behaviour in all high temperature steps during processing. The entire thermal history of the wafers is included, in order to obtain reliable and predictive simulations. Our simulation methods are based on experimentally confirmed models for phosphorus and boron diffusion as well as models for aluminum-, boron- and phosphorus-diffusion-gettering of metals which allow an accurate prediction of the impurity distribution.

Solar Cell Impurity Distribution Analysis Package

- measurement of the charge carrier lifetime and the Fe_i, Cr_i distribution before and after emitter diffusion and firing
- simulation of Fe_i distribution after emitter diffusion and firing (Sentaurus Process)

3 Measurement of the dissolved iron concentration (Fe_i in cm⁻³) in a vertical slice of the block produced in an extremely pure crucible. The very good agreement with the simulations can be seen in the superimposed images.



4 Overall density of iron precipitates in dependence on the cooling rate after solidification and the phosphorus diffusion process.

- determination of the impact of iron related defects on the charge carrier lifetime in different ingot regions after emitter diffusion and firing
- temperature profile optimization of the emitter diffusion process regarding the dominant impurities in processed wafers
- report of results and conclusions

Optionally Available Analysis

 simulation of the impact of iron related defects on the solar cell performance (Sentaurus Device)