Unraveling of Bulk and Surface Behavior in High-Quality c-Si Material via TIDLS

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***Abstract* — The current trend in silicon photovoltaics towards high-quality thin mono-crystalline silicon substrates makes the accurate representation of surface recombination of utmost importance. It has been shown by several authors that an effective way to study detrimental defects in silicon wafers is by means of temperature and injection dependent lifetime spectroscopy (TIDLS) coupled with the Shockley–Read–Hall recombination model. Given its high sensitivity this is an excellent technique to study high lifetime substrates. However, a thorough evaluation of the surface recombination velocity (SRV) dependence on injection level and temperature is vital to the extrapolation of meaningful results regarding the defects contained in the bulk of the material. Here, we present a TIDLS study of a-Si:H(i), a-Si:H(n) and a-Si:H(p) deposited on *n*-type low-resistivity FZ substrates. We evaluate the impact of every dielectric layer on the total SRV temperature- and injection dependence while demonstrating its fundamental role in τ_{eff} behavior of high-quality Si substrate.**

***Index Terms* — passivation, photoconductance, TIDLS, amorphous silicon, silicon.**

I. Introduction

In the last few years research on silicon photovoltaics has strongly shifted toward high-quality mono-crystalline silicon material fueled by the need of continuously pushing the efficiency/costs ratio. Particular attention has been given to *n*-type silicon which presents the obvious advantage over *p*-type material of being free of boron atoms and thus metastable defects such as B-O and Fe-B. The activity of these complexes are known to strongly downgrade the final device performance [1]-[4].

As the quality of PV silicon increases, the surface passivation quality of the substrate gains more and more relevance as its impact on the overall device performance is greatly augmented when compared to low-quality material. During the last decades, several passivation technologies have been developed as an alternative to the originally established SiO_2 in the attempt to eliminate the high-temperature step needed for the activation of this dielectric material. The oxidation process usually performed at temperatures above 900 °C is known to severely degrade the bulk lifetime of silicon samples [5]. Among these technologies the most important are SiN_x, Al_2O_3 and a-Si:H(i), with the first two owing their effect mainly to field effect passivation from the presence of fixed charges (positive for SiN_x and negative for Al_2O_3) [6]-[7] and the last one providing excellent passivation thanks to the superior electrical quality of the interface with c-Si due to the chemical passivation of dangling bonds provided by the hydrogen atoms [8]-[10].

The surface recombination velocity (SRV) is usually considered a figure of merit for the assessment of the overall quality of the passivation achieved by the dielectric layer, which includes the effect of chemical as well as field-effect passivation. Cell performance is known to vary with operating temperature and light intensity, but little is known on the fraction originating from variation in surface passivation properties. In this work we determine the SRV dependence for different passivation schemes on both temperature and injection level which we predict is crucial for an accurate understanding of the overall effective lifetime.

II. Experimental

A. Sample preparation

We used *n*-type (100) PV FZ wafers with a resistivity of 2.8 Ω·cm. The substrates were subjected to typical cleaning steps including RCA-b, Piranha and BOE solutions. Two series of samples with different thicknesses (150−250 nm) were obtained by subsequent etching into a mixture of hydrofluoric, nitric and acetic acid. The substrates were then double-side coated with 50 nm of a-Si:H(i) by plasma-enhanced chemical vapor deposition (PECVD) at 250 °C. Samples were annealed in a muffle furnace in air at 280 °C for 30 minutes. After a first cycle of lifetime measurements the samples were subjected to a new cleaning procedure before a second 10-nm-thick layer of either a-Si:H(n) or a-Si:H(p) was deposited on both sides by PECVD, on top of the a-Si:H(i) layer; no further annealing was applied.

B. Characterization

Temperature- and injection-dependent lifetime spectroscopy (TIDLS) measurements were performed with a

WCT-120TS Sinton lifetime tester [11]. The version used in this work is equipped with a heating stage which allows to acquire the lifetime vs injection curves in a range of temperature going from room temperature to 230 °C. All the measurements are made in transient mode and averaging over 20 data points to improve the signal-to-noise ratio..

III. Results and Discussion

The SRV values are obtained in this work by applying the wafer thickness variation method [12] on a series of chemically-thinned wafers. For double-side a-Si:H(i) coated samples with a minority carrier diffusion length greater than the sample width (W), and for sufficient low SRV, we can express relationship of the effective lifetime τ_{eff} to the bulk lifetime τ_{bulk} as[13]

$$\frac{1}{\tau_{eff}} = \frac{1}{\tau_{bulk}} + \frac{2 \cdot SRV}{W} \qquad (1)$$

Hence, the contribution of bulk recombination and SRV can be separated by measuring the lifetime on samples with varying thickness.

A. Passivation provided by a-Si:H(i) layer

The effective lifetime is measured for all the samples between 25 and 230 °C, with steps of 10 °C. Every measure is taken in the transient mode and is averaged over 20 acquisitions. Results are shown in Fig. 1 for the 250-µm-thick sample. All the other samples show a similar behavior although τ_{eff} is found to change with the samples thickness according to Eq. 1.

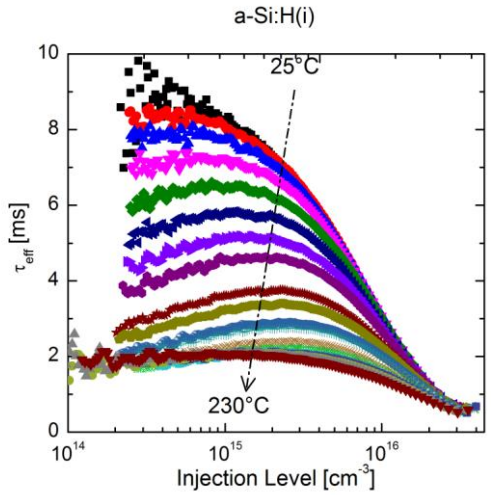

Fig. 1. Effective lifetime as function of injection level at different temperatures with a step size of 10 °C for the 250-µm-thick wafer coated with only a-Si:H(i) layer.

The resulting τ_{eff} is plotted as a function of temperature for three different injection levels in Fig. 2, for the same sample coated with a-Si:H(i).

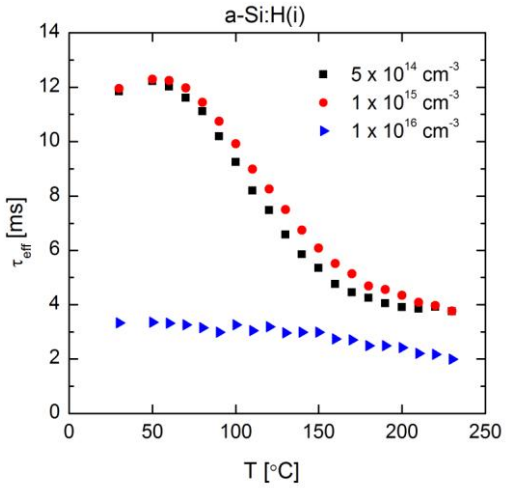

Fig. 2. Effective lifetime as function of temperature for three different injection levels for one of the samples analyzed with only a-Si:H(i) as passivation layer.

The effective lifetime is found to decrease substantially as the temperature increases for injection levels below 10^{16} cm^{-3} above which the lifetime is limited by the Auger recombination at all temperatures.

By measuring the effective lifetime of wafers with different thicknesses and following Eq. 1 we can extrapolate the surface recombination velocity at each injection level and temperature from the linear fit of data. An example of the results obtained with this method is shown in Fig. 3 using six samples with a thickness in the range 250–150 µm passivated with 50 nm of a-Si:H(i) at 100 °C.

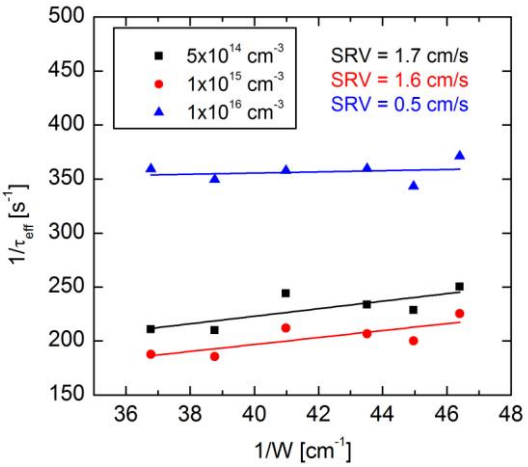

Fig. 3. Inverse of effective lifetime plotted vs. the inverse of thickness for extrapolation of SRV from the fit of data at each injection level and temperature, here at 100 °C for samples coated with a-Si:H(i).

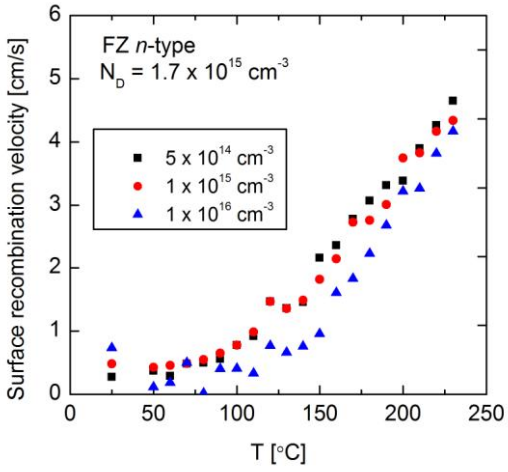

Fig. 4. Surface recombination velocity as function of temperature at three different injection levels for samples coated with a-Si:H(i).

The resulting SRV for the same three selected injection level values as shown in Fig. 2 at temperatures across the range 30 – 230 °C with a step size of 10 °C for samples coated with a-Si:H(i) is shown in Fig. 4. An outstanding surface recombination velocity is obtained with SRV below 0.5 cm/s at room temperature—to our knowledge this represents the best passivation provided by amorphous silicon on *n*-type substrates reported up to date. The SRV is found to increase as the temperature rises above 120 °C but remains lower than 5 cm/s in the whole temperature and injection level ranges. We think this trend originates from the decrement of Fermi level position with temperature which leads to the activation of a defect contained in the passivation layer. The correct position of the defect level within the bandgap and its very nature is currently a matter of investigation.

B. Passivation by a-Si:H(i)/a-Si:H(n) layer stack

As in real devices such as silicon heterojunction solar cells (SHJ) the intrinsic a-Si:H layer is always coupled to a doped a-Si:H layer working as a carrier-selective contact, we proceeded with the deposition of a 10 nm thick layer of a-Si:H(n) with an estimated doping density of 10^{19} cm^{-3} (100 Ω·cm from dark IV measurement) on top of the same samples used for the first part of this work. It must be noticed that the layers thicknesses don't correspond to those used in real devices but were chosen to provide a better temperature stability.

According to our understanding, the shift of Fermi level towards higher values due to the *n*-type doping of the additional layer should delay the activation of the defect level as the temperature rises, and lead to a shift in the temperature threshold at which the SRV starts to increase.

We observed a SRV now consistently below 1 cm/s for the whole range of temperatures and at all injection levels (data above the injection level of 10^{16} cm^{-3} are not shown but they are below the 1 cm/s threshold) (Fig. 5). This could mean that

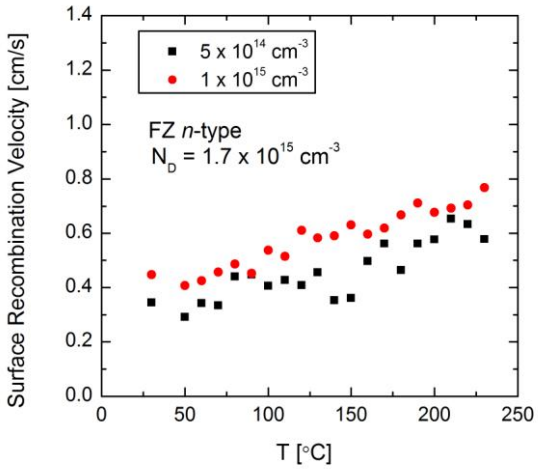

Fig. 5. Surface recombination velocity as function of temperature for two different injection levels for samples coated with the passivation stack a-Si:H(i)/a-Si:H(n).

the postulated shift of temperature threshold at which the SRV starts to increase is so substantial that it is above 230 °C and hence no increment in the SRV can be observed.

C. Passivation by a-Si:H(i)/a-Si:H(p) layer stack

We attempt to test this hypothesis by coating samples with a a-Si:H(p) layer which should affect the SRV in the opposite way, leading to an activation of the defect level at a lower threshold temperature. We prepared a second thickness series of 250- to 150-µm-thick wafers following the same procedure as the first one. An initial evaluation of τ_{eff} and SRV with only the a-Si:H(i) coating showed the same trends as for the first sample set. This time we deposited an additional 10-nm-thick a-Si:H(p) layer (18,000 Ω·cm from dark IV measurement). Following the method described above we extrapolated the SRV at every injection level and temperature. The results are shown in Fig. 6.

Despite a general decrement of the absolute SRV values and stronger scattering in the, we observe a similar increment happening at 120 °C as seen in Fig. 4 for samples passivated only with a-Si:H(i). We think this result to be due to the very low doping level of the additional a-Si:H(p) layer which is not sufficient to induce a shift in Fermi level position, as observed for the n-doped a-Si:H and thus didn't influence the energy threshold at which the defect level is activated.

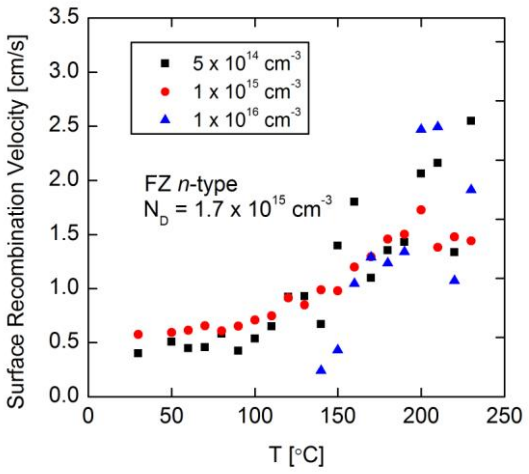

Fig. 6. Surface recombination velocity as a function of temperature for three different injection levels for samples coated with the passivation stack a-Si:H(i)/a-Si:H(p).

IV. Conclusions

The surface recombination velocity dependence on temperature and injection level of several passivation schemes was evaluated via the analysis of a chemically-thinned series of high quality *n*-type FZ c-Si samples. Very high level of passivation was demonstrated with a double-side 50 nm a-Si:H(i) layer coating alone, whereas a better temperature stability was provided by the addition of a 10 nm a-Si:H(n) layer on both surfaces; we attribute this behavior to a Fermi level shift provided by the doped layer preventing the activation of a defect level contained in the passivation layer.

On the other hand, the additional a-Si:H(p) coating did not modify the SRV trend with temperature compared to just the a-Si:H coating. We think that the doping in the a-Si:H(p) is not sufficient to induce a significant shift in the Fermi level position in the intrinsic layer and promote the expected activation of defect levels at a lower threshold temperature than for a a-Si:H(i) coating. Further investigation will provide a better insight of these results.

This work proves that SRV temperature- and injection-dependence varies greatly among different passivation layers. The dependence of SRV on temperature and injection level can't be ignored when analyzing high-quality substrates as its signature could hinder the contribution coming from the bulk. We predict that for an adequate modeling of TIDLS data, the extrapolation of the bulk lifetime will then be crucial for an accurate characterization of lifetime-limiting defects.

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