Characterization of Silicon Surface Passivation by Photoluminescence/Raman Spectroscopy

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Maximization of the power conversion efficiency (PCE) in nanostructured silicon/ PEDOT:PSS hybrid solar cells is an active area of photovoltaic research, due to the reduced thermal budget in production of such devices in comparison to conventional silicon solar cells [1]. Surface passivation of silicon at silicon/organic interface was found to be essential for high efficiency of silicon-based photovoltaics. Surface defects and dangling bonds significantly increase the recombination rate of minority carriers, may pin the Fermi level and cause undesirable band bending at silicon interfaces [2]. Passivation methods for planar silicon surfaces that are currently available [3] are not always compatible with the nanostructured and hybrid organic/inorganic devices, for which appropriate passivation should be developed. Measuring the state of surface passivation is essential in this process. We present a method for the characterization of surface passivation of silicon by simultaneous band gap photoluminescence and Raman spectroscopy.

Passivated surfaces have lower surface recombination velocities, thus more excess minority carriers are available for radiative recombination which results in increased intensity of band gap photoluminescence (PL) [3,5]. Many methods for characterization of surface passivation are based on PL intensity. Difficulty in those methods is the need for accurate calibration of PL intensity measurements [2-5]. Since the radiative bulk recombination in silicon is suppressed due to the indirect nature of its band gap, PL from silicon is highly inefficient and in intensity comparable to Raman scattering. When a Raman spectrum of silicon is taken with excitation energy slightly above the silicon band gap, a silicon TO() band can be observed superimposed to the band gap PL. Since Raman scattering is not sensitive to surface recombination, the ratio of integrated intensity of silicon TO() band to integrated PL intensity was used as a measure of silicon surface passivation.

A benchmark silicon passivation method is hydrogen passivation by immersion in hydrofluoric acid. While the HF passivation gives exceptionally low surface recombination velocities on freshly prepared surfaces, it is unstable under the ambient conditions and within hours transforms to non-passivated state due to the rapid oxidation and formation of surface defect states. We have taken a series of simultaneous Raman scattering and band gap PL spectra from HF passivated silicon sample during its aging under the ambient atmosphere. Excitation-intensity-dependent PL, as well as the PL at constant excitation intensity were measured in different time intervals during the sample aging. Exponential PL intensity decay in time was observed, as well as a linear dependence of PL intensity on excitation laser power. Surface passivation state was estimated by measuring the PL integrated intensities at constant excitation power, while Raman TO peak integrated intensity remained constant over time. We propose obtaining effective surface recombination lifetime ratios by taking the ratios of linear fit slopes of integrated PL intensities vs. excitation laser power at different times as another measure of surface passivation. This method will be further used for characterization of different nanostructured silicon passivation procedures in order to improve the properties of hybrid silicon/organic solar cells.



Figure 1 a) PL/Raman spectra of H-terminated Si, taken with 10 mW 1064 nm Nd:YAG laser excitation over 18h b) linear fits of integrated PL intensities vs. excitation laser power over a period of 18 hours.

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