6th International Conference on Silicon Photovoltaics, SiliconPV 2016

Modelling kinetics of the boron-oxygen defect system

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Abstract

Here we report on modeling kinetics of the boron-oxygen defect system in crystalline silicon solar cells. The model, as supported by experimental data, highlights the importance of defect formation for mitigating carrier-induced degradation. The inability to rapidly and effectively passivate boron-oxygen defects is primarily due to the unavailability of the defects for passivation, rather than any "weakness" of the passivation reaction. The theoretical long-term stability of modules in the field is investigated as a worst-case scenario using typical meteorological year data and the System Advisor Model (SAM). With effective mounting of the modules, the modelling indicates that even in desert locations, destabilisation of the passivation is no concern within 40 years. We also incorporate the quadratic dependence of the defect formation rate on the total hole concentration, and highlight the influence of changing doping densities or changing illumination intensity on the CID mitigation process.

1. Introduction

1.1. Boron-oxygen defect system in p-type Czochralski silicon

Crystalline silicon solar cells fabricated on boron-doped Czrochralski (Cz) grown silicon substrates are subject to a degradation of performance when exposed to carrier injection, which for solar cells, is typically induced by exposure to light [1]. This has been attributed to the formation of a boron-oxygen (B-O) complex, although the defect composition is still being heavily debated in the literature [2-7].

In 2006, Herguth *et al.* presented a method to passivate the boron-oxygen (B-O) defects based on illuminated annealing, hence permanently eliminating the B-O related carrier-induced degradation (CID) [8]. Earlier papers had focused on the temperature range of 50 °C – 230 °C and noted a reduced effectiveness of processes conducted at higher temperatures [8-12]. Similarly to the structure of the defect, significant contradictions have been reported on the mechanisms involved in the permanent passivation process [13-17]. However, strong evidence has shown the involvement of hydrogen [13,16,18-20], and in particular, the importance of hydrogen charge states in the passivation of the defect [14,21-24]. With the advancements in the understanding of the B-O defect and hydrogen passivation mechanisms, recent publications have demonstrated effective passivation of the defects at temperatures of 250 °C – 360 °C using patented hydrogenation processes [22,25-26], and this appears to be the temperature range adopted by tool manufacturers such as Centrotherm [27].

Warranties issued by solar panel manufacturers require that a certain level of performance be maintained for typically 25 years. Based on published reaction rates for the destabilisation reaction [28] and dissociation of the B-O defect [29], the passivated state of the B-O defect is more than 100 times stable than the defect itself for temperatures above 0 °C. However, due to the potential destabilisation of passivated B-O defects in the field, questions over long-term stability of the passivation are often raised.

1.2. Modelling the boron-oxygen defect system

Previous studies modelling the kinetics of the B-O defect system have investigated a variety of potential influences on the system. Those studies have typically used three-state models to describe the defect system, with simple reaction rates consisting of an attempt frequency and an activation energy [11, 30-33]. In those studies, no explicit influence of either the doping concentration or carrier concentrations were included. In another study, reaction rates involved normalised concentrations of substitutional boron, interstitial oxygen dimers and a mystery compound, X, that is now presumed to be hydrogen [9]. Again, in that study no dependence was included for the influence of carrier-injection. Gläser *et al.* included occupational probability of hydrogen charge states to participate in the defect passivation reaction [24]. However, the fractional concentrations of hydrogen charge states were assumed constant for a given illumination intensity, and hence no dependence on variations in the hydrogen charge state concentrations were considered throughout the process as the carrier lifetime evolves through the degradation-passivation cycle [24].

Studies exploring methods to accelerate the passivation of the defect have suggested that the speed of B-O defect passivation is primarily dependent on the time-constant for the passivation reaction [10]. However, that assumption did not include the influence of the availability of defects for passivation. In that study, time constants given for the destabilisation reaction were given at temperatures of 25 °C and 60 °C. It was concluded that the reported values of >8,800 years and >53 years, respectively, were sufficiently long that destabilisation would not be a major problem in the lifespan of a typical solar cell [10]. This was in agreement with earlier predictions by Herguth *et al.* [30], which also noted that any increased cell operating temperature would most likely be accompanied by illumination that could enable the passivation reaction to counteract the destabilisation reaction. However, operating temperatures of modules are highly variable, and in certain instances modules can operate well in excess of 60 °C.

Here we use a three-state model to describe the B-O defect system and perform a worst-case scenario numerical simulation of photovoltaic (PV) modules in operation to study the potential destabilisation of the B-O defect passivation. This is based on experimentally obtained values for the destabilisation reaction [28], predicted module temperatures using the System Advisor Model (SAM) (version 2015.06.30) from the National Renewable Energy Laboratory (NREL) [34-35] from typical meteorological year data. The study was extended to investigate the potential of passivating B-O defects in the field using the same principle.

We also discuss the model in terms of the rate-limiting reactions for the passivation of B-O defects. Our results show that in contrast to previous claims that the hydrogenation rate limits the speed at which defects can be passivated, with recently reported values of the passivation reaction rate, the speed at which defects are passivated is limited by the availability of defects for passivation, and therefore, the defect formation rate.

Further modifications are made to the model to reflect the enhanced understanding for the behaviour of the B-O defect, with the ability to accelerate the defect formation rate in p-type silicon by using high intensity illumination to increase the total hole concentration [36]. These include the quadratic dependence of the defect formation rate on the