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Current-induced and light-induced macroscopic changes in thin film solar cells: Device degradation mechanism

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ABSTRACT

We report on the formation of large voids in hydrogenated polymorphous silicon (pm-Si:H) PIN solar cells upon light-soaking. We could monitor *in situ*, the formation of macroscopic bubbles and holes during current-induced degradation of the same devices using optical microscopy. Forward bias, leading to a current-injection of 300 mA/cm^2, was applied to hydrogenated amorphous silicon (a-Si:H) and pm-Si:H PIN solar cells and series of optical images were taken on the same spot at various steps of current-injection. During the current-injection, the pm-Si:H PIN solar cells experience significant topological changes, which we could not detect in a-Si:H PIN solar cells. These effects were further characterized by complementary ex-situ techniques such as SEM, AFM and spectroscopic ellipsometry.

1. Introduction

Hydrogen plays two important roles in hydrogenated amorphous silicon (a-Si:H). On the one hand, it forms silicon-hydrogen (Si—H) bonds which passivate dangling bonds, reducing the defect density down to the level of 10^{15} cm^{-3}. This enables to make electronic devices such as photosensors, thin-film transistors, and solar cells. On the other hand, hydrogen is involved in metastable defect formation, resulting from the recombination of electron-hole pairs. Such metastable defect creation is known as the Staebler-Wronski Effect (SWE) Staebler and Wronski, 1977; Fritzsche, 2001; Shimizu, 2004. Conventional models of the SWE assume that a-Si:H is a continuous random network, which is disordered but homogenous, and the most favored model has been the hydrogen bond switching model (Fritzsche, 2001; Shimizu, 2004), which suggests that the dominant defects are isolated dangling bonds. However, in practice, a-Si:H is inhomogeneous and contains voids (Carlson, 1986), molecular hydrogen (Fedders et al., 2000), and various types of vacancies (Smets and van de Sanden, 2007). Nowadays, new discoveries in SWE, such as limited relevance of the traditional dangling bond defect to the SWE (Wronski and Niu, 2014), the role of hydrogen passivated internal surfaces (nanosized voids) Fehr et al., 2014; Melskens et al., 2015, and the agglomeration of the voids upon annealing (Duaand and Zhang, 2005; Mannheim, 2013; Schouten, 2013; Melskens et al., 2013; Bobela et al., 2011) or under light-soaking (Zhang and Branz, 2003), also support the inhomogeneous structure of a-Si:H. Moreover, it has been widely reported that hydrogen evolves during metastable defect creation (Carlson, 1986; Melskens et al., 2015; Duaand and Zhang, 2005; Takeda et al., 1997; Santos et al., 1991) and that its evolution introduces various structural modifications, initiated by the formation of bond-centered hydrogen (Zhang and Branz, 2003; Longeaud et al., 2002; Darwich et al., 1995; Godet and Roca i Cabarrocas, 1996). Recent research results also revealed that hydrogen passivated internal surfaces of voids play an important role in light-induced degradation compared to isolated Si—H bonds (Wronski and Niu, 2014; Fehr et al., 2014; Melskens et al., 2015).

In this work, we focus on hydrogenated polymorphous silicon (pm-Si:H), a nanostructured material consisting of a small volume fraction of nanocrystals embedded in an amorphous matrix, presenting improved medium range order (Roca i Cabarrocas, 2000). The crystalline fraction in pm-Si:H originates from plasma-generated silicon nanocrystals. In order to synthesize silicon nanocrystals in the plasma, the deposition of pm-Si:H is done at relatively higher working pressure (in a range of few Torr) compared to that of standard a-Si:H (Kim et al., 2017a). A feature characteristic of pm-Si:H films is detection of a middle stretching mode (MSM) in Fourier transform infrared spectroscopy (FTIR) measurements Lebib and Roca i Cabarrocas, 2004; Kim et al., 2017b. Recent

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results of Fischer et al. have shown that a-Si:H films having a MSM and a low level of high stretching mode (HSM) in their FTIR result in highly efficient solar cells (Fischer et al., 2015).

We have demonstrated that pm-Si:H solar cells show unusual light-induced degradation kinetics, such as irreversible degradation (Kim et al., 2012a, 2016), relaxation of internal stress (Kim et al., 2013), light-induced hydrogen migration (Kim et al., 2012b) and interface delamination at the substrate/p-layer interface (Kim et al., 2013) when submitted to standard AM1.5G light-soaking. Our previous results suggest that there is something more than conventional SWE in pm-Si:H solar cells. Such interesting light-induced effects in pm-Si:H solar cells can be regarded as an extreme case of light-induced structural changes in a-Si:H, which make its detection easier. Considering that metastable defect creation takes place mainly at hydrogen passivated internal surfaces, the heterogeneous structure of pm-Si:H material may lead to significant topological changes under standard light-soaking conditions (1 sun and 50 °C), while in the case of a-Si:H films such structural changes have been reported only under extreme light-soaking conditions (50 suns and 130 °C) (Carlson and Rajan, 1996) or annealing temperatures above 350 °C (Bobela et al., 2011).

Besides atomic-scale defect creation, large structural changes and hydrogen evolution may play crucial role on the degradation of the solar cells. Based on these previous understandings, we examine further the structural changes in pm-Si:H solar cells. The aim of this work is to study the physical origin of topological defect formation such as bubbles and holes in hydrogenated polymorphous silicon and metastable defect creation.

2. Experiment

The PIN solar cells were deposited at 175 °C by the radio-frequency (RF, 13.56 MHz) glow discharge PECVD method in a multiplasma-monochamber reactor (Roca i Cabarrocas et al., 1991). Standard a-Si:H was obtained by the dissociation of pure silane at low pressure (50 mTorr) and low RF power density (5 mW/cm^2). Intrinsic pm-Si:H films were deposited at a pressure of 2 Torr and a RF power density of 30 mW/cm^2. The solar cells had the following structure: Glass substrate/Cr /p-type hydrogenated amorphous silicon carbon (a-SiC:H)/a-SiC:H buffer/intrinsic layer/n-type a-Si:H/ITO contact. The area of the cells (0.0314 cm^2) was defined by the ITO top contact. The thickness of p and n doped layers were about 170 and 130 Å respectively, and the intrinsic layer thickness varied from 2000 to 5000 Å.

In addition, a set of pm-Si:H PIN layer stacks were also co-deposited on various substrates such as Corning Eagle glass, textured SnO_2:F (Asahi-U), and flat ZnO:Al, and were light-soaked (up to 500 h under 100 mW/cm^2). The changes in their topology were characterized by scanning electron microscopy (SEM), atomic force microscopy (AFM), and Spectroscopic Ellipsometry (SE). Veeco's Dimension 5000 was used for AFM, and Hitachi 4800 was used for SEM. Tapping mode was used in AFM measurements to prevent the cantilever from dragging across the surface and resulting in surface damage, as well as providing higher resolution. During the light-soaking, the PIN layer stacks were fan cooled to limit heating. In this way, the temperature of the PIN layer stacks, measured by PT100 thermometer during light-soaking, stayed under 50 °C. Spectroscopic ellipsometry spectra were taken before and after light-soaking. The resulting spectra were modeled using the Tauc-Lorentz dispersion model and the material parameters were obtained from the modeling (Jellison and Modine, 1996; Jellison et al., 1998).

Since light-soaking studies for SWE are time consuming, accelerated degradation tests such as current-induced degradation (CID) are also widely used to study the mechanism (Street, 1991; Dasgupta et al., 1998). The PIN solar cells were connected to a DC power supply and a forward bias of current density of 300 mA/cm^2 was injected to them. Such current density, which can be regarded as equivalent to an illumination under 20 suns (Street, 1991), was applied for 200 min, which is equivalent to 500 h of light-soaking under one sun illumination (Yang et al., 1991). During the CID, a series of optical images were taken in real time with an Olympus BX61 optical microscope for both a-Si:H and pm-Si:H PIN solar cells. The temperature of the PIN solar cells was monitored using a PT100 thermometer during the CID, verifying that the device temperature stayed under 80 °C.

3. Results

(1) **Light-induced degradation test:** The pm-Si:H PIN solar cell was light-soaked for 500 h and Spectroscopic Ellipsometry (SE) spectra of as-deposited and light-soaked state were measured. The measured spectra were modeled using the Tauc-Lorentz dispersion and the material parameters were obtained from the modeling (Jellison and Modine, 1996; Jellison et al., 1998). Fig. 1 summarizes the SE modeling of

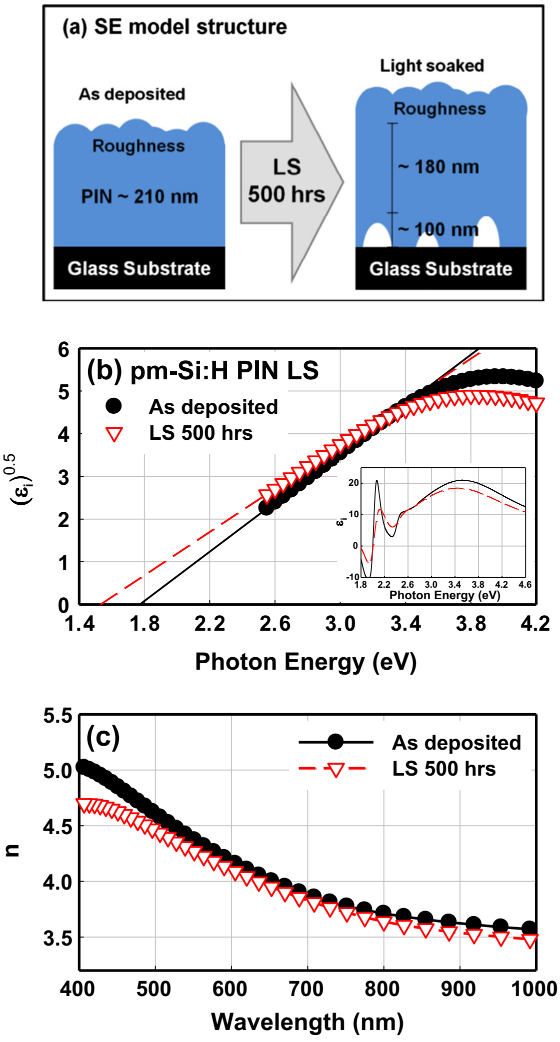

Fig. 1. Summary of SE modeling of pm-Si:H PIN solar cells deposited on glass before and after light-soaking during 500 h. (a) The optical model, (b) optical bandgap (E_{opt}) and raw ε_2 spectra (inset), and (c) modeled refractive index before/after light-soaking.