# The Improved Light-Induced Degradation and the Possible Mechanism in Deuterated Amorphous Silicon Alloy

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### 1. Introduction

The light-induced photoconductivity degradation was one of the most important topics in the studies of a-Si:H material. Many models have been proposed to explain this phenomena and it was generally accepted that the carrier capture and/or following recombination events are responsible for the creation of defects in the mid-gap, i.e., silicon dangling bonds, which result in the photo-degradation [1-4]. Recently, the hot electron degradation in Si metal oxide semiconductor transistor (MOSFET) has been found to be greatly reduced by passivating the Si/SiO<sub>2</sub> interface with deuterium instead of hydrogen [5]. It suggests that replacing hydrogen with deuterium in the amorphous silicon alloy (a-Si:D) may also solve the long-lasting light-induced photoconductivity degradation problem. In this paper, we confirm that the photoconductivity decay of a-Si:D alloy under AM1 illumination is indeed improved and propose a microscopic model to explain these results.

### 2. Results and Discussions

In our experiment, the a-Si:D films were prepared by the deuterium plasma treatment method. First, undoped a-Si:H films were deposited by plasma enhanced chemical vapor deposition (PECVD) at  $300^{\circ}$ C. After deposition, the a-Si:H films were annealed to expel all the hydrogen atoms out of the films. Then the annealed films were treated separately by H<sub>2</sub> (PT a-Si:H) and D<sub>2</sub> (PT a-Si:D) plasma until their electrical properties (dark and photoconductivities) were recovered.

Figure 1 shows the normalized photoconductivity  $\sigma_L / \sigma_{Lo}$  of three samples which are as-deposited a-Si:H (1(a)), PT a-Si:H (1(b)) and PT a-Si:D (1(c)) as a function of illumination time up to 250 hours. In general, the light-induced defect density N(t) or photoconductivity  $\sigma_L$  (inversely proportional to N(t)) of a-Si:H follows a stretched-exponential form [1]. But at the intermediated range, the photoconductivity exhibits a 1/n power law decay and gradually saturates at a certain value. At the intermediate range, it is found that the degradation curves obey the power law with power index close to 1/2, 1/2 and 1/4 for the lines (a), (b) and (c) in Fig. 1, respectively. The decay for deuterated a-Si films (line (c)) is the slowest. The saturation to initial photoconductivity ratio ( $\sigma_{sat}/\sigma_{ini}$ ) are 0.022, 0.020 and 0.12 for the as-deposited a-Si:H, PT a-Si:H and PT a-Si:D, respectively. The a-Si:D has the highest saturated photoconductivity.

According to the models proposed by Tzeng and Lee [3], Stutzmann et al. [4], the sufficient accumulation of the localized vibrational energy followed by its transfer and breaking the nearby weak Si-Si bonds is responsible for the generation of the light-induced defects (silicon dangling bonds). As illustrated in Fig. 2(a) [3], the energy which required to break these weak bonds are released from the non-radiative electron or hole capture to the nearby pre-exist defects. In a-Si:H, these capture events will occur at the Si dangling bonds and the energy is released to excite nearby localized vibration modes then the localized vibrational energy will flow out to the rest of the lattice through Si-Si phonon vibration. If enough localized energy is accumulated in a short period of time by multiple capture and recombination, the nearby weak bonds tend to be broken by this energy. The neighboring Si-H bond must switch to the broken bond position, as shown in Fig. 2(b), to stabilize the dangling bonds, otherwise the light-induced dangling bonds are going to reconnect [4]. During light soaking, if the localized vibrational energy can be coupled efficiently to the extended lattice mode (phonon), the energy accumulation near a single defect site becomes more difficult and the nearby weak bonds will be harder to break. Then the films become more stable under illumination.

Figures 3 show the IR spectra of the as-deposited a-Si:H, PT a-Si:H and PT a-Si:D films in the 400 to 2500 cm<sup>-1</sup> (stretching and wagging modes) range. In the a-Si:H and a-Si:D films, the phonon vibration of a-Si lattice is centered around 495 cm<sup>-1</sup>. The localized vibration modes which occur near 495 cm<sup>-1</sup> are Si-H and Si-D wagging modes at 640 and 510 cm<sup>-1</sup> for a-Si:H and a-Si:D, respectively. In a-Si:H, the vibration frequency of Si-H wagging mode (640 cm<sup>-1</sup>) is far away from the Si-Si lattice mode (495 cm<sup>-1</sup>). The energy coupling between these two modes is small and the energy transfer from Si-H to Si-Si matrix is slow. The rate of defect creation is fast and degradation of photoconductivity exhibits the small n value, i.e., n close to 2 for lines (a) and (b) in Fig. 1. But for the a-Si:D films, the Si-D wagging mode center around 510 cm<sup>-1</sup> which actually overlaps with the Si-Si lattice mode as shown in Fig. 3 and they may form a coupled vibration mode [6]. The energy can be easily transferred from the Si-D localized vibration mode to the Si-Si extended phonon mode. The energy accumulation near a single defect site becomes more difficult and the nearby weak bonds will be harder to break. This explains why a-Si:D film is more stable

under the same light exposure conditions, and the 1/n power law decay exhibits a larger n value (n close to 4 for the line (c) in the Fig. 1). This suggests that it requires three consecutive recombination events to break one weak bond [3].

### 3. Conclusion

In conclusions, it is found that the a-Si:D is more stable than a-Si:H under the same light exposure conditions. The strong coupling between localized Si-D wagging mode and Si-Si lattice mode is proposed to be responsible for the slowing down of photodegradation process.

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Fig.2 The schematic diagram showing the defect creation process of a-Si:H (a-Si:D): (a) electron capture non-radiatively, energy releases to localized Si-H (Si-D) wagging mode which eventually breaks neighboring weak Si-Si bond, (b) Si-H (Si-D) bond switches to the broken bond position to stabilize the newly created two dangling bonds.



Fig.1 The degradation of normalized photoconductivities of (a) as-deposited a-Si:H, (b) PT a-Si:H and (c) PT a-Si:D. The illumination intensity is AM1.



Fig.3 The IR spectra of as-deposited a-Si:H, PT a-Si:H and PT a-Si:D films. The spectra are ranged from 430 to 2500 cm<sup>-1</sup>, s and w in the figure represent the stretching and wagging modes, respectively.