



## Hydrogen kinetics in a-Si:H and a-SiC:H thin films investigated by real-time ERD



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### ABSTRACT

Hydrogen effusion from hydrogenated amorphous silicon (a-Si:H) and amorphous silicon carbide (a-Si<sub>1-x</sub>C<sub>x</sub>:H) thin films during a temperature ramp between RT and 600 °C was studied by in situ real-time elastic recoil detection analysis. Point to point contour maps show the hydrogen depth profile and its evolution with the ramped temperature. This paper proposes a diffusion limited evolution model to study H kinetic properties from total retained H contents recorded in a single ramp. In a compact a-Si:H layer where H predominantly effuses at high temperatures between 500 and 600 °C, an activation energy value of ~1.50 eV and a diffusion pre-factor of  $0.41 \times 10^{-4} \text{ cm}^2/\text{s}$  were obtained. Applied to a non-stoichiometric a-Si<sub>1-x</sub>C<sub>x</sub>:H film in the same range of temperature, the model led to reduced values of activation energy and diffusion prefactor of ~0.33 eV and  $0.59 \times 10^{-11} \text{ cm}^2/\text{s}$ , respectively.

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### 1. Introduction

Hydrogen plays an important role in Si based opto-electronic devices. In solar cells specifically, H has a beneficial role on the amorphous Si absorber – layer because it passivates a large part of the defects also known as dangling bonds. The hydrogen content has also been linked to the metastability change upon light exposure [1,2] and its bonding configuration has been reported to influence the structural properties of the material [3]. The hydrogen content and its depth profile in Si based thin films depend on the bond chemistry, the chemical reactions, solubility and on the microstructure properties that are themselves strongly influenced by the deposition techniques. It is thus of technological importance that not only the H content is accurately determined in the material but also its depth distribution and kinetic properties be established. For low H concentrations, H diffusion is often determined by secondary ion mass spectroscopy [4]. In a-Si:H and a-Si<sub>1-x</sub>C<sub>x</sub>:H, Fourier transform infrared spectroscopy is widely used to quantify and assign IR active vibrations bonds. Other methods such as thermal desorption spectroscopy have been employed for a long time to study H kinetics in a-Si:H from several ramped anneals [5].

Recently, Smeets et al. [6] have studied the hydrogen diffusion in a-Si formed by ion implantation using real-time elastic recoil detection analysis (ERDA). While several reports exist on the hydrogen kinetics in a-Si:H thin films, little literature exists on the kinetic parameters in non-stoichiometric a-SiC:H.

This paper reports on hydrogen diffusion kinetics in a-Si:H and a-Si<sub>1-x</sub>C<sub>x</sub>:H thin films in which the hydrogen is incorporated in various forms during the deposition by chemical vapour deposition (CVD) process. In the hydrogen evolution experiments for both films, the temperature is raised monotonically with the time between around 300 and 600 °C while collecting at a constant rate the ERD spectra; the total retained H content throughout this temperature range were obtained from the integration of the simulated content–depth curves. A diffusion-limited evolution model [7,8] was used to obtain both the activation energy and H diffusion coefficient from a single temperature ramp. It is assumed that no H resides in the used c-Si substrate.

### 2. Material and methods

Films of a-Si:H, and a-Si<sub>1-x</sub>C<sub>x</sub>:H around 1 μm thick were deposited onto Si(100) substrate by hot-wire chemical vapour deposition (HWCVD) using feed gas mixtures of SiH<sub>4</sub>/H<sub>2</sub> and SiH<sub>4</sub>/CH<sub>4</sub>/H<sub>2</sub> respectively at a low substrate temperature below 400 °C; a summary of the deposition conditions is given in Table 1.

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**Table 1**

A summary of the deposition conditions of the films studied.

Sample	Filament T (°C)	Substrate T (°C)	Pressure (μbar)	Feed gas (sccm)	Thickness (nm)
a-Si:H	1600	375	40	SiH <sub>4</sub> /H <sub>2</sub> :12/48	900
a-SiC:H	2000	280	150	SiH <sub>4</sub> /CH <sub>4</sub> /H <sub>2</sub> :2/4/100	1000

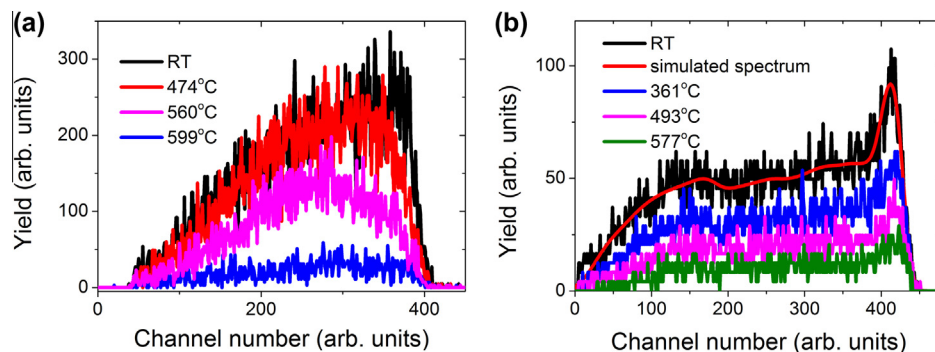
The studied grown a-Si<sub>1-x</sub>C<sub>x</sub>:H film is not stoichiometric but it instead incorporates an atomic C content  $x$  of ~7 at.% as it has been determined by EDX studies not given here. Real-time ERDA measurements were performed at iThemba LABS, Faure, South-Africa using the same experimental set-up and scattering details as in [9,6]. A 15 μm thick mylar (C<sub>10</sub>H<sub>8</sub>O<sub>4</sub>) was used as a stopper of the scattered He<sup>+</sup> in front of the solid state detector. The analysed spectra were obtained using an incident He<sup>+</sup> beam of 3 MeV while the channel – energies calibration experiment was done using spectra taken from a 125 μm thick Kapton (C<sub>22</sub>H<sub>10</sub>N<sub>2</sub>O<sub>5</sub>) foil at beam energies of 3, 2.5 and 2 MeV. For the a-Si:H sample, a rapid ramp from RT up to 300 °C was performed and subsequently a fixed slow ramp rate of 3 °C/min was applied over the range 300–600 °C. In a-Si<sub>1-x</sub>C<sub>x</sub>:H film where a low temperature H effusion was noted, the 3 °C/min slow ramp was initiated at a temperature of 250 °C. ERD spectra were saved every 30 s. The collected spectra were combined either in four or eight to form a slice of ERD spectra with improved statistics. The formed slices were thus representative of a temperature range of 6 and 12 °C, respectively. The simulations of the spectra were done using SIMNRA [10]. The non-Rutherford cross section of Baglin (HHeH-He30.R33) [10] in the energy range between 1 and 3 MeV and for a recoiled angle of 30° was chosen in the simulations process. The calibrated data of the experimental set-up, obtained from the

simulation of a Kapton foil spectrum (i.e., a simulation that reproduced the actual thickness and the hydrogen content in the foil), have been kept fixed during the simulation process of the studied samples' spectra.

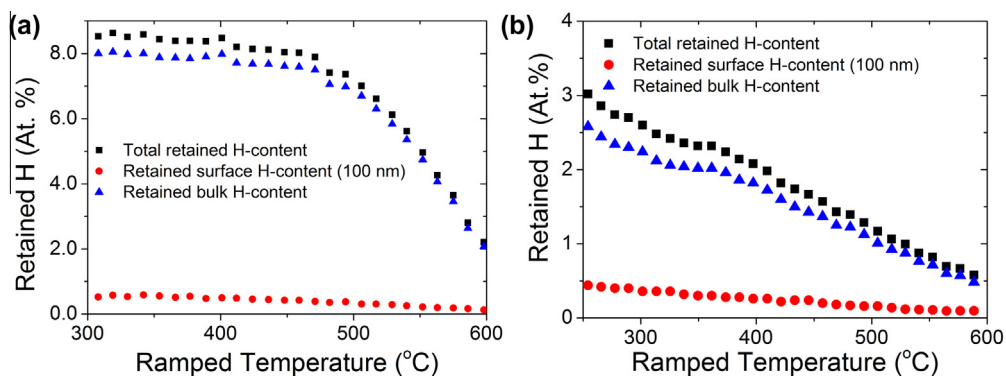
### 3. Results and discussion

Fig. 1 compares the profile of few selected ERDA raw spectra of temperature ramped a-Si:H and a-Si<sub>1-x</sub>C<sub>x</sub>:H films; the spectrum of the as-deposited a-Si:H sample in (a) shows that H was uniformly distributed throughout the thickness (the reader should note that in ERD spectra, the combined effect of the cross section and of the projectile's energy loss is such that the yield decreases rapidly with depth for the same number  $N_s$  of target atoms (i.e., same H content)) in contrast to a-Si<sub>1-x</sub>C<sub>x</sub>:H film in (b) where an inhomogeneous H profile was observed towards the interface. The stacked spectra in Fig. 1(b) indicate also that the H effusion starts at lower temperature in the a-Si<sub>1-x</sub>C<sub>x</sub>:H material. Fig. 2 that displays the total simulated hydrogen content as function of the temperature gives more details about the onset of the H effusion.

It is clear that only a high temperature H effusion process, starting at ~500 °C is observed in a-Si:H sample (Fig. 2(a)) while on the other hand a continuous loss of H can be seen to occur throughout



**Fig. 1.** Selected as-taken spectra (a) the a-Si:H, and (b) the a-Si<sub>1-x</sub>C<sub>x</sub>:H ramped from RT to 600 °C; the red solid curve on the top spectrum of (b) is a typical example of the simulation. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



**Fig. 2.** Measured retained H content obtained by simulation, as function of the ramped temperature (a) a-Si:H; (b) a-Si<sub>1-x</sub>C<sub>x</sub>:H.

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