Mechanisms for Defect Creation and Removal in Hydrogenated and Deuterated Amorphous Silicon Studied using Thin Film Transistors

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ABSTRACT

It has been widely observed that thin film transistors (TFTs) incorporating an hydrogenated amorphous silicon (a-Si:H) channel exhibit a progressive shift in their threshold voltage with time upon application of a gate bias. This is attributed to the creation of metastable defects in the a-Si:H which can be removed by annealing the device at elevated temperatures with no bias applied to the gate, causing the threshold voltage to return to its original value. In this work, the defect creation and removal process has been investigated using both fully hydrogenated and fully deuterated amorphous silicon (a-Si:D) TFTs. In both cases, material was deposited by rf plasma enhanced chemical vapour deposition over a range of gas pressures to cover the \( \alpha \rightarrow \gamma \) transition. The variation in threshold voltage as a function of gate bias stressing time, and annealing time with no gate bias, was measured. Using the thermalisation energy concept, it has been possible to quantitatively determine the distribution of energies required for defect creation and removal as well as the associated attempt-to-escape frequencies. The defect creation and removal process in a-Si:H is then discussed in the light of these results.

INTRODUCTION

The impressively rapid development of the active matrix (AM) liquid crystal display (LCD) over the last ten years has been enabled by hydrogenated amorphous silicon (a-Si:H) thin film transistor (TFT) technology. Each pixel in an AMLCD display employing this technology includes a bottom gate, inverted staggered structure TFT that controls the electric field across the liquid crystal. The dominance that a-Si:H has achieved in this area is due primarily to the fact that this material can be deposited uniformly over very large areas (upwards of 4 m\(^2\)) by rf plasma enhanced chemical vapour deposition (rf-PECVD) at glass compatible substrate temperatures. However, the amorphous structure introduces two deleterious consequences. First, the electron mobility in a-Si:H is very low (~1 cm\(^2\) V\(^{-1}\) s\(^{-1}\)) and therefore the switching speed in a-Si:H TFTs is too slow for them to be used for the display driving circuitry. Second, metastable dangling bond defects exist in the amorphous structure that produce localized electron states in the band gap of this material. When a gate voltage is applied to an a-Si:H TFT, these
defect states must be filled with electrons before free carriers can be accumulated in the channel, and this results in the device having a high threshold voltage, $V_{th}$. Furthermore, shifting the Fermi level towards the conduction band in a-Si:H induces the creation of dangling bond defects, and consequently, the threshold voltage of an a-Si:H TFT increases with time when a gate bias voltage is applied [1]. Defect creation is also observed upon light illumination of a-Si:H, and is known in this context as the Staebler-Wronski effect [2]. In an AMLCD, the duty cycle of each TFT is very low (much less than 10% for a 1000 line display) as the device is only regulating the charge stored on the capacitor across the liquid crystal. However, in the next generation of flat panel displays, the liquid crystal will be replaced by an organic light emitting diode (OLED) using either polymer or small molecule emitters [3]. In these devices, the active matrix transistors control the current flow through the light emitting diode. Consequently, the duty cycle is much greater and the threshold voltage shift in an a-Si:H TFT used in such a circuit becomes significant over the lifetime of the display. Hence, there is renewed interest in understanding the defect creation and removal process in a-Si:H.

Although it is generally accepted that the creation and removal of metastable dangling bond defects in a-Si:H is accompanied by some reordering of Si—H bonds, the exact mechanism by which this occurs is not fully understood. It is known that hydrogen exists in pairs in the a-Si:H structure from the experimental evidence that the defect density in the material is insensitive to the hydrogen concentration [4]. Two possible defect creation mechanisms have been identified based on this fact. In the first of these, the rate limiting step for defect creation is the breaking of an Si—H bond. The released mobile hydrogen atom diffuses through the a-Si:H network until it collides with a second mobile hydrogen atom to form a bound, paired hydrogen complex (SiHHSi) leaving behind two spatially separated silicon dangling bonds (db) in a reaction of the form [5]

$$\text{Si—Si + 2Si—H} \rightarrow \text{Si—Si + 2db + 2H}_{\text{mobile}} \rightarrow 2\text{db + SiHHSi} \quad (1)$$

In the second possible mechanism, the rate limiting step for defect creation is identified as the breaking of a weak Si—Si bond in close proximity to a doubly hydrogenated SiHHSi complex. This is accompanied by a local rearrangement of hydrogen atoms to leave two dangling bonds, each in close proximity to a hydrogen atom (SiHdb) in a reaction of the form [6]

$$\text{Si—Si + SiHHSi} \rightarrow 2\text{db + SiHHSi} \rightarrow 2\text{SiHdb} \quad (2)$$

Less attention has been paid to the defect removal process in a-Si:H. It is clear that there is no necessity for the defect removal process to be simply the reverse reaction of the defect creation process. Indeed, it would be surprising if this was the case, and previous studies of defect creation and removal in a-Si:H [7] and amorphous silicon-germanium alloys [8] support the view that the two processes are different. It would appear to be likely that some form of hydrogen motion must be required for defect removal to take place [9]. If the breaking of an Si—H bond is the first (and rate limiting) step in the defect removal process, the question then remains as to whether the hydrogen locally moves to passivate a nearby dangling bond or whether a long range diffusion process occurs before the released hydrogen atom rebonds in an SiHHSi complex.

In this paper, a systematic study of the defect creation and removal process is presented through the combination of a quantitative experimental study of the threshold voltage shift in
fully hydrogenated and fully deuterated amorphous silicon TFTs as a function of gate bias stress and annealing with no applied bias and a molecular dynamics simulation of hydrogen in silicon.

EXPERIMENT

A batch of fully deuterated and fully hydrogenated amorphous silicon, bottom gate, inverted staggered structure TFTs have been fabricated ($W/L = 38$ or 230) [10]. The channel (a-Si:H or a-Si:D), charge injection (n$^+$ a-Si:H or n$^+$a-Si:D) and gate insulator (hydrogenated or deuterated silicon nitride) layers were deposited by rf-PECVD at 13.56 MHz. It is well known that the stability of a-Si:H is strongly dependent upon the gas pressure in the reactor chamber during deposition [11, 12]. At low pressures, the a-Si:H growth rate is low as the plasma impedance is predominantly capacitive, and so there is a poor coupling between the external rf power and the plasma. Material deposited in this so-called $\alpha$-regime is highly metastable, but has a high field effect mobility. Above a transition gas pressure, the impedance of the plasma changes to being predominantly resistive due to the presence of negatively charged particles in the plasma produced by gas phase reactions between silyl species. More rf power is coupled into the plasma and a higher deposition rate results. Material deposited in this $\gamma$-regime is more stable, but has a lower field effect mobility. The higher mass of the deuterium atom compared to hydrogen means that, for the same nominal growth conditions, SiD$_x^+$ ions will have a higher energy than SiH$_x^+$ ions with the result that the $\alpha$-$\gamma$ transition is shifted to higher pressures in deuterated silane plasmas compared to their hydrogenated equivalent, as shown in Figure 1. Therefore, TFTs have been fabricated with a-Si:H and a-Si:D channel layers deposited over a range of deposition pressures to produce samples from the $\alpha$- and $\gamma$-regimes in both cases.

Measurements on the TFTs were performed on a Wentworth probe station enclosed within a light-tight Faraday cage. The sample stage was resistively heated using a low noise dc power supply (HP6642A) and the temperature monitored using a K-type thermocouple. A PC using a PID algorithm controlled the heating system. The same PC also drove an HP4140B picoammeter/dual voltage source which was used to measure the electrical characteristics of the TFTs.

Before attempting to measure the threshold voltage shift as a function of gate bias time, the TFTs were annealed at 466 K, with no bias applied, for two hours to minimise the defect density in the channel material. The sample temperature was then reduced to between 351.5 and 394 K. Once the temperature had stabilized, a “fast” gate transfer measurement was made by sweeping the gate voltage close to the threshold voltage whilst applying a drain source voltage, $V_{DS} = 0.25$ V. This allows the threshold voltage, $V_{th}$, to be determined without inducing a significant threshold voltage shift by performing the measurement. A gate bias stress field of 1 MV cm$^{-1}$ greater than the threshold field was then applied and the drain source current, $I_{DS}$, measured as a function of time with $V_{DS} = 0.25$ V. Any change in $I_{DS}$ is linearly related to the threshold voltage shift, $\Delta V_{th}$, if the device is operated in the linear regime, allowing $\Delta V_{th}$ to be determined implicitly as a function of time. This assumption is tested during measurement by periodically performing a “fast” gate transfer measurement to confirm $\Delta V_{th}$ explicitly.
Annealing measurements to study the defect removal process were performed by applying a gate voltage, $V_{GS}$, to TFTs such that a nominal electric field of $10^8$ V m$^{-1}$ exists in the gate insulator. The sample was then heated to 470 K whilst maintaining $V_{GS}$. This ensures that the defect density in the channel material is equilibrated for the applied electric field, resulting in the device having a threshold voltage that is almost equal to the stressing $V_{GS}$. The device is then cooled to the annealing temperature, $T$, whilst maintaining the stressing $V_{GS}$ to ensure that the defect density does not reduce. Once the annealing temperature is reached, $V_{GS}$ is set to 0 V for a time $\Delta t$ before performing a gate transfer measurement to determine $V_{th}$. The gate transfer measurement will tend to reintroduce defects into the channel layer, and if $\Delta t < 5000$ s, this will cause a significant change in $V_{th}$ compared to the change cause by the annealing process, and so the stressing $V_{GS}$ is reapplied and the device heated to 470 K for 900 s to restore the original defect density. This process is repeated for longer annealing times, $\Delta t$, until $\Delta t > 5000$ s, at which point the effect of performing the gate transfer measurement has a negligible effect upon the threshold voltage shift, so that bias stressing is no longer necessary between annealing steps. Measurements continue until the threshold voltage no longer changes, indicating that the defect density has been re-equilibrated.

**Figure 1.** The growth rate of a-Si:H and a-Si:D as a function of deposition pressure. The $\alpha$-$\gamma$ transition is shifted to higher pressures in deuterated silane plasmas.
DISCUSSION

Bias Stressing Results

The authors have previously reported that there is a clear increase in $V_{th}$ for both a-Si:H and a-Si:D TFTs as a function of gate bias stressing time due to the creation of dangling bond defects in the channel material at the interface with the gate insulator [10]. The threshold voltage will tend to shift towards the stressing voltage after long periods of time. Therefore, the time taken for the threshold voltage to shift by half of this maximum, $t_{0.5}$, can be taken as a very simple means of quantitatively comparing the defect creation rate in different samples tested under the same temperature and voltage stressing conditions [13]. If TFTs fabricated from a-Si:D and a-Si:H grown at the same pressure are compared, then the deuterated material generally appears to have a lower defect creation rate as shown in the left hand side of Figure 2. This correlates with reports by other groups of enhanced stability in a-Si:D solar cells and TFTs compared with a-Si:H devices deposited under the same growth conditions [14-17]. However, this does not take into account the shift in the $\alpha$-$\gamma$ transition as a function of pressure between SiH$_4$ and SiD$_4$ plasmas, and consequently, material with very different microstructures is being compared. The true effect of replacing hydrogen with deuterium in amorphous silicon can only be determined by comparing material with the same microstructure. The authors have previously shown that a-Si:H and a-Si:D deposited at the same growth rate have very similar microstructures [10]. When $t_{0.5}$ is plotted as a function of growth rate, as in the right hand side of Figure 2, then both a-Si:H and a-Si:D samples lie along the same trend line, indicating that there is indeed no discernable difference in stability between the two materials.

Further quantitative analysis of these results is possible using the concept of the thermalisation energy, $E_{th}$ [18]. It is clear that there is some energy barrier to defect creation in a-Si:H, and in practice, for an amorphous material with significant structural disorder, there will

![Figure 2](image-url). The variation in characteristic time for defect creation, $t_{0.5}$, at a stressing temperature of 394 K for a-Si:H and a-Si:D as a function of deposition pressure (left) and growth rate (right).
be a range of such energy barriers. The thermalisation energy concept states that, at a particular
temperature, \( T \), defects whose energy barrier to creation is less than or equal to \( E_{th} \) will have been
created after a time, \( t \), given by

\[
E_{th} = kT \ln(\nu t)
\]

where \( k \) is the Boltzmann constant. This permits \( \Delta V_{th} \) to be plotted as a function of energy
instead of time if the attempt-to-escape frequency, \( \nu \) (the number of attempts made by the
system to create a defect at a particular site each second) is known. This may be achieved by
measuring \( \Delta V_{th} \) for the same device at different stressing temperatures and plotting \( \Delta V_{th} \) as a
function of \( E_{th} \) for probable values of \( \nu \). Using this method, \( \nu \) has been found to be \( 10^9 \) Hz for
both a-Si:H and a-Si:D with an experimental error of less than half an order of magnitude [10].
Furthermore, the resulting curve has been found to be well described by a stretched hyperbola of the form

\[
\Delta V_{th}(E_{th}) = (V_{GS} - V_{th0}) \left( 1 - \left[ \exp\left( \frac{E_{th} - E_A}{kT_0} \right) + 1 \right]^{-2} \right)
\]

where \( V_{GS} \) is the stressing voltage applied to the gate, \( V_{th0} \) is the threshold voltage before bias
stressing the device, \( E_A \) is a measure of the mean energy barrier to defect creation and \( kT_0 \) is a
measure of the width of the distribution. Using this technique, \( E_A \) and \( kT_0 \) are found to vary with
growth rate for both a-Si:H and a-Si:D TFTs, but with no discernable difference in the trend line
between the two. This confirms that there is no measurable difference in stability between the
two materials. For material deposited in the \( \alpha \)-regime, \( E_A \) is found to be in the range 0.930 –
0.955 eV and \( kT_0 \) is in the range 54 – 61 meV. However, for material deposited in the \( \gamma \)-regime,
\( E_A \) is significantly increased to 0.96 – 0.98 eV and \( kT_0 \) is also increased to 63-69 meV [10].

![Figure 3](image-url)

**Figure 3.** Normalised threshold voltage shift as a function of annealing time for an a-Si:H TFT at four different annealing temperatures.
Zero Bias Annealing Results

Figure 3 shows the normalized threshold voltage shift as a function of annealing time at four different annealing temperatures for an a-Si:H TFT. As expected, the defect removal rate is greater at higher annealing temperatures, resulting in a faster restoration of the threshold voltage. A similar behaviour is also observed in a-Si:D TFTs. As with the defect creation analysis, it is possible to convert the time dependence of the threshold voltage shift into an energy dependence if the attempt-to-escape frequency, $\nu$, for defect removal is known.

It has previously been reported that $\nu$ is $\sim 10^{13}$ Hz for defect removal, which is the same order of magnitude as most bond oscillation frequencies. It is also believed that the breaking of an Si—H bond is the rate limiting step to defect removal. It would seem reasonable to consider each oscillation of an Si—H bond in a defect site to be an attempt to break the bond and so remove the defect state, in which case the bond oscillation frequency should be taken to be $\nu$.

Therefore, a molecular dynamics simulation has been performed to determine the bond oscillation frequency for both the Si—H and Si—D bonds in amorphous silicon. Simulations were performed using the Cambridge Serial Total Energy Package (CASTEP) in which the bonding electron states for each atom are represented by a pseudopotential, and a summation of plane waves are then used to iteratively solve the Schrödinger equation [19]. The supercell chosen for this simulation is shown in Figure 4. It consists of sixteen silicon unit cells with the addition of two hydrogen (or deuterium) atoms in the H$_2^+$ configuration in which one H atom is in a bond-centred (BC) site and the other is in a tetrahedral (T$_d$) site using the Si—H bond length in the silane molecule as an initial condition. Device quality amorphous silicon is normally slightly compressively stressed, and this has been simulated by reducing the supercell size by 10% in all dimensions compared with the zero stress crystalline silicon structure. The labeled Si—Si bond has also been shortened by a further 10% to introduce an element of structural disorder into the system. All atoms are permitted to move in the simulation, which is performed

![Figure 4](image_url) **Figure 4.** The supercell structure employed in the molecular dynamics simulation of Si—H/D bond oscillation. Silicon atoms are shown in grey and H/D atoms are shown in black.

![Figure 5](image_url) **Figure 5.** The simulated variation in Si—D bond length at the T$_d$ site with time.
at a temperature of 400 K with a plane wave cut-off kinetic energy of 250 eV for 500 fs in 1 fs steps. The simulation shows that, after a short stabilization period, both the BC and T_d Si—H/D bonds settle into a well defined oscillation consisting of a slow rocking motion superposed on a stretching oscillation along the length of the bond. Figure 5 plots the variation in the length of the Si—D bond at the T_d site as a typical example of this stretching oscillation. From such graphs, it is possible to determine the oscillation frequency for the BC and T_d Si—H/D bonds, and the results are summarized in Table 1 together with the average oscillation frequency in each case. The ratio of the oscillation frequencies should depend upon the reduced mass, \( \mu \), of the Si—H/D systems. Therefore, the increased mass of D relative to H should lead to the Si—D bond having an oscillation frequency that is 1.39 times slower than that of the Si—H bond, and the ratio of \((1.30 \pm 0.12)\) from the simulation data is in agreement with this. Conversion of these average oscillation frequencies into wavenumbers gives \((1470 \pm 100)\text{cm}^{-1}\) and \((1900 \pm 100)\text{cm}^{-1}\) for the Si—D and Si—H bonds respectively, which is consistent with the stretching modes of these bonds observed in the infrared absorption spectra for a-Si:D and a-Si:H [20].

Using these average values of the bond oscillation frequencies as the attempt-to-escape frequency in equation 3 allows the threshold voltage shift for both a-Si:H and a-Si:D TFTs during annealing to be plotted as a function of thermalisation energy. This results in all of the annealing curves produced at different temperatures forming a coincident line for each material, as shown in Figure 6, which verifies that the bond oscillation frequency is an appropriate value for \( \nu \). Furthermore, the resulting data points are well described by the stretched hyperbola function of equation 4, and a fit to the data yields values for \( E_A \) and \( kT_0 \) summarised in Table 2.

### Table 1. Summary of the bond oscillation frequencies measured by molecular dynamics simulation.

<table>
<thead>
<tr>
<th>Bond</th>
<th>BC Oscillation Frequency [Hz]</th>
<th>T_d Oscillation Frequency [Hz]</th>
<th>Average Oscillation Frequency [Hz]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si—H</td>
<td>((5.6 \pm 0.4) \times 10^{13})</td>
<td>((5.8 \pm 0.4) \times 10^{13})</td>
<td>((5.7 \pm 0.3) \times 10^{13})</td>
</tr>
<tr>
<td>Si—D</td>
<td>((4.4 \pm 0.3) \times 10^{13})</td>
<td>((4.4 \pm 0.3) \times 10^{13})</td>
<td>((4.4 \pm 0.3) \times 10^{13})</td>
</tr>
</tbody>
</table>

![Figure 6](image-url)

**Figure 6.** Variation in normalized threshold voltage shift as a function of thermalisation energy for (a) an a-Si:H TFT and (b) an a-Si:D TFT. In each case, the solid line is a fit of a stretched hyperbola to the data.
Defect Creation and Removal Processes

The results from the bias stressing and zero bias annealing of the a-Si:H and a-Si:D TFTs throws light on the defect creation and removal process. The absence of any evidence of a giant isotopic effect in a-Si:D compared with a-Si:H of similar microstructure is significant. If the breaking of an Si—H/D bond is the rate limiting step to defect creation, then the fact that the energy of the Si—D and Si—H bonds differs by ~0.1 eV, being 3.136 eV and 3.040 eV in their respective diatomic molecules [21], should result in a significantly improved stability in deuterated devices compared with their hydrogenated equivalent. Equation 4 can be rewritten in terms of the time taken for the threshold voltage to shift by half of its maximum, \( t_{0.5} \), defined earlier. At this time \( \Delta V_{th} = (V_{GS} - V_{th0})/2 \), giving

\[
t_{0.5} = \frac{1}{\nu} \exp\left[\frac{T_0}{T} \ln(\sqrt{2} - 1) + \frac{E_A}{kT}\right]
\]

If the difference in the Si—H and Si—D bond energies is taken to be the difference in \( E_A \) for the deuterated and hydrogenated samples, then \( t_{0.5} \) should be over 16 times greater in the a-Si:D TFTs compared with the hydrogenated equivalent at 394 K, assuming that \( T_0 \) and \( \nu \) are the same in both cases. Figure 2 shows that such a level of enhanced stability is absent which strongly suggests that the breaking of an Si—H bond is not the rate limiting step for defect creation. Furthermore, it has previously been shown that there is a strong correlation between \( E_A \) and intrinsic stress in a-Si:H TFTs deposited under a range of deposition conditions [22]. As the structural backbone of a-Si:H are the Si—Si bonds, the compressive stress found in a-Si:H will result in a shortening of these bonds, resulting in a reduction in the energy required to break the bond. The fact that variations in \( E_A \) appear to follow changes in the energy required to break Si—Si bonds in different a-Si:H samples, combined with the absence of enhanced stability in a-Si:D TFTs, leads to the conclusion that the defect creation process is described by equation 2 in which the breaking of an Si—Si bond is the rate limiting step for defect creation.

In the case of the defect removal process, however, a clear quantitative difference is observed in the variation of the threshold voltage as a function of time between a-Si:H and a-Si:D TFTs. It has already been shown that the attempt-to-escape frequency, \( \nu \), for defect removal is well fitted by the Si—H and Si—D bond oscillation frequencies determined by molecular dynamics simulation. Furthermore, it has been reported that the activation energy for deuterium diffusion in undoped amorphous silicon is \((1.53 \pm 0.15)\) eV [23] whilst that for hydrogen is 1.5-1.6 eV [24, 25]. These values are very similar to the activation energies of

<table>
<thead>
<tr>
<th>Material</th>
<th>( E_A ) [eV]</th>
<th>( kT_0 ) [meV]</th>
</tr>
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<tbody>
<tr>
<td>Si—H</td>
<td>1.552 ± 0.003</td>
<td>41 ± 3</td>
</tr>
<tr>
<td>Si—D</td>
<td>1.559 ± 0.003</td>
<td>47 ± 2</td>
</tr>
</tbody>
</table>
defect removal measured in this study (Table 2). This would suggest that it is the energy required to make hydrogen mobile that limits defect removal. It has already been seen that the Si—D bond energy is slightly greater than that of the Si—H bond by ~0.1 eV, and this too is reflected in the difference in $E_A$ measured here between the deuterated and hydrogenated materials.

Electron spin resonance (ESR) [26] and nuclear magnetic resonance (NMR) [27] experiments also provide important information on the structure of a-Si:H both before and after defect creation. From NMR data, it is known that hydrogen exists in two phases in a-Si:H – a clustered phase, which is considered to be associated with hydrogen on the inner surface of microvoids of the material, and a dilute phase of hydrogen atoms bonded to silicon in which only one hydrogen atom is bound to any one silicon atom. The dilute phase is consistent with the SiHHSi complex of two hydrogen atoms separated by a distance of between 0.6 and 0.8 nm. The ‘double T_d’ model of the SiHHSi complex satisfies this requirement [6]. In this model, the two hydrogen atoms sit in the tetrahedral (T_d) positions on two silicon atoms that would otherwise have been bound, as shown in Figure 7. Assuming that the Si—Si bond length found in crystalline silicon is the distance between these two unbonded silicon atoms, that the Si—H bond length is also that found in crystalline silicon and that all four atoms are collinear, this gives an separation distance of 0.531 nm. However, a molecular dynamics simulation using CASTEP of the ‘double T_d’ complex reveals that, in practice, the two silicon atoms move apart in the absence of a bond between them, increasing their separation by ~60% to sit approximately in plane with

Figure 7. The results of a molecular dynamics simulation of the structure of the ‘double T_d’ SiHHSi complex. The two hydrogen atoms are shown in black. They are each bound to a silicon atom. The dotted black line denotes where a bond would have existed between the two silicon atoms in the complex, and the two atoms have moved apart in the absence of a bond between them.
the other three silicon atoms to which each is bound (Figure 7). The two hydrogen atoms in this configuration are then ~0.7 nm apart, which is consistent with NMR data. Recent NMR studies of a-Si:H that has had a large number of defect states created by light soaking suggests that hydrogen undergoes a change in configuration upon defect creation, taking up a new structure in which the two hydrogen atoms are only 0.23 nm apart [28, 29].

Collecting together all of the available experimental evidence, it would appear that defect creation occurs through the breaking of a weak Si—Si bond in the vicinity of a ‘double $T_d$’ SiHHSi complex. The defect state is then stabilized through the localized reconfiguration of the hydrogen atoms into a new state in which their separation distance is reduced. Defect removal then occurs through the breaking of an Si—H bond. The newly mobile hydrogen atom(s) may then passivate dangling bond defects, but it is not clear whether this occurs locally or after a long-range diffusion of hydrogen.

CONCLUSIONS

It has been shown that fully deuterated and fully hydrogenated amorphous silicon TFTs provide an excellent means of quantitatively investigating the defect creation and removal process in these materials. In the case of defect creation, activation energies for defect creation in the range of 0.93 to 0.98 eV are measured with an associated attempt-to-escape frequency of $10^9$ Hz with no discernable difference in stability between the hydrogenated and deuterated materials with similar microstructures. The activation energy for defect removal is $(1.552 \pm 0.003)$ eV and $(1.559 \pm 0.003)$ eV for a-Si:H and a-Si:D respectively which correlates with the activation energy of hydrogen diffusion in amorphous silicon and the fact that the Si—D bond energy is slightly greater than that of the Si—H bond. Furthermore, the attempt-to-escape frequency corresponds to the stretching mode oscillation frequency of the Si—H or Si—D bond. This leads to the conclusion that defect creation is limited by the breaking of an Si—Si bond in the vicinity of an SiHHSi complex, which is most likely to be in the ‘double $T_d$’ configuration. A localized rearrangement of hydrogen atoms then occurs to stabilize the defect state. Defect removal, on the other hand, is limited by the breaking of an Si—H bond to create mobile hydrogen which may then passivate dangling bond defects.

ACKNOWLEDGMENTS

The authors are grateful to Philips Research Laboratories, Redhill, UK, for their financial and technical support for this work and to P. W. Peacock for assistance in setting up the molecular dynamics simulations.
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