Model-simulation of light-induced defect creation in hydrogenated amorphous silicon

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Abstract. The processes of light-induced defect creation in hydrogenated amorphous silicon consist of self-trapping of holes in a weak Si-Si bond adjacent to a Si-H bond, nonradiative recombination of self-trapped holes with electrons, the Si-H bond switching towards the weak Si-Si bond, and hydrogen-hopping or tunneling along the weak Si-Si bond. The Si-H bond switching and hydrogen movements are treated by Monte-Carlo computer simulation in a simple cubic lattice. From the result of \(\langle r^2 \rangle \) vs \(t\) in which \(r\) and \(t\) designate diffusion distance of hydrogen and diffusion time, respectively, the density of light-induced defects is estimated in a good agreement with the observed density.

1. Introduction

The mechanism of light-induced defect creation in hydrogenated amorphous silicon (a-Si:H) has received much attention from viewpoints of physics and applications such as solar cells. Prolonged illumination causes Si dangling bonds (DBs) to be created, so that the conversion efficiency of solar cells decreases. So far the consensus has not yet been obtained for the mechanisms of light-induced defect creation although many models have been proposed. We have already proposed a mechanism of light-induced defect creation [1], in which the breaking of a weak Si-Si bond adjacent to a Si-H bond (specific weak Si–Si bond) and hydrogen movement are key factors, as mentioned below. In this paper, we present model-simulation for the light-induced defect creation process in the following way: A Si-H bond adjacent to a weak Si-Si bond is switched towards the weak Si-Si bond, i.e., hydrogen occupies a central site of the weak Si-Si bond by use of an energy associated with nonradiative recombination of an electron with a self-trapped hole in the weak Si-Si bond under illumination, and then a normal DB is created behind. The switched hydrogen at the central site is bonded to a neighboring Si atom, and then this Si-H bond is switched towards its neighboring Si-Si bond in the same way as before. Such a switching of the Si-H bond is repeated, and a DB having hydrogen at the nearby site (hydrogen-related DB) is created at a certain time \(t\) after the first switching of the Si-H bond occurs. In figure 1, these processes are illustrated in simple cubic lattice sites, in which the Monte Carlo computer simulation of such a Si-H bond switching and diffusion processes is performed. The mutual distance of two types of DBs, i.e., a normal DB and a hydrogen-related DB, has been estimated to be about 13Å from the width of spin packet of the ESR line due to DBs [1].

In Section 2, the Monte-Carlo computer simulation as well as its results are presented. In Section 3, these issues are discussed. In Section 4, a conclusion is drawn.
2. Monte-Carlo computer simulation

Monte-Carlo computer simulation is performed in a simple cubic lattice, that is, different 10 lattices with 300×300×300 sites are attempted. The hydrogen-silicon bond energy distributes with a Gaussian shape of the density of states, as given by

\[
D(E) = \frac{1}{2\pi\sigma} \exp\left[-\frac{(E-E_0)^2}{2\sigma^2}\right]
\]

(1)

where \(\sigma\) and \(E_0\) are the standard deviation and the central energy, respectively. We put

\[E_0 = k_BT_0\] and \(\sigma = k_BT_\sigma\),

(2)

where \(k_B\) is the Boltzmann constant.

The calculated mean square hopping distance of hydrogen, \(<r^2>\), is shown as a function of the number of steps, \(s\), for various lattice temperature, \(T\), in figure 2. The log \(<r^2>\) vs. log \(s\) plot forms a slope in the range of large steps, as shown in figure 2.

\[<r^2> = a s^\alpha,\]

(3)

The value of \(\alpha\) depends on \(T\), as shown in figure 3.

As mentioned in Section 1, the distance between a normal DB and a hydrogen-related DB is \(r = 13\text{Å}\). This distance corresponds to the hopping distance of hydrogen to create two type of DBs. We obtain

Figure 1. A schematic illustration of hydrogen movements in a simple cubic lattice.
from figure 2 that the number of step corresponding to \( r = 13 \text{ Å} \) is 37.4. Thus, the time necessary for creating two types of DBs is estimated from the Si-H bond switching time and the number of steps, i.e., is 37.4. The Si-H bond switching time is estimated to be the reversal of the Si-H bond switching frequency, that is given by

\[
\nu = \nu_0 \exp \left[ -\frac{\Delta E}{k_B T} \right],
\]

where \( \nu_0 \) and \( \Delta E \) are the pre-factor and the barrier height, respectively. We take \( \nu_0 = 1 \times 10^{12} \text{ s}^{-1} \) and \( \Delta E = 40 \text{ meV} \) [2]. For \( T = 300 \text{ K} \), the time necessary for creating two types of DBs, \( \Delta t \), is

\[
\Delta t = \nu_0^{-1} \exp \left[ \frac{\Delta E}{k_B T} \right] \times (\text{number of steps})
\]

\[
= 1.8 \times 10^{-10} \text{ s},
\]

In the following, we consider how many two types of DBs are created through the Si-H bond switching and movement during 1 hr illumination from xenon-arc lamp with infrared cut at 1.3 Wcm\(^{-2} \) with \( G \) (generation rate of free carriers) = \( 1.9 \times 10^{22} \text{ cm}^{-3} \text{ s}^{-1} \) [3]. The light-induced DB creation begins with self-trapping of a hole at a specific weak Si – Si bond. After then, the Si – H bond switching and movement are repeated to create two types of DBs separated by 13 Å, as shown in figure 4. Now, we take the case of 1 hr illumination, during which the above light-induced DB creation process is repeated by \( 2.0 \times 10^{13} (= 3600 \text{ s} / 1.8 \times 10^{-10} \text{ s}) \). It is assumed that eight Si – Si bonds are broken by hole trapping during one period, i.e., the time necessary for hydrogen reaching on the surface of radius 13 Å. Here, the efficiency of bond breaking, \( \eta \), is taken to be 0.1 [4]. The ratio of the self-trapped hole density in specific weak Si – Si bonds to the total density of trapped holes in weak Si – Si bonds, \( \xi \), is taken to be \( 10^{-3} \) at room temperature[4]. The hole density, \( p \), is estimated from (5) in [5] to be \( 1.9 \times 10^{14} \text{ cm}^{-3} \).
Then, the light-induced DB density is given by

\[ N_d = p \xi \eta^8 \times (2.0 \times 10^{13}), \]  

(6)

The above values of \( p, \xi, \) and \( \eta \) are inserted into (6), then we obtain \( N_d = 3.9 \times 10^{16} \) cm\(^{-3}\). This is in a good agreement with the observed value of \( 3.0 \times 10^{16} \) cm\(^{-3}\) [3], as will be mentioned in Section 3.

3. Discussion

First, we discuss the light-induced DB creation considered in the Monte-Carlo computer simulation. The mutual distance between a normal DB and a hydrogen-related DB is estimated to be 13 Å, as mentioned in Section 1. This distance almost corresponds to the atomic configuration of two types of DBs, as shown in Fig. 4. This is of course a typical configuration corresponding to \( r = 13 \) Å. For simplicity, it is assumed that eight weak Si – Si bonds are broken when a hole is self-trapped at each weak bond, as mentioned in Section 2. The observed light-induced DB density has been measured by electron spin resonance measurements for various types of a-Si:H samples and for illumination times, e.g., \( 3 \times 10^{16} \) cm\(^{-3}\), for 1 hr illumination by xenon-arc lamp with infrared cut for device-quality a-Si:H samples prepared at substrate temperature of 250 °C [3].

Secondly, we discuss the temperature dependence of \( \alpha \) in (3). As shown in figure 3, the value of \( \alpha \) tends to 1 above 100 K that is equal to \( T_{\sigma} \), corresponding to almost the full width of half-magnitude (FWHM) of the Gaussian shape in a unit of temperature. This is in contrast with the case of exponential density of states of hydrogen-site energy, in which \( \alpha \) is proportional to temperature [5].

4. Conclusion

Two types of DBs, i.e., a normal DB and a hydrogen-related DB, are created through the Si – H bond switching and movement under illumination. The time necessary for separating two types of DBs with 13Å is estimated from the Monte-Carlo computer simulation in a simple cubic lattice. Using this time, light-induced DB density is estimated and is compared with the observed density in a good agreement.

References

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