

Note on the Positron Annihilation Spectroscopy Measurements in Hydrogenated Amorphous Silicon –Their Interpretation in terms of Light-Induced Defects–

by

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Abstract

The results of the positron annihilation spectroscopy measurements by Melskens et al. (Phys. Rev. B **91** (2015), 245207) in hydrogenated amorphous silicon are interpreted in terms of our model of light-induced defects, i.e., normal dangling bonds and hydrogen-related dangling bonds. As a model of microvoids, a sphere is presented, whose inner surface is occupied by light-induced defects, and whose size is estimated, using the mutual distance between a normal dangling bond and a hydrogen-related dangling bond.

Keywords: Positron annihilation spectroscopy; Amorphous silicon; Defect.

1 Introduction

Light-induced defect creation processes have been investigated during four decades in hydrogenated amorphous silicon (a-Si:H) [1], but they are still unresolved until now. In this paper, we consider recent positron annihilation spectroscopy (PAS) measurements [2, 3] on the basis of our model of light-induced defect creation processes and nature of light-induced defects in a-Si:H [4–6].

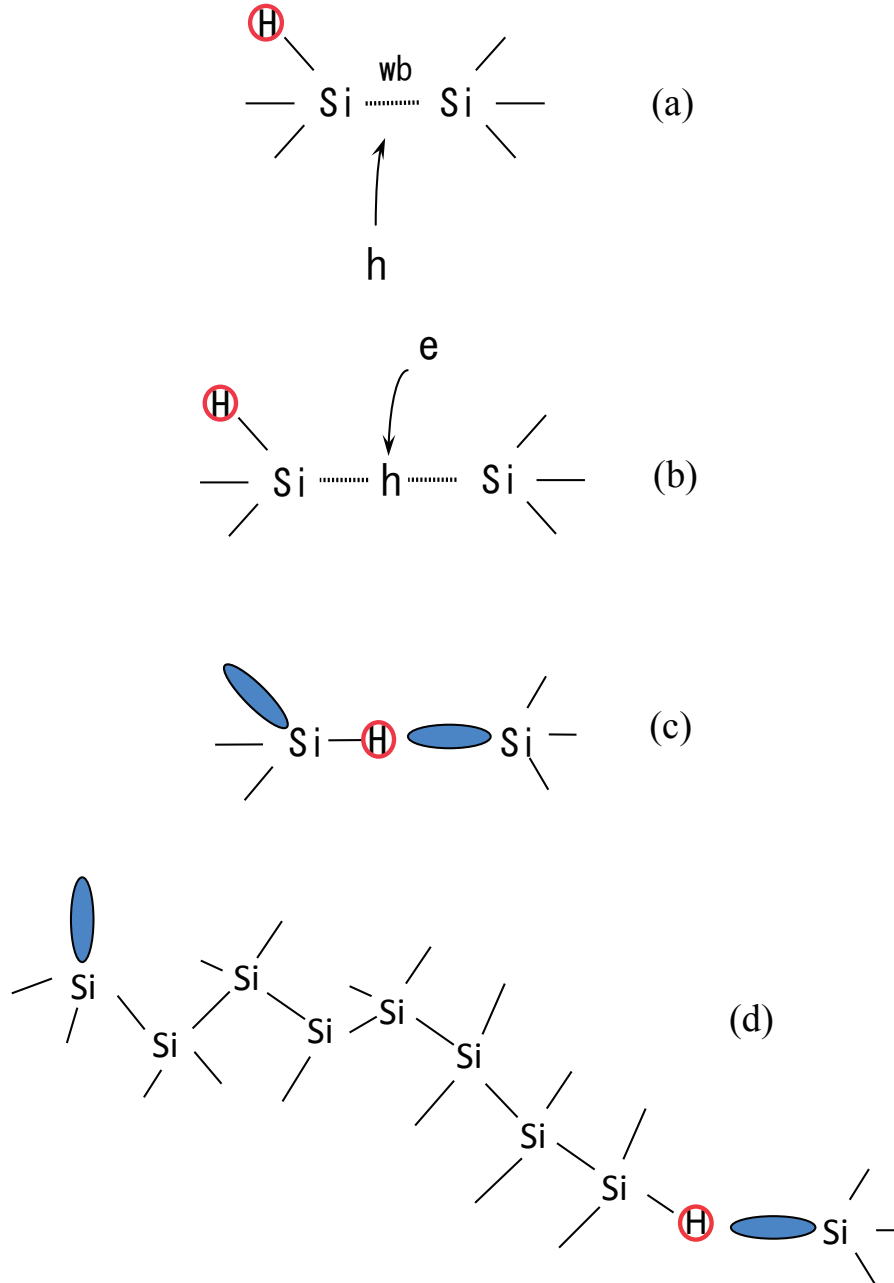


Figure 1: Atomic configurations involved in the formation of two types of dangling bonds, i.e., normal dangling bonds and hydrogen-related dangling bonds, under illumination: (a) self-trapping of a hole in a weak Si-Si bond (wb) adjacent to a Si-H bond, (b) electron-hole recombination at a weak Si-Si bond, (c) switching of a Si-H bond towards the weak Si-Si bond, leaving a dangling bond behind, (d) formation of two separate dangling bonds through hydrogen movement after repeating the processes shown in (a) – (c).

2 Light-Induced Defect Creation Processes

Those light-induced defect creation processes which we have proposed are given below: Under illumination by light with band to band energy, electrons and holes are generated. A hole is self-trapped in a specific weak Si-Si bond that is a weak Si-Si bond adjacent to a Si-H bond (Fig. 1(a)) and

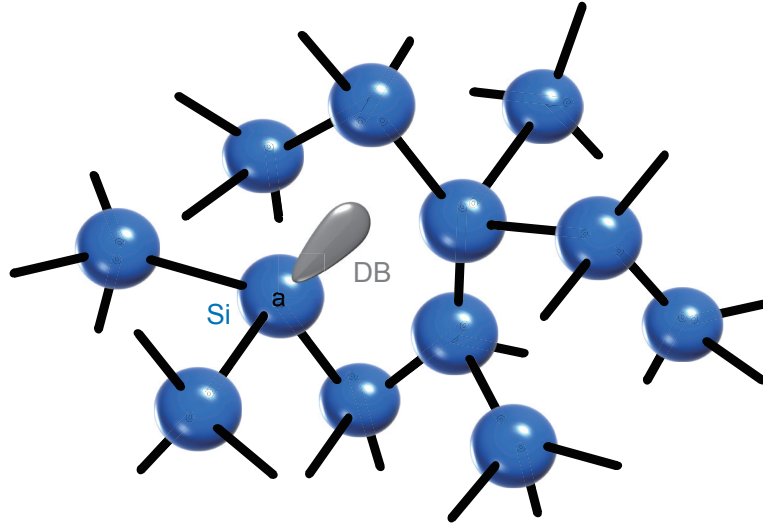


Figure 2(a): Schematic illustration of the normal dangling bond in a-Si:H.

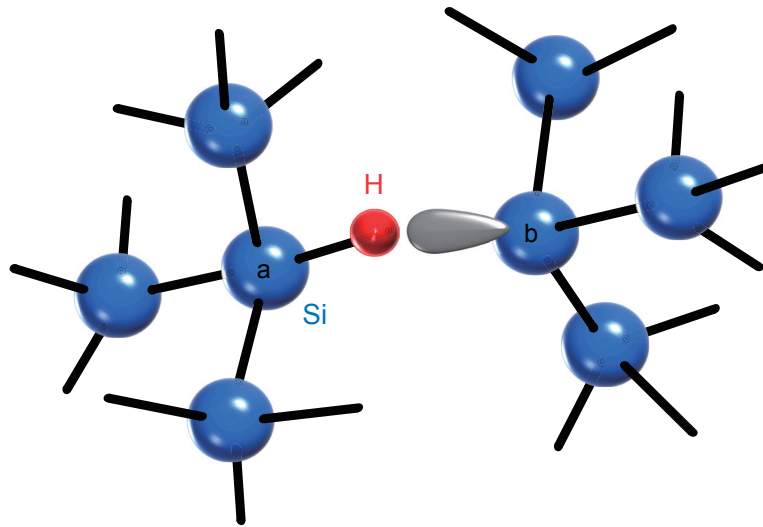


Figure 2(b): Schematic illustration of the hydrogen-related dangling bond in a-Si:H.

then is recombined with an electron most nonradiatively (Fig.1(b)) and eventually the weak bond is broken. Using the recombination energy associated with nonradiative recombination between the electron and the hole, the Si-H bond is switched towards the weak Si-Si bond (Fig. 1(c)). After switching of the Si-H bond (Fig. 1(c)) and breaking of the weak Si-Si bond, the two close dangling bonds created under illumination are separated by movement of hydrogen due to hopping and/or tunneling (Fig. 1(d)) and eventually two separate dangling bonds (Fig. 1(d)), i.e., a normal dangling bond and a hydrogen-related dangling bond are created under illumination, as shown in Fig. 1(d). A couple of a normal dangling bond and a hydrogen-related dangling bond is created in such a way. Some of such two separate dangling bonds become more separate so as to be isolated normal dangling bonds (Fig. 2(a)) and isolated hydrogen-related dangling bonds (Fig. 2(b)), as have been shown by calculations based on the above light-induced creation processes [5]. Detailed accounts on the light-induced defect creation mentioned above have been presented in [4–6].

3 Doppler-Broadening Positron Annihilation Spectroscopy (DB-PAS) Measurements

Melskens et al. [2, 3] have reported the results of the Doppler-broadening positron annihilation spectroscopy (DB-PAS) measurements in a-Si:H. This technique is a powerful means for investigating the size of defects and voids in solids. They discussed the results of DB-PAS measurements along with those of electron-spin echo (ESE) measurements [7]. These measurements were carried out before illumination and after illumination. They prepared a-Si:H films in various conditions, i.e., dilation ratio of hydrogen gas to silane gas R , substrate temperature T_s , gas pressure, reaction power, etc. They have observed that for device-quality films (i.e., dense films $R = 0$, $T_s = 160^\circ\text{C}$), before illumination, the amplitudes of the fast- and slow-decay components of the ESE signal correspond to $N_s = 2.1 \times 10^{15} \text{ cm}^{-3}$ for both and, after illumination, to $N_s = 9 \times 10^{16} \text{ cm}^{-3}$ for both and the values of $S/S_{\text{c-Si}}$ are 1.02 for both before and illumination, where S is called the S parameter defined by the ratio of the top area to the tail area of the electron energy distribution due to the Doppler shift of γ -ray. $S_{\text{c-Si}}$ is the S parameter of crystalline silicon. For instance, if a positron is annihilated with an electron at an atomic vacancy, the value of the S parameter becomes high compared to the case without a vacancy, because the probability of positron annihilation with an inner shell electron in the former case decreases compared to the latter case. Thus, the measurement of the S parameter as a function of depth from the surface of the film provides with us information of the existence of vacancies inside the film.

According to their measurement, the defects in the as-deposited state (i.e., before illumination) exist mostly in the large open volume deficiencies, and after illumination (after light-soaking) the fast-decay component may be mostly linked to light-induced defects in isotopically distributed small open volume deficiencies or linked to isotopically distributed defects present in the matrix which surrounds the open volume deficiencies and which is similar to a continuous random network. The slow-decay component largely corresponds to light-induced defects created in large open volume deficiencies.

Melskens et al.'s results [3] obtained for device-quality a-Si:H films are summarized below: (1) After illumination, the value of $S/S_{\text{c-Si}}$ does not change compared to before illumination. (2) After illumination, the intensity of the slow- and fast-decay components of the ESE signal increases compared to before illumination. The first result indicates that illumination is nothing to do with the formation of small and large open volume deficiencies. The second result suggests that the density of defects responsible for slow- and fast-decay components increases after illumination.

In our model, the fast-decay component is due to a couple of a normal dangling bond and a hydrogen-related dangling bond, and the slow-decay component is due to isolated normal dangling bonds or isolated hydrogen-related dangling bonds in the matrix [8]. In our model, these dangling bonds exist in the matrix that is a continuous random network. Small and large open volume deficiencies may certainly exist in the matrix, as shown from the DB-PAS measurements, but some broken bonds in their inner surface may be terminated by hydrogen atoms or connected by two broken bonds. This is a great difference in the interpretation between two models, that is, our model and Melskens et al. model [3].

In the following, we consider the microvoid whose inner surface sites are occupied by a couple of a normal dangling bond and a hydrogen-related dangling bond and isolated normal dangling bonds and isolated hydrogen-related dangling bonds. For simplicity, we assume the microvoid to be a sphere

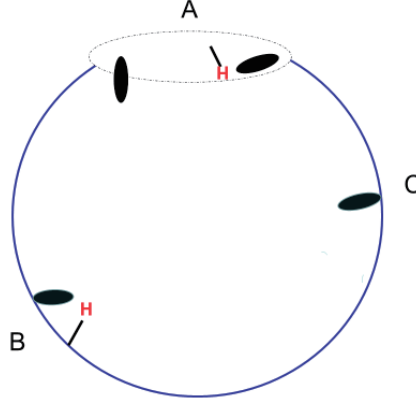


Figure 3: Schematic diagram for the normal dangling bond (n-DB) and the hydrogen-related dangling bond (H-DB) in the inner surface of the sphere. (A) a couple of n-DB and H-DB, (B) H-DB, and (C) n-DB.

such as shown in Fig. 3. The inner surface sites of such a sphere are occupied by a couple of a normal dangling bond and a hydrogen-related dangling bond. The mutual distance between a normal dangling bond and a hydrogen-related dangling bond is $13 \text{ \AA}$ [5], which has been derived from the width of the spin-packet of the ESR line due to dangling bonds. From the distance of $13 \text{ \AA}$, the radius of the sphere r is statistically derived by a formula of the mean distance between two sites is equal to be r/π . Putting the distance of $13 \text{ \AA}$ into the formula, r is estimated to be $40.8 \text{ \AA}$. The radius of the microvoid has not been estimated from the DB-PAS measurements. The above consideration has been performed on the basis of our model of light-induced defects.

Further, we would like to point out the result of the Monte-Carlo computer simulation in a cubic lattice model [9], in which hydrogen can diffuse from site to site in the cubic lattice site to be $13 \text{ \AA}$. The diffusion time necessary for this distance is obtained by Monte-Carlo computer simulation, from which the light-induced dangling bond density can be obtained to be $3.9 \times 10^{16} \text{ cm}^{-3}$ on the basis of our light-induced defect creation model. This value is compared to an observed value of $3.0 \times 10^{16} \text{ cm}^{-3}$ with a good agreement. This means that the mutual distance of a normal dangling bond and a hydrogen-related dangling bond of $13 \text{ \AA}$ is a reasonable value.

4 Discussion

Our model of light-induced defects is based on a couple of two types of dangling bonds, i.e., a normal dangling bond and a hydrogen-related dangling bond. Further, isolated normal dangling bonds and isolated hydrogen-related dangling bonds are also created in the matrix. In this paper, we extend this model to the distribution of light-induced defects over the inner surface of microvoids, as suggested by Fehr et al. [7, 10]. On the other hand, Melskens et al. [3] postulate the existence of open volume deficiencies. Further investigations are necessary for elucidating this issue.

5 Conclusion

In this paper, we interpret reasonably the results of Doppler-broadening positron annihilation

spectroscopy measurement in terms of our model of light-induced defect creation processes and of light-induced defects in a-Si:H. Thus, we conclude that the results of the measurement may support our model by extending the distribution of light-induced defects in the matrix to that over the inner surface of microvoids.

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