Visible Light Irradiation Effects on Atomic-Scale Observations of Hydrogenated Amorphous Silicon Films by Scanning Tunneling Microscopy

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1. Introduction

Hydrogenated amorphous silicon (a-Si:H) films contribute to the electronic industry of today, because they are widely used in various fields such as optical sensors, solar cells, photosensitive materials and thin film transistors. To realize higher performances in these devices, it is essential to control the structure of a-Si:H in an atomic level. For example, a-Si:H films are well known to be degraded during the exposure to intense visible light. It has been predicted that this degradation is related to the creation of dangling bonds, and the change of atomic configurations inside the film during the light exposure. But the atomic configuration of a-Si:H films, or the interaction between a-Si:H and external light has not been clarified yet. Scanning probe techniques are widely spread to investigate surface structures in an atomic level. When the atomic structure of a-Si:H surfaces are clarified with these techniques, peculiar phenomena to a-Si:H such as photodegradation can be understood in an atomic scale. However, only a few attempts have been made so far on amorphous materials, and atomic images on a-Si:H films have not been reported.

In this study, atomic-scale images are obtained on intrinsic a-Si:H films at a negative sample bias by scanning tunneling microscopy (STM) under visible light irradiation. During an observation, monochromatic visible light irradiation (630nm, 1.96 eV) plays an important role to enhance the electric conductivity. It is demonstrated that the light irradiation increased the tunneling current between a probe (Pt-Ir) and an a-Si:H surface at negative sample biases, and the mechanism is discussed.

2. Experimental

Sample preparation

As a substrate, a p-type doped Si(001) wafer was wet-cleaned with HF containing solutions, and the surface was hydrogen-terminated. Thin films of a-Si:H were deposited on the substrate by the plasma chemical vapor deposition (CVD) in which an atmospheric pressure plasma with a rotary electrode was employed. The detailed explanation of the plasma CVD method is described elsewhere [1]. It is reported that dopants near the surface influence the electronic structure of the surface, which makes the analysis of STM images difficult [2]. To avoid this situation, P or B to enhance the electric conductivity was not implanted to the film. Hydrogen terminated a-Si:H surfaces were prepared by dipping in a diluted HF solution after dipping in $H_2SO_4+H_2O_2$. Hydrogen termination on the surface was confirmed by XPS (X-ray photoemission spectroscopy) measurements. Then the sample was transferred into an ultrahigh vacuum chamber for STM. During STM observations with Pt-Ir tips, a background pressure of about 3.0×10^{-8} Pa was achieved with neither thermal treatment nor baking.

I-V characteristics under light irradiation

Figure 1 shows I-V curves (a)with, and (b) without continuous visible light irradiation. In Fig. 1(a), monochromatic light (630 nm) from a Xe lamp (500 W) and a monochromator was irradiated continuously on the a-Si:H surface. The photon energy (1.96 eV) is greater than the measured optical gap of the a-Si:H film ($1.6 \sim 1.7 \text{ eV}$). The intensity of the irradiated light was much weaker than that to induce photodegradation to a-Si:H films.



Fig. 1 I-V characteristics (a) with, and (b) without continuous light irradiation (630 nm) on a 200-nm-thick a-Si:H film.

It is obvious that tunneling current increases dramatically at negative sample biases ($V_{sample} < 0$) with the light irradiation, although I-V characteristics do not change at positive sample biases. Without the light irradiation, the tunneling current at a negative sample bias is low, and the I-V curve shows a rectifying behavior, as shown in Fig. 1(b). If tunneling current is too low to sustain a stable STM feedback, a probe touches a sample surface frequently. Hence, STM observations are performed on a-Si:H surfaces at a negative sample bias under continuous visible light irradiation. *Atomic-scale images on a-Si:H film under irradiation*

Figure 2(a) is a typical STM image (40x40 nm²) on a 20-nm-thick-a-Si:H surface under the continuous light irradiation. The sample bias was set to negative (-2.3 V). Bright dots forming the surface structure are well resolved in

relatively flat areas in Fig. 2(a). A typical close-up image $(2.2x2.2 \text{ nm}^2)$ on the a-Si:H surface is shown in Fig. 2(b). As a reference, the image of the substrate surface (HF-cleaned Si(001)) is shown in Fig. 2(c). The separation between the dots in Fig. 2(b) is quite similar to that between regularly distributed dihydrides shown in Fig. 2(c). Consequently, the bright dots in Fig. 2(b) are supposed to be SiH_n (SiH-, SiH₂-, SiH₃-) in which dangling bonds on the a-Si:H surface are capped with H atoms. Here, a highly-resolved image like Fig. 2(a) and 2(b) was not obtained at a positive sample bias like +2.3 V, or without light irradiation. As shown in Fig. 1, high tunneling current is obtained only when the a-Si:H surface was exposed to the monochromatic light and negative sample biases were applied. It is supposed that the high tunneling current under the monochromatic light irradiation on the intrinsic a-Si:H film achieved stable STM feedback, which enables us to obtain highly-resolved images like Figs. 2(a) and 2(b).



Fig. 2 A typical STM image of (a) 40x40 nm², and (b)2.2x2.2 nm² on the 20-nm-thick a-Si:H film under visible light irradiation. Tunneling current was 0.3 nA. (c) A reference image of 2.2x2.2 nm² of a substrate Si(001) surface after HF cleaning.

Mechanism to increase tunneling current under irradiation

Why does tunneling current increase dramatically only at negative sample biases by the external light irradiation? To answer this question, the energy band diagram of the probe (Pt-Ir) and the a-Si:H surface, as shown in Fig. 3, is analyzed. Parameters were taken from literatures [3],[4].

It is suggested that the increased tunneling current at negative sample biases in Fig. 1(a) is induced by tunneling of photoexcited electrons (as minority carriers) to the probe at the Schottky junction between a Pt-Ir tip and an a-Si:H film. At first, let us consider how tunneling occurs without the light irradiation. It is likely that holes contribute to the electric conduction in a-Si:H films although the a-Si:H film itself is intrinsic, because a-Si:H films were deposited on a p-typed Si substrate. Figures 3 and 4(a) show that a Schottky barrier to holes is formed at the tunneling junction between the probe (Pt-Ir) and the sample (a-Si:H). In this case, a rectifying behavior is expected. This corresponds to the experimental result shown in Fig. 1(b). Here, when photons with greater energy than the







Fig. 4 Schematic of the energy band diagram between the probe (Pt-Ir) and the sample (a-Si:H) under light irradiation.
(a) At zero external bias. Schottky barrier(_{Bp}) to holes is formed at the tunneling junction. (b) In the forward bias (V_{sample}>0). (c) In the reverse bias (V_{sample}<0).

optical gap of the a-Si:H film arrive at the tunneling junction, they are absorbed inside the a-Si:H film to create electron-hole pairs. Created electron-hole pairs are separated by the band bending (electric field) in the a-Si:H film. In the forward bias ($V_{sample}>0$), photoexcited holes reach the a-Si:H surface. However, tunneling current does not change by the light irradiation, because holes exist much at the a-Si:H surface, as shown in Fig. 4(b). In the reverse bias ($V_{sample}<0$), photoexcited electrons (as minority carriers) are drifted to the a-Si:H surface through the conduction band at the Schottky structure. They tunnel to the empty states of the Pt-Ir tip to increase tunneling current dramatically as shown in Fig. 4(c). This corresponds to the experimental result shown in Fig. 1(a).

3. Conclusions

Atomic-scale images are obtained on an intrinsic a-Si:H film at negative sample biases with STM under monochromatic visible light irradiation. The increased tunneling current under the irradiation is induced by a Schottky structure at the tunneling junction and photoexcited electrons. This realizes stable STM observations. This work represents an initial step toward an atomic-scale understanding of a growth process and photodegradation on a-Si:H films.

References

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