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Interaction of SiH_3 radicals with deuterated (hydrogenated) amorphous silicon surfaces

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Abstract

Interactions of SiH_3 radicals with surfaces of deuterated amorphous silicon (a-Si:D) and hydrogenated amorphous silicon (a-Si:H) films were studied using attenuated total reflection Fourier transform infrared spectroscopy and molecular-dynamics simulations, respectively. SiH_3 radicals abstract surface silicon deuterides through an Eley–Rideal abstraction reaction. Surface deuteride abstraction occurs on the same time scale as SiH_3 insertion into Si–Si bonds over the substrate temperature range of 60–300 °C. Some fraction of SiH_3 adsorbing on the a-Si:D/a-Si:H films dissociates and releases H into the subsurface. These observations are consistent with the temperature independent reaction probability of SiH_3 and the temperature dependent smoothening mechanism of a-Si:H thin films.

Keywords: Amorphous surfaces; Amorphous thin films; Chemical vapor deposition; Plasma processing; Silane; Silicon; Surface chemical reaction

1. Introduction

Hydrogenated amorphous silicon (a-Si:H) thin films used in photovoltaic devices and thin-film transistors for flat panel displays are deposited from SiH_4 containing plasmas [1,2]. The microstructure and electronic properties of plasma-deposited a-Si:H films depend strongly on the interactions of reactive radicals produced in the discharge (SiH_x: $0 \leqslant x \leqslant 3$, H) with the film surface [2,3]. Of the radicals that impinge on the a-Si:H growth surface, SiH_3 is believed to be the

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dominant precursor for device-quality a-Si:H film growth [4]. There are several key observations in a-Si:H film deposition, for which the microscopic mechanisms are not yet completely understood. For example, surfaces of the a-Si:H films deposited under conditions where SiH_3 is the dominant precursor are remarkably smooth (~10 Å root-mean-square roughness). The smoothness of these device-quality a-Si:H films is attributed to the high mobility of SiH_3 on an H-terminated surface [5] which has a very low fractional dangling-bond coverage ($\sim 10^{-2}$–10^{-3}) [6]; the mobility of SiH_3 on a-Si:H surfaces has been confirmed by molecular-dynamics (MD) simulations [7]. Several experiments have also shown that the overall surface reaction probability, $\beta \sim 0.3$ [4,5,8–12], for SiH_3 is independent of the deposition temperature at temperatures below 400 °C [4,5,11,12].

A better knowledge of the various reactions of SiH_3 with a-Si:H surfaces is required to address these outstanding issues in a-Si:H deposition. In this article, we report on the reactions of SiH_3 with an a-Si:D surface examined using surface-sensitive in situ attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopy [13,14]. We also discuss MD simulation results for the dissociative adsorption of SiH_3 radicals on the a-Si:H surface and the subsequent release of H atoms into the subsurface region of the a-Si:H film, which corroborate our experimental observations. In our experiments, we have used a-Si:D films in order to observe the replacement of D atoms in the film with H atoms from SiH_3 using infrared (IR) spectroscopy.

2. Experimental

The experiments were conducted in a high-vacuum parallel-plate capacitively-coupled plasma reactor with equipment for in situ ATR-FTIR spectroscopy. The ATR-FTIR setup is identical to that described in a previous publication [15]. In this study, the plasma was generated by applying radio frequency (rf) power at 13.56 MHz between two stainless-steel parallel plates. The distance between the parallel plates was 4 cm and the applied rf power was 20 W. a-Si:D films were deposited on GaAs substrates placed on the grounded electrode, whose temperature was maintained at 300 °C during the 20-min film deposition time. The flow rate of SiD_4 (2% SiD_4, 98% Ar) into the plasma chamber was 25 standard cm^3/min, while the pressure was maintained at 50 mTorr. After deposition of the a-Si:D films, their surface was exposed to SiH_3 radicals produced by thermally dissociating SiH_4 on a resistively heated tungsten filament as shown schematically in Fig. 1. Thermal dissociation of SiH_4 produces other radicals, such as Si and H, in addition to SiH_3 [16] and care must be taken to separate SiH_3 from the other radicals. To accomplish this, the line of sight between the hot filament and the GaAs substrate was blocked with a shutter and

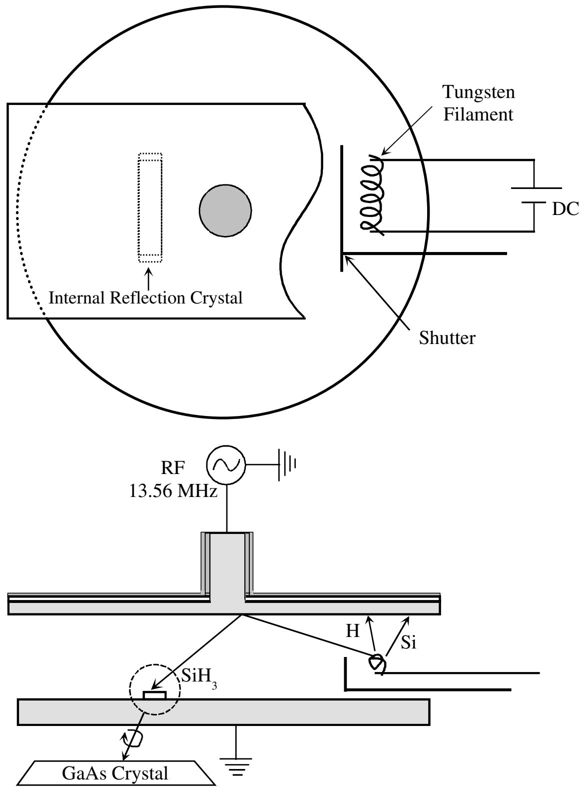

Fig. 1. Top and side view of the experimental setup for SiH_3 exposure of a-Si:D films deposited using a parallel-plate capacitively-coupled plasma. SiH_3 exposure was through the dissociation of SiH_4 on the hot wire with the line of sight between the GaAs substrate and the hot wire blocked with a shutter. This eliminated radicals other than SiH_3 also produced on a hot filament, such as Si and H, from reaching the substrate.