

Hydrogen incorporation in a-Si:H - growth studies on an Expanding Thermal Plasma

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At a rate of 10 nm/s a-Si:H has been deposited with an AM1.5 photoconductivity of $6 \times 10^{-5} \Omega^{-1} \text{cm}^{-1}$ and a photoresponse of 2×10^4 using a remote argon/hydrogen plasma. Because of the pressure gradient between the plasma source -a DC thermal arc typically operated at 0.5 bar and 5 kW- and the deposition chamber -pressure is 0.2 mbar-, a plasma jet is created with a flow velocity of about 10^3 m/s. Near the plasma source, typically 600 sccm of silane is injected into the jet (flow about 4 slm).

In order to understand the possible contribution of the flux of atomic hydrogen towards the substrate, a number of isotope studies have been carried out: in one series, the hydrogen in the feedgas was replaced by deuterium, and in another series the silane was replaced by SiD_4 . A number of observations are done:

1. In the $\text{Ar}/\text{D}_2/\text{SiH}_4$ experiment, the $\text{D}/(\text{H}+\text{D})$, as determined by ERDA, was approximately 0.10; in the cross-experiment with $\text{Ar}/\text{H}_2/\text{SiD}_4$ this ratio was approximately 0.90. From this we can conclude that by far the dominant part of the hydrogen remaining in a-Si:H originates from the silane radical but that there still is a contribution from the atomic H (or D) in the plasma.
2. In the $\text{Ar}/\text{D}_2/\text{SiH}_4$ experiment, the formation of deuterated silanes is observed using a mass spectrometer. It can be shown that the $\text{SiH}_3\text{D}/\text{SiH}_4$ ratio in the deposition chamber is about 0.04. If SiH_3D and SiH_4 are assumed to behave identically in the plasma, the gas phase contribution of deuterium to the film would yield a $\text{D}/(\text{H}+\text{D})$ ratio of less than 0.01. The dominant deuterium incorporation mechanism appears to be $\text{H} \leftrightarrow \text{D}$ exchange at the surface. This suggests that the H (or D) flux to the substrate is of the same order of magnitude as the flux of silane radicals.
3. The behavior of the film refractive index -and thus the corresponding hydrogen or deuterium content- as a function of the substrate temperature is identical for the $\text{Ar}/\text{H}_2/\text{SiH}_4$ and the $\text{Ar}/\text{H}_2/\text{SiD}_4$ series; the tested range is from 100 to 500 °C. This implies that the responsible mechanism, a thermally activated cross-linking reaction between silicon atoms releasing hydrogen molecules, is independent of the H or D isotope.