

## **MICROSTRUCTURE OF HELIUM DILUTED a-Si:H PREPARED BY D.C. PECVD**

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### **ABSTRACT**

This work investigates the effect of helium dilution of silane on the microstructure of plasma enhanced chemical vapour deposition (PECVD) hydrogenated amorphous silicon (a-Si:H) deposited on c-Si substrates. The a-Si:H thin films studied were prepared by d.c. PECVD from the discharge of helium diluted silane. Gas mixtures containing different helium to silane flow-rate ratios have been used to produce these films. The films have been analysed using X-ray diffraction, infrared transmission spectroscopy and atomic force microscopy (AFM). The X-ray diffraction results clearly indicate the presence of nanocrystalline structures within the amorphous structures of the film when the helium to silane flow-rate ratio was between two and four. However, further helium dilution resulted in a purely amorphous film structure as in films produced from the discharge of pure silane. The chemical bonding properties, microstructure parameter and surface morphology of the films were obtained from the infrared transmission spectra of the films. The surface morphologies of the films were analyzed from the AFM images of the films. The effects of the presence of nanocrystalite structures in the film on these properties were investigated.

### **INTRODUCTION**

The hydrogenated amorphous silicon films are recognized as attractive semiconductor materials because of the use of these films as highly-sensitive photodetectors or photoreceptors in electrophotography. Recently, the characterization of these films with helium diluted silane has become more important, since microcrystalline structure of the amorphous materials with very interesting properties can be produced. For instance, the combination of amorphous and crystalline silicon in the micromorph tandem cell is found to improve stabilised efficiency up to 10.7% [1]. Knights et al [2] distinguished that the coarseness of the microstructure was greatly dependent on silane dilutant. Several workers have studied the microstructure of thin films [3]. The general conclusion is that the helium dilution approach can be used as an alternative to hydrogen dilution for making microcrystalline-silicon thin films.

## EXPERIMENTAL PROCEDURES

The a-Si:H samples described in this paper are deposited by in-house horizontal d.c. plasma glow discharge. Films have been grown through thermal decomposition of silane ( $\text{SiH}_4$ ) in a 10 cm long quartz tube having two electrodes 5 mm apart. The deposition parameters useful to control the growth kinetics are pressure, substrate temperature and ionisation current. The pressure was fixed at 1.5 mbar, while the temperature and ionisation current was maintained at  $200^\circ\text{C}$  and 10mA respectively. High-resistivity polished crystalline-silicon (c-Si) wafers have been chosen as substrates for measuring infrared-absorption spectra. Surface structure was studied by means of atomic-force microscopy (AFM) in air. Crystallinity, in turn, was investigated by glaze-angle X-ray diffraction.

## RESULTS AND DISCUSSIONS

The absorption spectra of a-Si:H of all samples are shown in figure 1. From the spectra, as helium was introduced into the system, the spectra showed slight changes where the stretching-mode absorption band was observed to shift towards lower wave number, i.e. from  $2038\text{ cm}^{-1}$  and  $2110\text{ cm}^{-1}$  (sample with pure silane) to around  $2020\text{ cm}^{-1}$  and  $2096\text{ cm}^{-1}$  respectively for helium diluted samples. Both hints are attributed to an important changes in the density of  $\text{SiH}_2$  and/ or  $(\text{SiH}_2)_n$  groups.

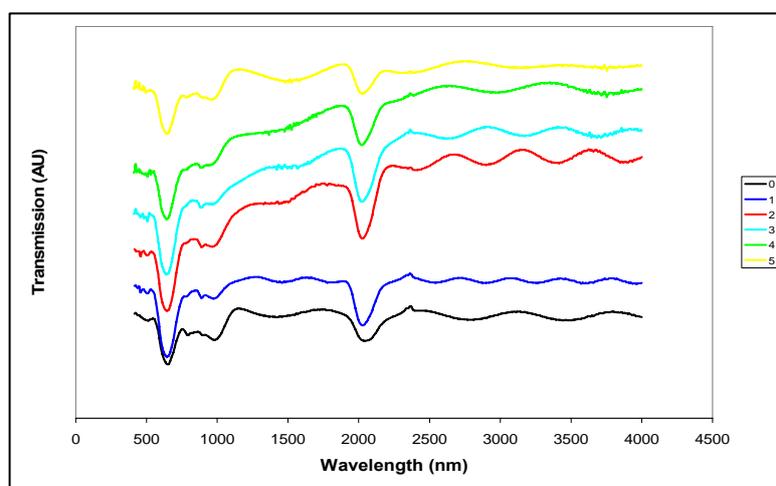


Figure 1: The FTIR transmission spectra of a-Si:H films prepared from pure silane and helium diluted silane at different helium to silane flow-rate ratio

Figure 2 shows the variation of the integrated intensities at  $2000\text{ cm}^{-1}$  and  $2090\text{ cm}^{-1}$  with helium to silane flow-rate ratio. Absorption peaks at  $2000\text{ cm}^{-1}$  and  $2090\text{ cm}^{-1}$  indicate the presence of Si-H and Si-H<sub>2</sub> stretching modes respectively. As could be observed from the figure, the integrated intensity of both bands show different behaviour as soon as helium is introduced into the silane plasma where  $I_{\text{SiH}_2}$  decreases significantly while  $I_{\text{SiH}}$  increases at this stage. However, as the helium to silane flow-rate ratio increases further, the integrated intensity of both bands showed similar trend where both intensities decreases as the flow-rate ratios increases. High helium dilution also reduces impurity atoms like O and N to be bonded to Si

atoms. This is clearly seen from figure 1 where the absorption peak at  $1000\text{ cm}^{-1}$  is decreased when the helium to silane flow-rate ratio is 5.

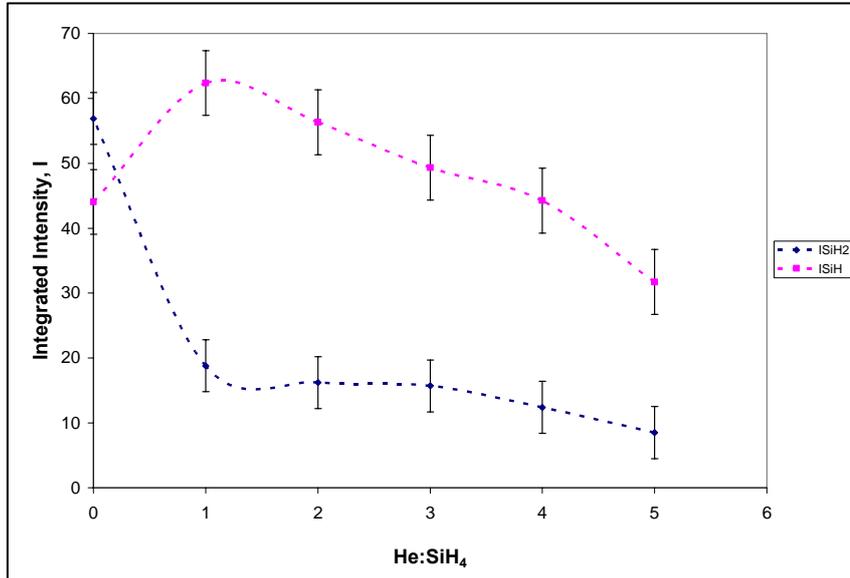


Figure 2: Variation of the integrated intensities at  $2000$  and  $2090\text{ cm}^{-1}$  with helium to silane flow-rate ratio.

Figure 3 shows the microstructure parameter, R with helium to silane flow-rate ratio. From the figure, the microstructure parameter decreases significantly when the helium gas was introduced into the silane plasma. With these results, it can be concluded that helium hindered the formation of microstructures in the film.

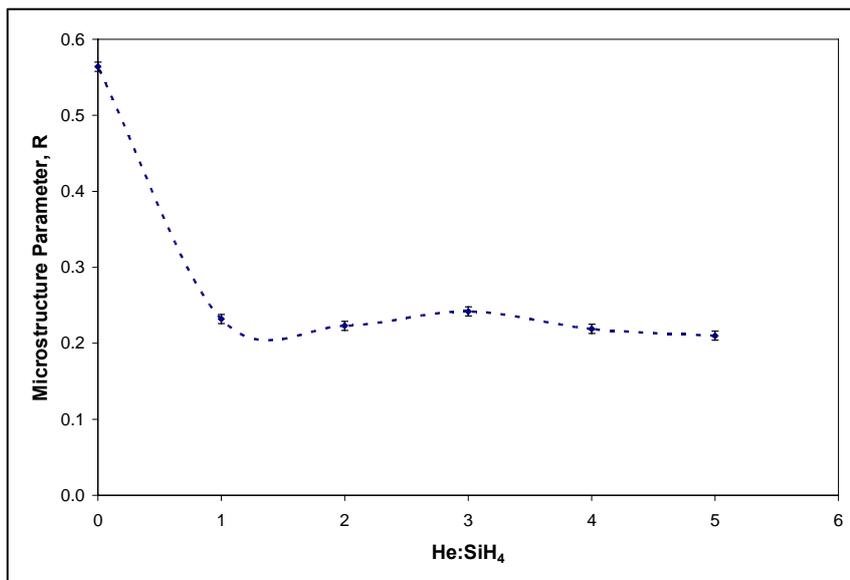


Figure 3: Variation of microstructure parameter, R with helium to silane flow-rate ratio

Figure 4 presents the X-ray diffractograms (XRD) of the a-Si:H films on c-Si substrates prepared from pure silane and helium diluted silane at different helium to silane flow-rate ratio. Evidence of microcrystallinity is observed for films prepared at helium to silane flow-rate ratio of 2, 3 and 4. The peaks are observed at  $28.4^\circ$  and  $56.1^\circ$  which correspond to (111) and (311) planes of Si crystal respectively. The average crystallite size corresponding to this peak as calculated using Scherrer's equation for films prepared at helium to silane flow-rate ratio of 2, 3 and 4 are 24, 23 and 22 nm respectively.

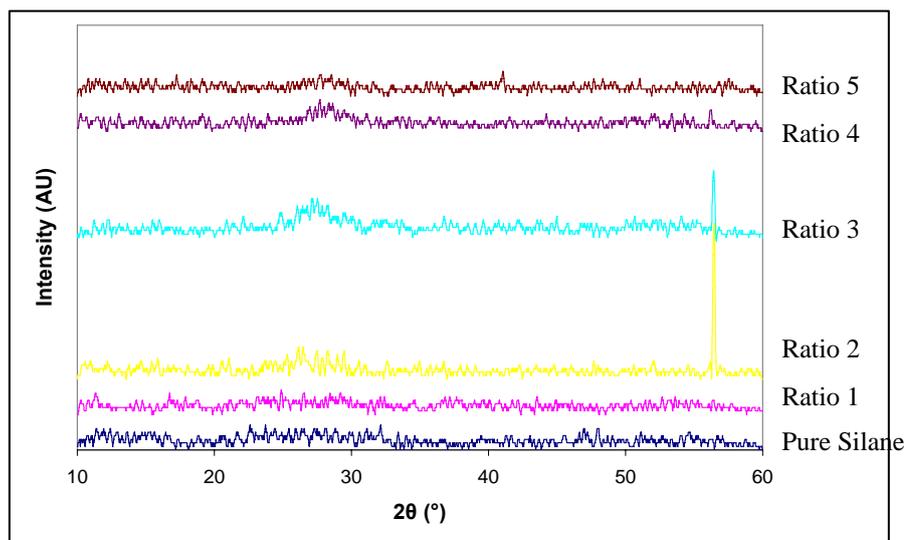
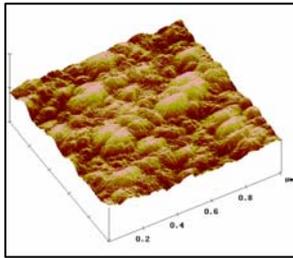
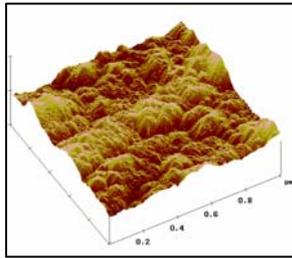


Figure 4: XRD of a-Si:H films prepared from pure silane and helium diluted silane at different helium to silane flow-rate ratio

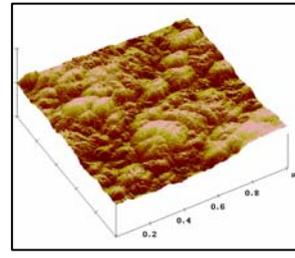
The AFM images of the a-Si:H films studied in this work are displayed in figures 5. Figure 5(a) displays the AFM images scanned over  $1 \times 1 \mu\text{m}^2$  area of a-Si:H films prepared from pure silane. The granular features appear to be sharp and jagged. The granular structures are clustered together and is formed by  $(\text{SiH}_2)_n$  bonds as confirmed from figure 2 where the concentration of  $\text{SiH}_2$  bonds are higher than the Si-H bonds in these films. The clusters form ridges separated by narrow valleys in some parts. From figure 2, these films have higher concentration of Si-H bonds as compared to  $\text{Si-H}_2$  bonds. Thus these clusters are actually Si-H bonds clustered together resulting in  $(\text{Si-H})_n$  bonds. The higher deposition rate for films on c-Si substrates contribute to the formation of long ridge like features on the AFM image. Figure 5(e) and (f) shows the surface morphology of a-Si:H films prepared from helium dilution of silane at helium to silane flow-rate ratio of 4 and 5 respectively. The granular clusters decreasing in size as compared to the film prepared using helium to silane flow-rate ratio of 3 (figure 5(d)). These features is consistent with the results featured from the infrared spectroscopy results in figure 2 where Si-H bonds are more dominant than  $\text{Si-H}_2$  bonds in these films and the concentration of Si-H bonds in the films are also smaller than the film prepared from lower helium to silane flow-rate ratio. Thus, clustering of Si-H bonds is reduced and more isolated Si-H bonds are present forming a very homogenous film structure.



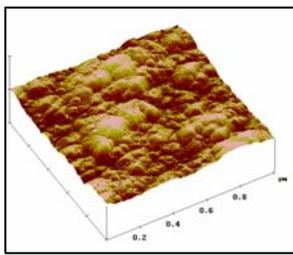
(a) Pure silane



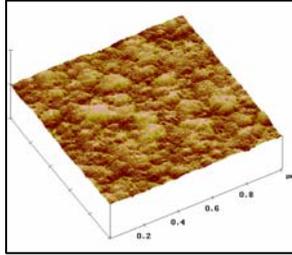
(b) He:SiH4 = 1



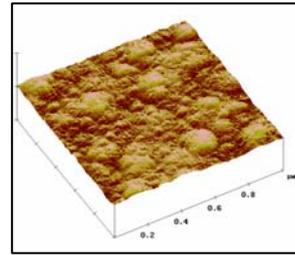
(c) He:SiH4 = 2



(d) He:SiH4 = 3



(e) He:SiH4 = 4



(f) He:SiH4 = 5

## CONCLUSIONS

The microscopic structure of thin films made by PECVD of pure silane and helium diluted silane at different helium to silane flow-rate ratio has been investigated. AFM, XRD and IR spectroscopy have rendered mutually consistent results with a number of more or less coalescent microcrystals are embedded in an amorphous tissue.

## ACKNOWLEDGEMENTS

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