Optical properties of sputter deposited amorphous hydrogenated silicon films

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Abstract: Optical properties of room temperature microwave plasma pulsed DC sputter deposited amorphous hydrogenated silicon are presented. Results show controllable and reproducible reduction in absorption edge and refractive index with increasing hydrogen concentration.

OCIS CODES: (310.1860) Deposition and fabrication; (310.3840) Materials and process characterization; (310.1860) Thin films, optical properties

1. Summary

Evaporated or sputtered amorphous silicon without hydrogen (aSi) is a material containing a high concentration of dangling and weak covalent bonds (of the order of 10^{19} cm^{-3} [1] and 3 x 10^{21} cm^{-3} [2] respectively). Moreover, the electron energy levels of the dangling bond lie in between the bonding (valence band) and antibonding (conduction band) and give high optical absorption at high wavelength (typically 1um – [3]), precluding use of deposited aSi as an optical thin film material for wavelengths < 1um.

It has been demonstrated that the midgap electronic density of states in amorphous silicon can be reduced by several orders of magnitude when hydrogen is introduced during preparation (deposition) of the material - hydrogen passivates the dangling bonds and reducing concentration to typically 10^{16} cm^{-3} [4]. Hydrogenated amorphous silicon (a-Si: H) has properties which are similar to that of crystalline semiconductors [4], with the hydrogen in a-Si: H responsible for the fact that low defect densities can be obtained compared to pure a-Si. However, hydrogen not only saturates the dangling bonds and decreases the density of defect states but also play active roles in reducing the structural disorder, enlarging the band gap [5] and consequently shifting the absorption edge towards lower wavelengths in line with broadening of the optical gap.

Therefore, to make aSi material adaptable for optical usage at wavelengths < 1um, the presence of hydrogen in the network of a-Si is necessary [6].

2. Experimental Results

Deposition was carried out using a pulsed DC reactive sputtering process with microwave plasma for chamber pre-conditioning and substrate pre-clean. The deposition system uses a horizontal axis rotating drum in which deposition of each layer can be achieved with multiple passes across a rectangular planar DC magnetron source and assisted microwave plasma region [7]. Drum rotation speed is such that one to two monolayers is deposited per pass across the magnetron target. Controlled hydrogen introduction was via a hydrogen generator. Pulsed DC sputtering is employed to suppress arcing, necessary to ensure that required coating cosmetic quality is achieved.

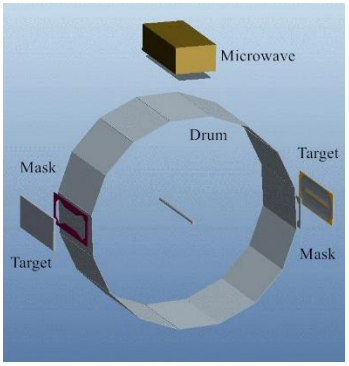

Fig.1. Schematic of Microdyn

Deposition conditions provided in following table – primary variable is hydrogen flow with power and current ranges shown.

Table1: Hydrogenated Silicon Deposition Conditions

Ar Flow (sccm)	H_2 Flow (sccm)	Power (kw)	Current (A)	Voltage (V)	Pulsed DC Frequency (KHz)	Preclean MW Power (kw)	Preclean Time (Mins)
190	0 to 15sccms	5.1 to 7.40	9.64 to 7.40	530	54	3	3

Spectral Transmittance & Optical Constants

Spectral tranmittance is show in Figure 2 – measurements using Hitachi visible/ near infra red spectrophotmeter as a function of hydrogen flow during deposition. As can be seen absorption edge moves towards shorter wavelengths (increased bandgap) in accord with reducing dangling bond density..

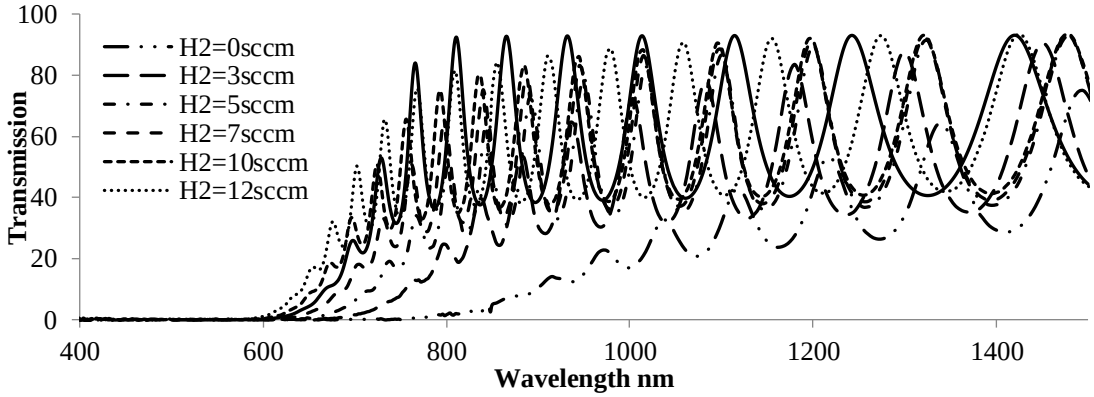

Fig.2. Spectral Transmittance

Figures 3 and 4 indicate refractive index and absorption coefficients as a function of hydrogen flow, derived from measured spectral photometric data shown in Figure 2.

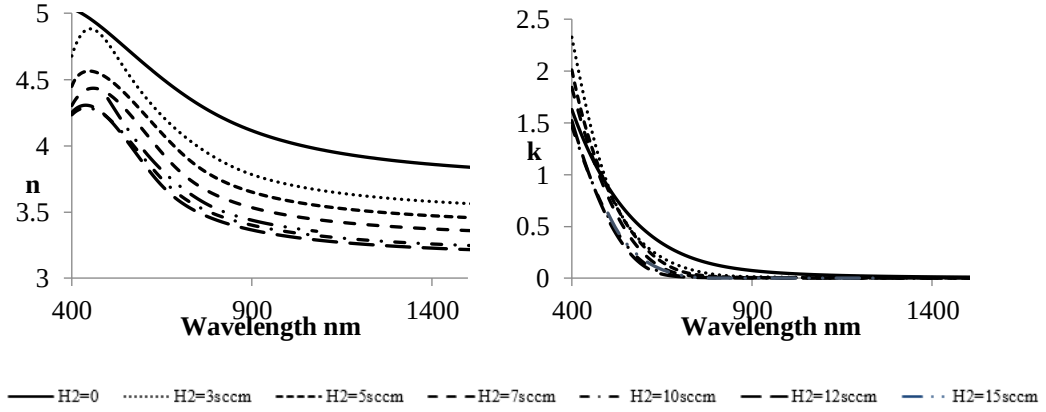

Fig.3. n v Wavelength

Fig.4. k v Wavelength

Bandgap

The optical gap values are determined using the OJL interband transition model for amorphous materials [7]. Assume in this case that the valence band and conduction are parabolic and the value of bandgap energy (E_G) with an absorption coefficient [Eq 1: α(ω); ω = oscillator frequency]

$$\alpha(\omega) \sim \frac{1}{\omega}(h\omega - E_0)^2 \ldots\ldots\ldots\ldots (1) \qquad \sqrt{\omega\alpha(\omega)} \sim h\omega - E_0 \ldots\ldots\ldots\ldots (2)$$

Hence a plot of Eq 2 versus energy should lead to a straight line whose intersection with the y-axis gives E_G , often used to characterize the optical properties of amorphous materials. values of E_G for all samples are presented in column 3 of Table 3.

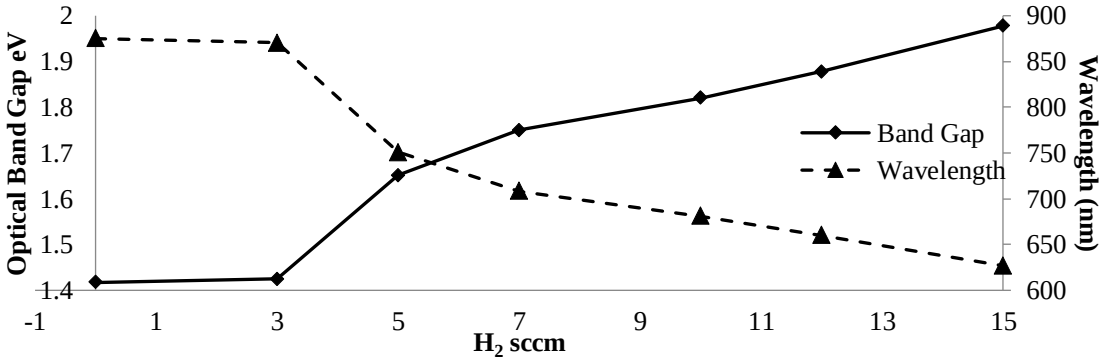

Fig.5. Bandgap (in nm) v Hydrogen flow

3. Conclusions

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