WIDE OPTICAL GAP BINARY Si:H ALLOYS PREPARED BY GLOW DISCHARGE OF DISILANE

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Physical properties of hydrogenated amorphous silicon (a-Si:H) depend greatly on both the incorporated hydrogen content and the Si-H bond configuration. At the highest hydrogen content limit, that can be realized by the polysilane $(SiH_2)_n$ structure, extremely different physical properties are expected. Up to the present, one group, Wolford et al.¹⁾, have reported on a preparation technique for the polysilane. However, the structure and the relation between the microscopic structure and the macroscopic physical quantities have not been clarified yet.

This letter presents binary Si:H alloys having large optical gap values, up to 2.4 eV, prepared by the glow discharge of disilane. The microscopic structure of the films was investigated by infrared absorption techniques. The relations between $(SiH_2)_n$ chain length, Si-H bond length, and physical properties are discussed.

Glow discharge conditions were selected to ensure a successive growth of SiH₂. Disilane was essentially used because it is dissolved into monosilane and SiH₂. To obtain this dissociation homogeneously, the RF power was set at an extremely low level $(2X10^{-3}W/cm^2)$. The substrate was held at very low temperature (220-370K) during deposition in order to prevent hydrogen diffusion and adsorption, which take place above 400K. These conditions are quite different from those for solar cell preparations.

Figure 1 shows the relation between the substrate temperature and the optical gap. The optical gap is quite sensitive to the substrate temperature. By cooling the substrate down to 220K, the 2.4 eV optical gap value was obtained. This value is greater by 0.6 and 0.37 eV than those of the previously obtained films prepared by glow discharge of monosilane and disilane¹⁾, respectively. As a result of a wide optical gap, the present binary alloys showed a visible (red-orange) photoluminescence at room temperature. The spectrum had a peak near 0.8 μ m and a broad band from 0.5 μ m to above 1 μ m infrared region.

The infrared absorption spectrum for the present typical specimen is shown in Fig.2. Stretching absorption peak is shifted from 2000 $\rm cm^{-1}$

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to 2100 cm⁻¹ due to SiH₂ or $(SiH_2)_n$ group formations²). The absorption peaks near 850 and 890 cm⁻¹ relevant to $(SiH_2)_n$ wagging and $(SiH_2)_n$ or SiH₂ bending modes²⁾, respectively, are also observed. It should be noted that only near-neighbor pairs of SiH2 or large chain segment $(SiH_2)_n$ contribute to a strong absorption near 850 cm⁻¹.

Figure 3 shows the infrared absorption gravity-center for stretching vibrations and the peak absorption coefficient ratio $\alpha(850 \text{ cm}^{-1}) / \alpha(890 \text{ cm}^{-1})$ as a function of the optical gap. The frequency shift for stretching vibrations and the change in the $\alpha(850 \text{ cm}^{-1})/\alpha(890 \text{ cm}^{-1})$ value indicate the change in the Si-H bond

length and the $(SiH_2)_n$ chain length²⁾, respectively. The origin of the change in the Si-H bond length may be effective electronegativity differences arising from the change in the (SiH₂)_n chain length. From Fig.3, it can be said that the present increase in the optical gap value is caused by the increase in the Si-H binding energy which comes from the formation of large chain segments, (SiH₂)_n.



Fig.2 Infrared absorption spectrum for a specimen prepared from disilane at 298 K.







Fig.3 Infrared absorption gravitycenter for stretching vibrations ω and peak absorption coefficient ratio $\alpha(850 \text{ cm}^{-1})/\alpha(890 \text{ cm}^{-1})$ as a function of optical gap E_q^{opt} . References; 1) D.J.Wolford et al., Appl.Phys.Lett.42(1983)369.

2) G.Lucovsky et al., Phys.Rev. 19(1979)2064.