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Effect of Hydrogenation on Optical Transmission and Energy Bandgap of Mg/Al Thin Films

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***Abstract*-Bilayer Mg/Al (150nm) thin film were prepared by using D.C. magnetron sputtering unit. The prepared films were rapid thermal annealed (RTA) using halogen lamp to get a homogeneous mixture of bilayer thin films. To see the effect of hydrogenation on optical properties of Mg/Al thin films, hydrogen gas was introduced at different hydrogen pressure (20 & 40 psi) in the hydrogen chamber, where samples were kept. The UV–Vis transmission spectra of thin films with and without hydrogenation were carried out at room temperature in the visible range of wavelength (300 to 800nm). The variation in the optical band gap was noted after hydrogenation and found to be increased with hydrogen pressure. Hence it was suggested that optical band can be tailored using hydrogen gas in thin films structure. All investigations indicates that Mg/Al thin films can be used for hydrogen storage purpose.**

***Index Terms*- Thin Film, Annealing, Hydrogenation, Transmission, Energy Band gap.**

I. INTRODUCTION

Metal hydrides find a wide range of applications of which the most prominent is reversible hydrogen storage. Hydrogen is the most abundant element on earth, scores over all renewable fuels regarding reversibility, energy density and compatibility with the environment [1, 2]. The behavior of hydrogen in metals has attracted scientific attention for many decades and is interesting from both basic research and technological points of view. Most of hydrogen's interesting properties relate to the high mobility of the hydrogen atoms, which reaches to the values similar to those of ions in aqueous solutions. This high mobility exists because the hydrogen atoms occupy interstitial positions in the host lattice due to an interstitial diffusion mechanism and the contribution from quantum-mechanical tunneling [3]. Metal hydride technologies have reached more practical and applied stages in recent years.

The hydriding / dehydriding kinetics of metal hydrides are relevant to areas of design and applications of various metal hydride devices, especially in energy conversion devices such as heat pumps, refrigerators, automobiles, power generators, batteries and thermal energy storage units [4].

Mg is considered to be one of the most promising materials for hydrogen storage. In spite of the fact that MgH_2 satisfies the requirement set by the U.S. Department of Energy, with a theoretical capacity of 7.6 wt. % hydrogen, lightweight and low cost. Its high thermodynamic stability, resulting in a low partial hydrogen pressure at ambient temperatures, prevents it from being adopted as hydrogen storage material. Moreover, MgH_2 suffers from slow hydrogenation kinetics [5]. The problem with using magnesium as a storage material is that it has high binding energy with hydrogen, since it desorbs hydrogen at high temperature (300-350^{o}C). Alloying of magnesium with transition metals can result in a substantially improved dissociation activity due to the presence of d-electrons in transition metals [6]. Alloys of Mg with the transition metals (TM) Ni, Co, Fe, Mn, V have been found to switch with hydrogen [7]. Mixed metal thin films containing magnesium and a first-row transition element exhibit very large changes in both reflectance and transmittance on exposure to hydrogen gas [8, 9]. Similar behavior have been presented in Mg-rare-earth films and magnesium transition-metal alloys, such as Mg_2CoH_5 [10], $Mg_6Co_2H_{11}$ [11] and Mg_2FeH_6 [12], the band structure calculations which support experimental evidence for semiconductor behavior in these materials [10, 12].

II. EXPERIMENTAL

The bilayer thin films were prepared by using D.C. magnetron sputtering unit. Mg (99.99%) & Al (99.99%) pure were used for present study, the glass substrates cleaned by plasma sputtering technique were placed in the substrate holder and bilayer Mg/Al thin films (Mg-100nm & Al-50nm) were prepared on glass substrates. To get homogeneous structure and intermixing of prepared thin films, rapid thermal annealing (RTA) was done by halogen light lamp (1000 W). For this process, bilayer thin films were kept in quartz tube at 200^{o}C and then rapid thermal annealed by halogen light lamp for two minutes. The hydrogenation of annealed Mg/Al thin films were performed by keeping samples in hydrogenation cell, where hydrogen gas was introduced at different hydrogen pressure 20 & 40 psi for half an hour. The UV-1800 Shimadzu spectrophotometer was used to get UV–VIS transmission at room temperature in the visible range 300-800 nm of wavelength.

III. RESULTS AND DISCUSSION

Fig.1. shows the optical transmission spectra of Mg/Al thin films. The optical transmission of thin films were studied at room temperature in the visible range of wavelengths (300-800nm). It was observed that the transmission for each sample was increased after hydrogenation. Fig.2. shows the bandgap spectra of Mg/Al thin films. The optical bandgap of

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the samples have been calculated by using Tauc relation [13].

$$\alpha h\nu = A(E_g - h\nu)^m$$

Where Eg, is the optical bandgap, α, is the absorption coefficient, hν, is the photon energy and A is a constant. Here, m has been taken as 0.5 for direct bandgap material, the direct bandgap was determined by plotting (αhν)2 vs hν spectra, with the extrapolation of the linear vicinity to lower energies.

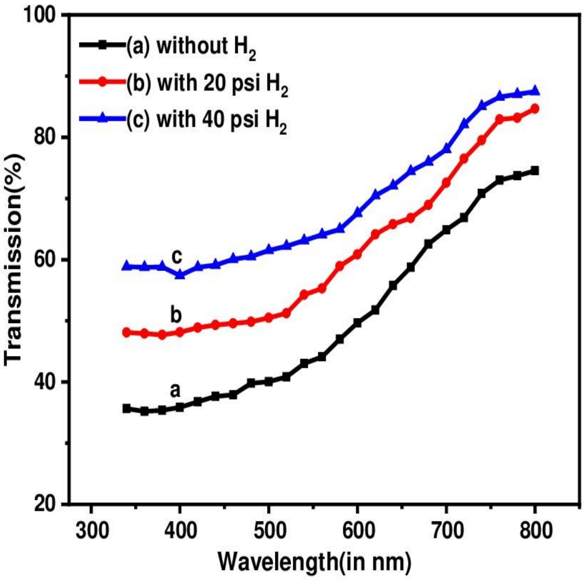

Fig. 1. Transmission spectra of Mg/Al thin films

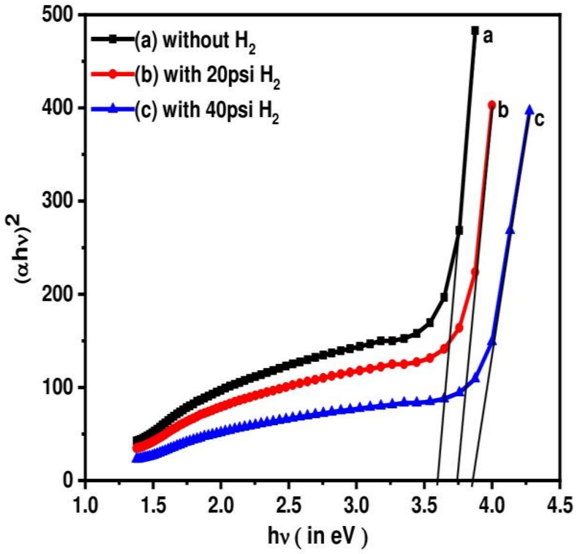

Fig. 2. Optical band gap spectra of Mg/Al thin films

Table-1. Optical bandgap of Mg/Al thin films

Hydrogen pressure	Optical Bandgap (eV)
without H_2	3.59
with 20 psi H_2	3.73
with 40 psi H_2	3.85

It was observed from the bandgap spectra that the bandgap increases after hydrogenation of the thin films Table-1. The variation in the bandgap may be explained as that the hydrogen accumulates at interface and takes electrons from the interface of thin film which support the anionic model [14]. The variation in optical bandgap for Mg/Mn and Mg/Ti thin films have also been reported and found to be increased with hydrogen pressure in both cases [15, 16]. The variation in optical band due to hydrogenation suggests phase changes from metal to semiconductor. The theoretical calculations have been reported by many researchers and suggest that MgH2 under goes various phase transitions as a function of hydrogen pressure [17, 18]. The variation in optical bandgap for various complex hydrides have been observed and found 1.6 eV in case of Mg2NiH4 [19], 1.9 eV in case of Mg2CoH5 [20] and 2.56 eV for Mg3MnH7 [21].

IV. CONCLUSION

In the present work, hydrogenation effect on optical properties have been studied and found that hydrogen tailored the optical properties of Mg/Al thin films. The variation in optical transmission was observed and found to be increased after hydrogenation of thin film. Also optical band gap of Mg/Al thin films was increased with hydrogen pressure. The prepared thin film structure shows the semi conducting behavior with variable optical bandgap with hydrogenation. These results indicates that Mg/Al thin films can be used to hydrogen storage applications.

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