Yttrium hydride films as switchable mirrors: optical characterization and electronic structure

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ABSTRACT

The development of switchable mirrors based on yttrium hydride thin films is shown. Yttrium is deposited on regular glass under ultra-high vacuum conditions. Upon hydrogen pressure the transition from light-reflecting metal YH_2 to transparent insulating YH_3 is induced. Surface and optical characterization is performed to improve the deposition and hydrogenation conditions. A good variable transparency is achieved, with transmittance up to 70% in the visible range for the completely hydrogenated sample. The electronic structure of the YH_3 phase is calculated by considering strong correlation corrections to the crystal potential. We obtain a gap in the quasiparticle spectrum that agrees with the optical transmittance of the YH_3 phase. A prototype device based on these films is proposed.

Keywords: yttrium, metal hydrides, switchable mirrors, strong coupling electron systems, optical transition

1. INTRODUCTION

The discovery of the drastic change in the optical properties of yttrium (Y) and rare-earth hydrides upon hydrogen concentration has triggered the interest in these compounds [1,2]. YH_2 is a metal with no transmittance in the visible range whereas YH_3 is an insulator with a 75%-90% transmittance. This metal-insulator transition is abrupt and reversible when diminishing the hydrogen pressure. Such a dramatic change in both the optical and electronic properties of these materials makes them good candidates to develop optoelectronic devices, as hydrogen sensors, optical modulators or switchable mirrors [3]. The studies performed so far on yttrium hydride thin films use quartz and saphire as substrate [3,4]. However, in order to develop windows of controllable transparency based on these materials, the use of regular glass substrates is desirable. For this purpose we study yttrium hydride thin films deposited on commercial glass and perform surface and optical characterization.

2. RESULTS

The yttrium films were prepared under Ultra-High Vacuum (UHV) conditions and capped *in situ* with a palladium (Pd) layer that protects against yttrium oxidation while being permeable to hydrogen. Commercial glass, previously cleaned in an ultrasound bath and submitted to Argon bombardment of high purity, is used as substrate. Surface characterization of the samples by Scanning Electron Microscopy and Energy Dispersive X-ray spectroscopy is performed to select the most homogeneous films [5]. The selected thin films were hydrogenated under a 3 atm pressure of pure hydrogen during 3 hours. Fig. 1 shows the change in transparency of one of the samples after hydrogenation. This result reproduces those of references [1-3] where quarz and saphire substrates are used.

Samples were grown with different yttrium and Pd thickness. Their optical transmittance after hydrogenation was measured. The results (see Fig. 2) show that good transparency is reached with very thin yttrium layers (case (b)). For yttrium layers of hundreds of nanometers the transmittance diminishes to less than 20%. The higher transmittance of the Pd uncapped sample (d) with respect to sample (e) indicates, in contrast to previous studies [6], that hydrogenation of an oxidized yttrium layer is possible, although it is poorly efficient. X-ray Photoemission Spectroscopy (XPS) profile measurements of dehydrogenated samples show, in addition, that yttrium oxide retards the dehydrogenation [5].

The dehydrogenation process is studied by measuring the time evolution of the transmittance for sample (c). After 5 minutes the sample transparency has fallen in a 75%, reaching total dehydrogenation after 4,5 hours. The evolution is more or less homogeneous in wavelength during the first minute, but after 5 minutes a transmittance peak at ~700 nm remains before total dehydrogenation is reached. This effect occurs because the yttrium hydride goes through all the non-stoichiometric phases [1,2]. These results agree with those reported in the literature [3].

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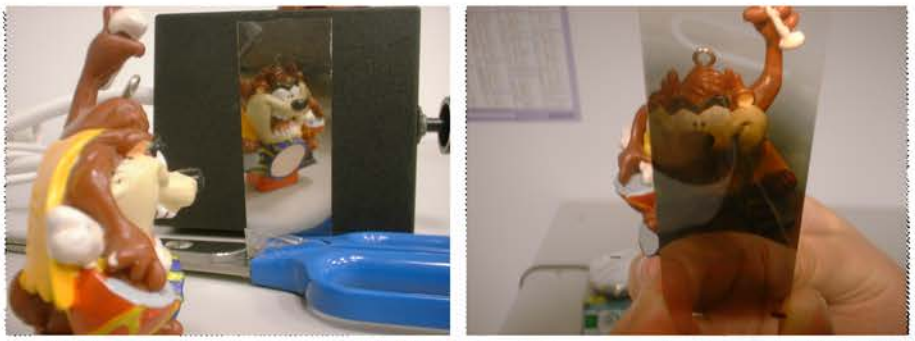

Figure 1. (a) Reflective non hydrogenated Y-Pd thin film (b) transparent hydrogenated Y-Pd thin film.

The hydrogenation and dehydrogenation reactions induced by submitting the yttrium films to H_2 pressure are very slow. This is a handicap for developing switchable mirrors based on these films. The reaction rate is enhanced significantly by performing the hydrogenation electrochemically. With this idea, we have developed a switchable mirror prototype. It consists of a 0.01 molar KOH electrolytic solution "sandwiched" between an Y and Pd layer deposited on glass, and a 15 nm Pd layer framed by an insulator material (polyvinylchloride) to avoid the ohmic contact. A 1.5 volt direct (inverse) polarity is enough to hydrogenate (dehydrogenate) the yttrium film in a few seconds.

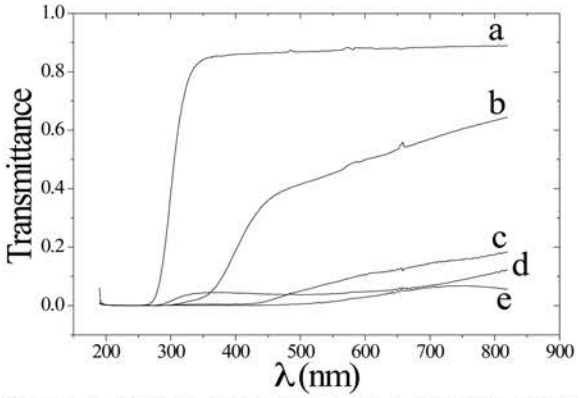

Figure 2. Optical transmittance as a function of the wavelength for different samples. a) Glass substrate, b) Y: 65 nm, Pd: 15 nm, c) Y: 300 nm, Pd 15 nm, d) Y: 100 nm, no Pd, e) Y: 400 nm, Pd 15 nm.

The optical transition of yttrium films upon hydrogenation is concomitant with a change in their crystal structure [1,2]. However, such structural phase transformation does not occur for other hydrides with similar switchable optical properties, as LaH_{2+x} [1,2]. Thus, an electronic origin of this phenomena is suggested. Band structure calculations in the Local Density Approximation (LDA) are unable to predict the magnitude of the semiconducting gap of the trihydrides. Strong electron correlations, which are underestimated in LDA, may be the reason for this misdescription [1,2]. We have calculated the electronic structure of YH_3 by considering self-energy correlation corrections to the LDA crystal potential, as explained in previous work [7]. Our results improve significantly the description of the electronic structure of the insulating phase, yielding a gap that agrees with the transmittance measurements of Fig. 2.

3. CONCLUSIONS

We have shown that low-cost commercial glass can be used as substrate for depositing yttrium hydride thin films. The selection of adequate deposition and hydrogenation conditions leads to samples of switchable transparency of fairly good quality. Optical transmittance up to 70% in the visible range of completely hydrogenated samples confirms the existence of a semiconducting gap. This is coherent with the electronic structure of the YH_3 phase, calculated by introducing self-energy corrections to the LDA crystal potential. Sample dehydrogenation and XPS data indicate the role of oxygen contamination as a dehydrogenation retarder. We have developed a simple switchable mirror prototype with galvanostatic (de)hydriding. This work shows the viability of switchable mirrors based on yttrium hydride films.

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