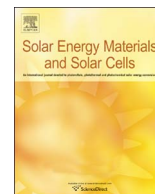




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Solar Energy Materials and Solar Cells

journal homepage: www.elsevier.com/locate/solmatComposition of photochromic oxygen-containing yttrium hydride films[☆]Dmitrii Moldarev^{a,b,c}, Daniel Primetzhofer^c, Chang Chuan You^b, Smagul Zh. Karazhanov^{b,*}, Jose Montero^b, Fredrik Martinsen^b, Trygve Mongstad^b, Erik S. Marstein^b, Max Wolff^c^a Department of Materials Science, National Research Nuclear University "MEPhI", 31 Kashirskoe sh, 115409 Moscow, Russia^b Department for Solar Energy, Institute for Energy Technology, P.O. Box 40, NO-2027 Kjeller, Norway^c Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden

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ABSTRACT

In this work, the composition of oxygen-containing yttrium hydride (YHO) thin films was investigated. The films were prepared by reactive sputter deposition, and were found to have oxygen contents on the order of several tens of per cents. We present depth-resolved atomic composition profiles of photochromic YHO films to study the connection between composition, photochromic properties and growth parameters. Two films, deposited at different pressures, were prepared and characterized using ion beam analysis techniques, i.e. Rutherford backscattering spectrometry and elastic recoil detection analysis. We found that an increase of deposition pressure results in larger [O]/[Y] ratios, while the ratio [H]/[Y] becomes reduced. We also report a gradual oxidation of the films exposed to air as well as hydrogen release under ion bombardment.

1. Introduction

Chromogenic materials attract increasing attention in the scientific community. This fact is related to the wide range of possible technological applications, such as smart windows, sensors, sunglasses or visors, as well as displays or light modulators [1,2]. Electrochromic materials are applied in commercial devices already. However, such materials have long response times and high fabrication and implementation costs limiting the range of applications. Thermochromic and photochromic materials can potentially overcome these challenges.

Yttrium hydride foils made of metallic YH_2 and insulating YH_3 exhibit photochromic properties only at high pressure [3]. At ambient conditions, yttrium trihydride crystallizes into a hexagonal structure with $P\bar{3}c1$ symmetry [4]. A phase transition to face-centered cubic (fcc) and the closure of the band gap was found in first principle calculation [4] at a pressure of ~ 20 GPa. Experimentally this transition was verified at 8 GPa [5]. Theory predicts that the presence of O in YH_{3-x} leads to an increased band gap and stabilizes the fcc phase at ambient conditions [6]. The latter was confirmed by X-ray diffraction studies [7]. The oxygen-containing yttrium hydride shows a photochromic behavior at room temperature [8]. From Rutherford backscattering spectrometry [9] (RBS) and neutron reflectometry [10] a large amount of oxygen, [O]/[Y] of up to 1.67, has been reported in the YHO films deposited by reactive sputtering. Mongstad et al. [9] found an even distribution of O

atoms throughout the thickness of the films encapsulated by a thin layer of Mo. Although the oxygen is incorporated in the films during the deposition process, there was no specific analysis of that point. Later, systematic studies of the films have shown that the oxygen is incorporated after exposing the films to air [11]. For YHO, the band gap depends on the deposition pressure [12] and exceeds 2.6 eV similar to YH_3 in the hexagonal phase [13]. Theoretical studies (Ref. [6]) suggest that the change in band gap is related to the increased oxygen content in the films. Similar changes of the band gap of oxidized Gd-hydride were reported [14] earlier. In the present work, we perform a compositional analysis of YHO films. We relate the deposition pressure of the film's to their composition and follow the oxidation processes in air. We present results from RBS and Time-of-Flight - Energy Elastic Recoil Detection Analysis (TOF-E ERDA) measurements on YHO films, synthesized by reactive sputter deposition on glass substrates at two different deposition pressures.

2. Experiment

The YOHO films were reactively sputtered on glass substrates using a Leybold Optics A550V7 sputtering system. The deposition was carried out at room temperature in a mixed atmosphere of argon and hydrogen (H_2 flux = 40 sccm; Ar flux 160 sccm) at two deposition pressures, namely 1 Pa and 6 Pa. The nominal purity of the gases was 99.999% for

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Ar and 99.9999% for H₂. The base pressure in the sputter chamber was $\sim 10^{-4}$ Pa prior to film deposition. A metallic yttrium target of purity 99.99% was used. The thickness of the films, measured by profilometry, was around 500 nm. More details about the deposition process can be found in Ref. [15] and the optical properties are reported in Ref. [12]. The samples in this work represent two extreme cases with close to the absence of a photochromic effect for the films grown at 6 Pa and a strong photochromic effect ($\sim 30\%$ optical response) for films grown at 1 Pa [12]. For the current samples, the photochromic properties were qualitatively verified in a solar simulator directly after deposition.

The RBS measurements were performed with the 5 MV NEC tandem accelerator at Uppsala University. The incident particles were helium ions with an energy of 2 MeV. The backscattered particles were detected under an angle of 170°. The RBS spectra were analyzed by the SIMNRA software [16]. The TOF-E ERDA measurements were performed at the same accelerator using iodine ions with an energy of 36 MeV. The energy and TOF detectors were located at an angle of 45° with respect to the incident projectile direction. The samples were irradiated at an angle of 67.5° with respect to the surface normal. The software CONTES [17] was used to analyze the spectra and calculate depth profiles for each element.

3. Results and discussion

Fig. 1(a) shows a TOF-E ERDA coincidence spectrum for the film deposited at 1 Pa one week after deposition. Simultaneous measurements of energy (x-axis) and time of flight (y-axis) permit the separation of recoil particles with different masses. The main constituents of the films are identified as yttrium, oxygen, and hydrogen, but traces of other chemical elements such as carbon, nitrogen, fluorine, silicon, sodium, and calcium are detected as well. The dashed line at high energy marks recoils expelled from the surface of the sample, while the low energy part corresponds to signal stemming from close to the substrate. The energy loss curves for the respective elements are used for quantification of the atomic concentrations in the TOF-ERDA. Since the yield of the detected ions is proportional to their concentration the energy loss curves for oxygen in Fig. 1(b) can be interpreted as the oxygen concentration plotted against depth. As seen from these curves, films deposited at 1 Pa show an oxygen-enriched surface layer, while the oxygen concentration below the near-surface region is lower compared to the film deposited at 6 Pa. Note, that the observed increase with increasing energy loss is primarily an effect of changing scattering cross sections and stopping power. With exception of oxygen, all elements are found distributed evenly throughout the film thickness.

The quantitative depth profile for each element can be extracted from the yield of recoil particles as a function of energy loss by solving a system of linear equations [18]. In CONTES this is done by a so-called inverse iteration [19] with projectile fluence as an adjustable parameter. The projectile fluence as a function of depth is depicted in Fig. 1(c). The actual fluence does not depend on depth, but for the conversion algorithm, it is a free parameter. For each depth bin it can deviate slightly from constant values like it is observed for the 1 Pa sample in Fig. 1(c). A significant deviation close to the surface of the 6 Pa sample indicates the presence of high porosity.

Results from TOF-E ERDA are subject to uncertainties from two main sources: firstly, the detection efficiency in the TOF-detector [20], and secondly, the unknown specific energy loss of the detected ions lead to systematic uncertainties in the derived concentrations. This uncertainty is at most 5% for heavy elements, but increases and may significantly exceed 10–20% for lighter elements. Note, that a relative

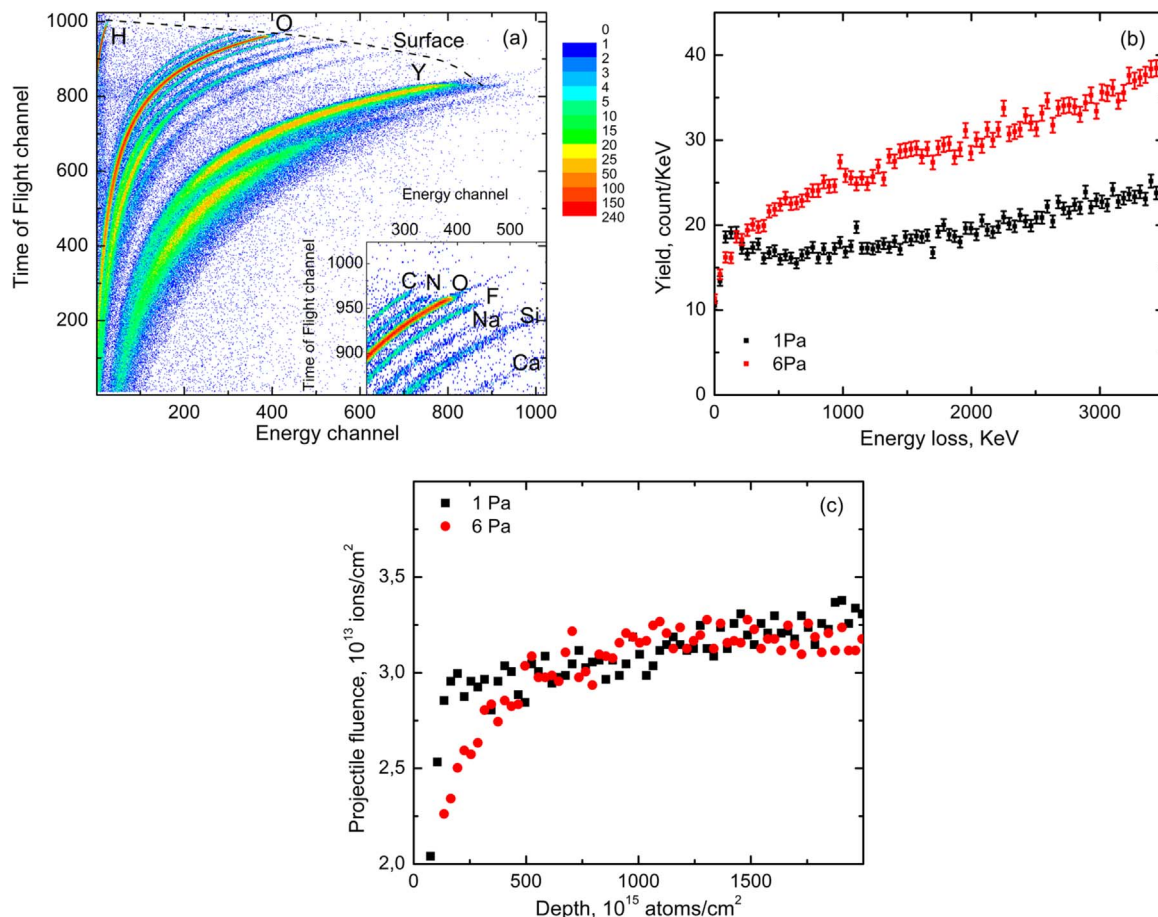


Fig. 1. (a) ERDA spectrum for the film deposited at 1 Pa, (b) energy loss histograms of oxygen and (c) projectile fluence as a function of depth for the films deposited at 1 Pa and 6 Pa measured 1 week after deposition.

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