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Report:

Yttrium hydride is an inorganic material which has been thoroughly studied because of the fascinating reversible optical transition that accompanies hydrogen uptake [1]. Thin-films of Pd-coated yttrium subjected to an external hydrogen pressure transform from a metallic to a transparent phase, where the optical switching is observed between the cubic (fcc) YH_2 to the hexagonal YH_3 phase. The transparent YH_3 is a semiconductor with a band gap of 2.6 eV [2]. For thin-films of yttrium hydride prepared by reactive sputtering (sputtering of yttrium in hydrogen atmosphere), described in [3], we observe a photochromic effect where initial transparent samples absorbs up to 50% of visible light after one hour of visible or ultraviolet light irradiation at moderate intensity [4]. The change in optical transmission is accompanied by a persistent increase in conductivity.

In the reactively sputtered films, the photochromic effect is observed at room temperature and ambient pressure. The effect is reversible and the yttrium hydride thin films return to their initial transparent state when left in the dark over time. In general, the bleaching relaxation is slower than the photo-darkening, and is highly dependent on the duration of the photo-excitation. The transparent yttrium hydride films are strongly textured (preferred orientation) and have a cubic phase with elongated unit cell axes (a~5.35Å) compared to typical "bulk" cubic yttrium hydride (a = 5.20 Å), and contains both oxygen and hydrogen with an approximate chemical composition of $YO_{0.3}H_{2.4}$. In addition to the transparent yttrium hydride films, strongly absorbing "black" films with less hydrogen content and contracted fcc unit cell compared to the transparent films (a_{black}~5.26Å, see [3]) can be made by reactive sputtering.

The Yttrium Hydride thin-films were studied at BM01A using the single-crystal diffractometer KUMA KM6-CH equipped with a CCD detector with a monochromatic beam. Measurements with different orientations of the films were performed to exclude texturing effects in the refinements of the interstitial oxygen atoms, and to estimate the texture (preferred orientation) of the films. *In-situ* experiments with light excitation were also performed to study the structural changes during switching. The photochromic effect in oxygen containing yttrium hydride films was found to be related changes in unit cell axes during the optical transformation. Figure 1 below shows how the unit cell volume contracts during the bleaching process.

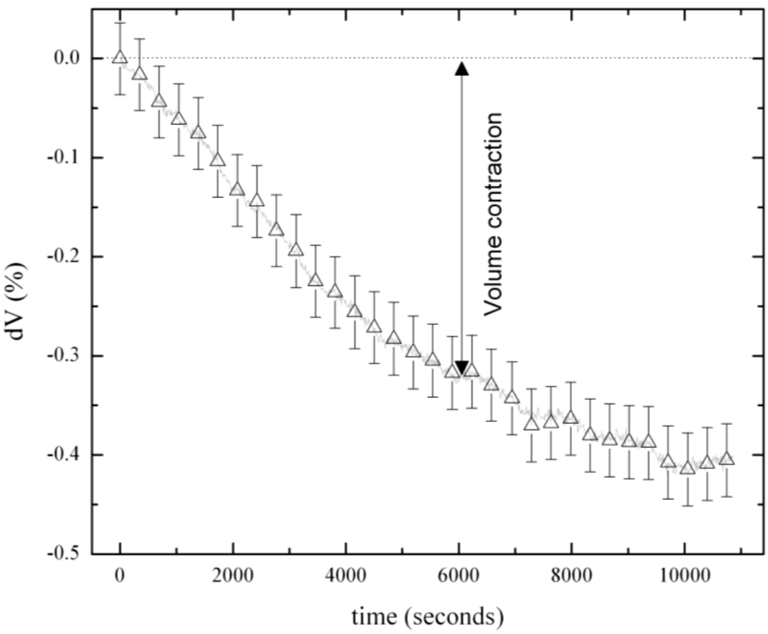

Figure 1*: Unit cell volume of oxygen containing yttrium hydride thin film during switching from transparent to opaque (from Rietveld-type fitting of in-situ SR-XRD data; symbol for each 30. point (xrd-dataset), rest is shown as a grey line).*

We did texture analysis for different samples using the software Maud [5]. Diffraction patterns from four different φ orientations of the sample were devided into sectors of 5º in η angles going from η = -70º to η = +70º. We fitted the data using an E-WIMW parametrization of the texture, and reconstructed the pole plots from the best fits of the simulated diffraction patterns. The best fit were obtained using a multi-parameter Rietveld fit. In the texture analysis, we did not take into account the possible differences that oxygen occupancy of sites in the lattice could present, which could have enhanced the fit but would not give substantial changes in the texture. Figure 2 shows the reconstructed pole plots for black and transparent samples of yttrium hydride (see [3]). The two different optical states of yttrium hydride films prepared by reactive sputtering both exhibit a fcc lattice, with slightly different lattice parameters (a = 5.24 Å for black and a = 5.35 Å for transparent). The texture analysis shows that these two types of samples, although very similar in crystal structure, have a large difference in the prefferred orientation. The transparent sample is strongly oriented in the 200 direction, and exhibit circular symmetry. On the other hand, the black sample does not show so clear orientation, and is observed to not be symmetric. The texture analysis explains why the 200 peak on the transparent samples is observed to have a very strong intencity when doing standard θ – 2θ diffraction experiments, while the intencity of the peaks is more evenly distributed in such experiments for black samples [3]. This information can help understanding θ – 2θ diffraction data, and might result in the revelation of the oxygen ion positions in the lattice of the transparent samples.

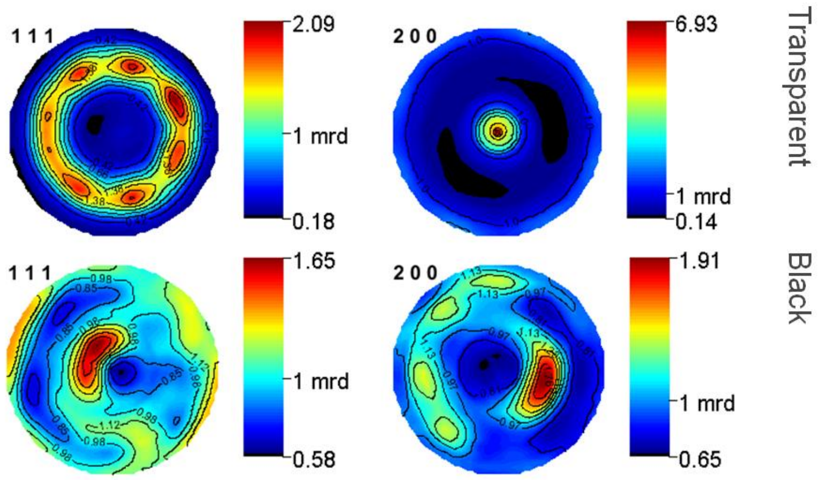

Figure 2*: Reconstructed pole plots from obtained from 2D diffraction patterns taken at four different φ orientations of the sample. Upper left: For the 111-orientation of the transparent sample*
Upper right: For the 200 orientation of the transparent sample
Lower left: For the 111-orientation of the black sample
Lower right: For the 200 orientation of the black sample

References

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