



**Experiment title:**  
**Dynamics of structural domain formation in epitaxial yttrium- hydride films**

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**HS 560**

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**Report:** The  $\beta$ - $\gamma$  phase transition in yttrium-hydride films is of great current interest due to the spectacular changes in the optical transmission and its potential industrial applications. Cubic  $\text{YH}_2$  ( $\beta$ - phase) films are metallic reflecting while hexagonal  $\text{YH}_3$  ( $\gamma$ - phase) films are transparent insulators with a band gap of 1.8 eV. In thin epitaxial Y- films this phase transition is completely reversible without any loss of structural coherence [ 1].

The present experiment was intended to temporally and spatially resolve the distribution of  $\beta$ - and  $\gamma$ - domains in a 50 nm thick Y- film during the  $\beta$ -  $\gamma$  phase transition. The Y (00.1)- film was grown on a  $\text{Al}_2\text{O}_3/\text{Nb}$  buffer (50 nm) and capped successively with Nb and Pd. While the buffer guarantees epitaxial growth, the Pd cap layer serves as hydrogen window and as protection against corrosion. For the first time monochromatic x- ray diffraction topography has been used to spatially resolve structural phases within a thin metallic film. Fig.1 shows reflections from the  $\beta$ - and  $\gamma$ - phase in the coexistence region. Domains of both phases must be smaller than 1-2  $\mu\text{m}$  (film resolution). The intensity of both reflections is distributed almost homogeneously, though there is a slight tendency of domains of one phase

to gather together.

To visualize the dynamics of lateral hydrogen diffusion a partially Pd- covered Nb film on sapphire was prepared. As an example fig.2 presents three topographs of the Nb and sapphire reflections taken at different times during the diffusion process.  $\text{Al}_2\text{O}_3$  does not solve H, thus its reflection stays at the same position, serving as a reference. Upon hydrogenation, the Nb lattice underneath the Pd- cap expands immediately by 8% and the reflection shifts to the other side of the substrate reflection. The H- concentration gradient between the unloaded part of the sample and the hydrogen saturated region leads to a steady shift of lattice parameter. Then lateral diffusion starts. The movement of the diffusion front can clearly be observed by the position of the substrate reflection which is unaffected by hydrogen.

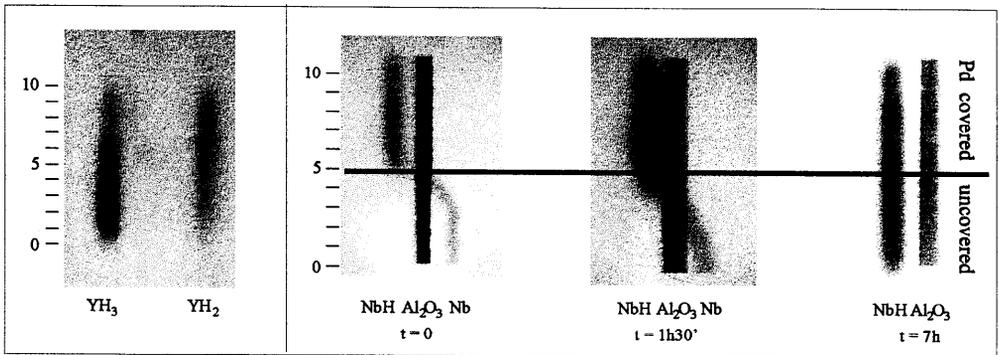


Fig. 1

Fig. 2

*Fig.1 X-ray diffraction topographies of  $\text{YH}_2$  and  $\text{YH}_3$  in phase coexistence.*

*Fig.2 Time series of topographies visualizing H- diffusion within the 50 nm thick Nb- buffer. at  $200^\circ\text{C}$  in an H atmosphere of 16 mbar. The scale shows mm. The horizontal bar marks the line up to which the sample is covered with palladium.*

This experiments demonstrate the feasibility of XDT to study structural properties like the dynamics of phase transitions and hydrogen diffusion in thin epitaxially films and superlattices in the nanometer regime.

[1] A. Remhof, G. Song, K. Theis-Bröhl, and H. Zabel, Phys. Rev. B 56 (1997) R2897.