

## MS44-P03

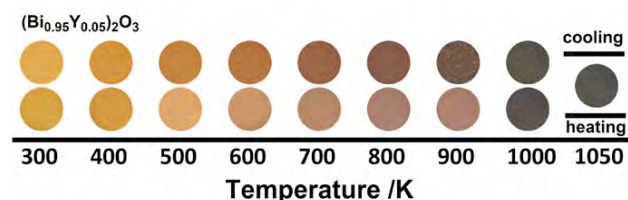
**Yttrium substituted Bismuth oxides as high-temperature thermochromic materials**Thorsten M. Gesing<sup>1,2</sup>, Anne Staubitz<sup>1,2</sup>, Xi Liu<sup>1</sup>

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Polymorphs of bismuth oxide and its yttrium substituted solid solutions ( $(\text{Bi}_{1-x}\text{Y}_x)_2\text{O}_3$  ( $0.00 \leq x \leq 0.25$ )) exhibit excellent thermochromic properties in the range from room temperature to 1050 K. The colors change mostly from yellow at low temperatures to various brown hues at high temperatures. The compounds in this nominal series were examined between 293 K and 1050 K using X-ray powder diffraction, UV-Vis spectroscopy, and dynamic scanning calorimetry. A combination of Tauc and DASF methods were applied to determine the band gap energies and types from the diffuse UV-Vis spectra for these semiconducting oxides. It is well known that reversible monoclinic (low temperature) to defect fluorite-type cubic (high temperature) or tetragonal (low temperature) to defect fluorite-type cubic (high temperature) phase-transitions occur on heating and cooling for pure bismuth oxide and the solid solution with 10% cation substitution, while none in the solid solutions with  $x > 0.1$  without annealing. Thermochromic behavior is observed for all samples studied in this series to be generally a gradual darkening as the temperature increases at the regions without any phase transitions, and a more abrupt color change at the stage where a phase-transition happens (Figure 1). The UV-Vis reflectance spectra show the room-temperature absorption edges of all samples in the range between 2.4 eV to 2.8 eV. The spectrum of pure  $\alpha\text{-Bi}_2\text{O}_3$  show a sharper threshold at the absorption edge comparing to the rest samples, which contain high concentration of vacancies on the anion sites. At higher temperatures, the absorption edges extend into longer wavelength regions, resulting in darker colors.

Figure 1: Optical color change of  $(\text{Bi}_{0.95}\text{Y}_{0.05})_2\text{O}_3$  between 300 k and 1050 K.



**Keywords:** thermochromic materials, high-temperature powder diffraction, phase-transition

## MS44-P04

**HEIMDAL@ESS – Fast neutron powder diffraction for material science**Jürg Schefer<sup>1</sup>, Jonas Birk<sup>2</sup>, Sonja L. Holm<sup>2</sup>, Dan Mannix<sup>3</sup>, Kåre Iversen<sup>3</sup>, Rodion Kolevatov<sup>4</sup>, Bjørn Hauback<sup>4</sup>, Kim Lefmann<sup>2</sup>, Lukas Keller<sup>1</sup>, Mogens Christensen<sup>3</sup>

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New functional materials are in the focus for cutting-edge materials as demanded for example to minimize energy consumption, reducing waste and optimizing recycling processes. Such new materials must be probed under working conditions by a wide range of methods including neutron diffraction, covering a length scale from millimeters down to atomic distances below  $<1$  nm.

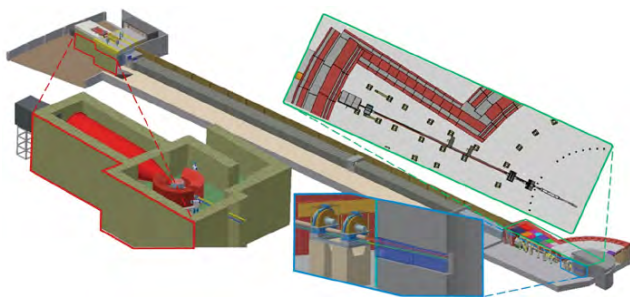
The HEIMDAL [1,2] instrument at the new spallation neutron source ESS is exactly covering these needs, combining powder diffraction (NPD), small angle scattering (SANS) and neutron imaging (NI) in a single instrumental setup. It is essential to have time dependent information from the sample using different probes to give access to all length scales. In a first stage, we will complete the powder diffraction part, later upgrade the instrument by the SANS and imaging option.

A key component of the instrument is a double guide delivering thermal and cold neutrons. Extracting neutrons through two separated guides was a consequence of the different optics needed for the transport of cold and thermal neutrons, respectively. Our solution allows the optimization of the flux-sensitive NPD using thermal neutrons down to  $0.5\text{\AA}$ . The NPD takes full advantage of the long pulse of ESS: HEIMDAL can deliver high flux as well as high resolution by adjusting the pulse width within seconds. We can adapt exactly to the need for the materials science community, where phase transitions and structural parameters can be envisaged.

As we expect a less trained user community in this field, we and the Data management and software center (DMSC) in Copenhagen will make a big effort to offer a wide range of easy-to-operate software packages, such as 2D Rietveld refinement.

**Figure 1:**

The layout of the new HEIMDAL instrument at the European Spallation Neutron Source ESS in Lund, Sweden: A dedicated instrument for *in-situ* and *in-operandi* studies for materials science in the long experimental hall.



## References:

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- [1] S.L. Holm et al., Nuclear Instrument and Methods (2016) 782, 1-8.  
 [2] K. Anderson and Instrument Groups, Instrument park at ESS, in preparation (to be submitted to NIM)
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**Keywords:** Neutron Diffraction, In-Operandi, In-Situ

## MS44-P05

## Temperature-dependent structure changes of complex aluminium hydrides with Rb and Cs as metal cations

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Complex aluminium hydrides are interesting materials with respect to the release and uptake of hydrogen. Since hydrogen is part of the crystal structure of the hydrides, such compounds can serve as solid hydrogen storage materials. The temperature dependent behaviour of most of the complex aluminium hydrides with alkali and earth alkaline metals has been studied intensively.<sup>[1]</sup> The crystal structures of complex aluminium hydrides are built from isolated  $[\text{AlH}_4]^-$  tetrahedra which coordinate the metal cations. The decomposition of aluminium hydrides with alkali metals proceeds via the formation of intermediate hexahydride structures consisting of isolated  $[\text{AlH}_6]^{2-}$  octahedra. This formation is associated with a first hydrogen release step before simple metal hydrides form after a second step. However, *in situ* X-ray diffraction experiments have shown that their decomposition route cannot easily be transferred to  $\text{CsAlH}_4$  and  $\text{RbAlH}_4$ .<sup>[2]</sup> The transformations are more complex and do not proceed via the known hexahydride structures. *In situ* synchrotron measurements have been performed in order to study the processes and the phases formed during the dehydrogenation of both hydrides.

## References:

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- [1] Mamatha, M., Weidenthaler, C., Pommerin, A., Felderhoff, M., & Schüth, F. (2006) J. Alloys Compds, 416, 303.  
 [2] Weidenthaler, C., Felderhoff, M., Bernert, T., Sørby, M. H., Hauback, B. C., & Krech, D. (2018). Crystals, 8(2), 103.
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**Keywords:** complex aluminium hydride, hydrogen storage, *in situ* powder diffraction