caused by thermal cycling like elastic and plastic deformation of film and substrate, recrystallisation, phase transformation, annealing of defects [1,2]. The purpose of this contribution is to present a new complex high-temperature X-ray diffraction (XRD) approach which can be used to *in-situ* characterize structural changes occurring in thin film structures during thermal cycling. The novelty of the approach resides in the characterization of a free standing thin film-substrate composite which can bend freely in the high-temperature chamber (DHS900, Anton Paar GmbH). This gives an opportunity to characterize the substrate curvature by measuring substrate symmetrical reflections at different sample positions [3]. In this way, the macroscopic stress imposed on the film can be correlated with other structural parameters like elastic strain, size of coherently diffracting domains, point defect density. The approach provides thus an opportunity to perform a complex thermo-mechanical and structural characterization of films. By comparing measured stress and strains, absolute magnitude of temperature dependent X-ray and mechanical elastic constants can be determined. In the case of multilayered coatings, a comparison of the macroscopic stresses imposed on the whole film composite with the elastic strain behaviour of individual sublayers can be used to study thermo-mechanical effects in complex thin films structures. The new approach was applied to a variety of thin film systems *e.g.* TiN, CrN/Cr, Al, Cu, CrN on Si(100) measured using laboratory and synchrotron sources (BESSY and Hasylab) in the temperature range -100 to 550°C [4]. In the case metal thin films with the thickness down to 50 nm, the approach was used to determine flow stresses which exceed 800 MPa in Al. Moreover, first high-temperature X-ray elastic constants of textured Cu, Al and TiN thin films were evaluated. In the case of hard CrN films with an average crystallite size of about 10 nm deposited on Si(100) and steel, the new approach allowed for the calculation of exact XECs and quantify intrinsic and extrinsic stresses. Also other examples of high-temperature XRD analysis of thin films will be provided.

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MS37 O4

Structural and Compositional Investigation of Yttrium-doped HfO_2 Nano-films

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Keywords: anomalous scattering, epitaxial structures, synchrotron radiation

Cubic phase yttrium-doped HfO_2 (YDH) ultra-thin films were grown epitaxially on GaAs (001) and Si (111) substrates by molecular beam epitaxy (MBE). The C-V and I-V measurements of a film of 7.7 nm thick yield an enhanced dielectric constant □~32 and thus an equivalent oxide thickness ~0.94 nm, close to the theoretical value of cubic phase HfO_2. Thorough structural and morphological investigations by x-ray scattering and transmission electron microscopy reveal the YDH thin films are epitaxially grown on the substrates. The interfaces between YDH and these substrates are atomistic sharp and free of reacted interfacial layer. We have also determined yttrium content of YDH films to be 19% by using anomalous x-ray diffraction (AXD) across Y *k*-edge and angle resolved X-ray photoelectron spectroscopy (AR-XPS). The agreement between the AXD and AR-XPS results manifests that the incorporated Y atoms indeed homogeneously substitute Hf atoms in the crystalline lattice and form a substitutional solid solution.

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Generating High Brilliance X-ray Beams for X-ray Diffraction and Scattering Applications

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Today a large fraction of the X-ray analytical systems used in two-dimensional diffraction and scattering applications are still equipped with non-optimized beam-generating schemes that combine high power sealed tubes or rotating anodes with large source-sizes with inefficient optical schemes. With the advent of single reflection graded multilayer optics and efficient, low power micro-focus sealed tubes, it has become advantageous and cost-effective to replace these high power systems with this more efficient and robust technology.

The key to this new technology are Xenocs' high performance, single reflection X-ray optics that couple optimally to small x-ray sources. The relative figure-of-merit for X-ray beams is the brilliance, which typically is expressed as photons/mrad²/mm²/s in the relevant part of the spectrum (i.e. Cu K-alpha), and which can never exceed the brilliance of the source (Liouville's Theorem). Xenocs' single reflection optics optimally conserve the brilliance of these sources, resulting in extremely bright X-ray beams.

The GeniX product line from Xenocs combines a micro-focus X-ray tube with high-efficiency Xenocs X-ray optics, and offers a high performance solution with clearly defined characteristics (beam size, divergence, spectral purity, flux…). Compared to high power sealed tubes, the Genix solution offers superior brilliance enabling faster data collection in a package with a small footprint, low power consumption, and low facility requirements. The low maintenance requirements of this solution also make it appealing as a replacement for traditional rotating anodes.

In addition to presenting the GeniX product platform we present data obtained with the GeniX to demonstrate its performance and its value as an efficient, cost-effective X-ray beam delivery solution for a variety of applications including single crystal and protein crystallography, high pressure diffraction, and SAXS.