MS14-P34 | Hexagonal Bariumtitanate stabilized as ultra-thin film on Pt(111): An X-ray diffraction and electron-energy-loss spectroscopy study

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Bariumtitanate ($BaTiO_3$) is one of the most intensely studied oxides. Besides the perovskite- (PV) type phases, a high-temperature hexagonal (h) phase exists, which is stable above 1705 K. The h- type structure is distinctly different from the PV-type, as it contains TiO_6 octahedra linked by common faces rather than by common corners. Many attempts have been made to stabilize h-$BaTiO_3$ at ambient conditions, but thus far only a mixture of PV- h-type (17%) $BaTiO_3$ could be obtained in crystals of 140 nm in size [1].

We present an x-ray diffraction (XRD) and electron-energy loss spectroscopy (EELS) study in combination with theoretical simulations which shows that h-$BaTiO_3$ exists as a 7 nm thick film on Pt(111) deposited by radiofrequency magnetron sputtering. The film forms a (2x2) superstructure with respect to the Pt(111) surface unit cell. XRD experiments carried out at the ESRF in Grenoble indicate that the h-$BaTiO_3$ unit cell parameters are in-plane contracted by -3.04% and vertically expanded by +3.89% relative to the bulk parameters (a=b=5.724 Å, c=13.965 Å). Based on the fitting of the intensities of 14 symmetry independent reflections the formation of h-$BaTiO_3$ is unambiguously confirmed. Along the c-axis the film is disordered by the presence of two terminations of the h- $BaTiO_3$ unit cell. In parallel, comparison of EELS spectra collected for PV-type $BaTiO_3$ and for the film with simulations also confirm the h- $BaTiO_3$ formation.

[1] M. Yashima, T. Hoshina, D. Ishimura et al., J. Appl. Phys. 98, 014313 (2005)