Pulsed laser deposition of In_2O_3 thin films on YSZ(111)

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In_2O_3 is a wide band-gap semiconductor and belongs to the class of transparent conductive oxides, which combine high electrical conductivity and optical transparency in the visible region. Undoped In_2O_3 and especially Sn doped In_2O_3 find application in optoelectronic devices [1-2], e.g. flat panel displays, solar cells or organic light emitting diodes. Additionally, In_2O_3 changes its conductivity depending on exposure to oxidizing and reducing gases, which makes it an interesting candidate for gas sensing applications [3-5].

In many applications the interface to a different material, e.g., an organic layer or ambient conditions, plays a key role in the performance. This is characterized by the geometric arrangement and electronic properties at the surface, the reactivity towards gaseous species, the band alignment and conductivity within heterostructures. Thus, achieving a better understanding of the atomic-scale surface characteristics by investigating well-defined single-crystal model systems is of paramount importance to optimize the functionality of devices. Recently, In_2O_3 single crystals were used to investigate with scanning probe techniques the precise atomic-scale structure of In_2O_3(111) surfaces, as well as its reactivity towards water [6].

Undoped In_2O_3 single crystals are not commercially available, and synthetically grown ones are usually very small, measuring only 1-2 mm in diameter. While the small size is not critical for scanning probe techniques, area averaging techniques such as TPD and XPS, require larger samples of homogeneous composition for qualitative and quantitative investigations of e.g., the reactivity of the surface and its electronic properties. Thus, larger single crystalline samples would allow the use of a variety of techniques for In_2O_3.

To compensate for the lack of large In_2O_3 single crystals, we have prepared well-ordered and atomically flat In_2O_3(111) thin films, with a thickness of few hundreds of nanometers. The films were grown on Y-stabilized zirconia (111) substrates by pulsed laser deposition (PLD). Their structure, chemical composition and morphology were characterized by electron (RHEED, LEED) and x-ray diffraction (XRD), XPS, atomic-force microscopy (AFM), and scanning tunneling microscopy (STM). By optimizing the growth parameters (temperature and oxygen background pressure) and investigating their effect on the film morphology and structure we could obtain In_2O_3(111) films exhibiting properties comparable to the best single crystalline samples available. Such films exhibit atomically-flat regions a few hundreds of nanometers wide, separated by hexagonal pit-like structures a few nanometers deep. XRD reveals that the structure of the films is relaxed to the bulk lattice of bixbyite In_2O_3 in the out-of-plane direction, with typical peak widths comparable to those of single-crystalline samples.

These films appear to be promising candidates to be used as an equivalent replacement of In_2O_3(111) single crystals, allowing combination of atomic-scale surface-science analysis and investigation of the electronic structure of such surfaces via area averaging spectroscopic techniques, as well as characterization of their reactivity to different chemical species.

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