

Role of interfacial defects and strain in the metal-insulator transition of epitaxial VO₂ films

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Vanadium dioxide (VO₂) undergoes a first-order metal-insulator transition (MIT) from a high-temperature metal phase to a low-temperature insulator phase around 68°C. This transition is accompanied by (i) a structural phase transition, from the monoclinic M1 phase (insulator phase) to the rutile R phase (metal phase), (ii) an abrupt variation, over several orders of magnitude, of the optical and electrical properties. This phase transition can be triggered not only by temperature but also by electric field, light and strain. These properties make VO₂ a promising candidate for fundamental researches and industrial applications, such as sensor devices, meta-materials, ultrafast optical switching and memory devices.

In this work, pure-phase VO₂ epitaxial thin films with different thickness, have been grown on (001)-oriented Al₂O₃, and (100)-, (001)- and (111)-oriented TiO₂ substrates using electron beam evaporation. The structural properties of the films have been investigated using both room-temperature and temperature-dependent high-resolution X-ray diffraction (XRD). The temperature-dependent electrical properties of the film have been investigated using 4-probe resistivity measurements. All samples clearly exhibit a insulator-to-metal transition, with a resistivity jump covering more than four orders of magnitude proving the high crystalline quality of the films. The analysis of the XRD data allows to determine the level of strain and the relative amount of each phase during the transition.

It is shown that the films grow in a strain-relaxed state and tensile strain is stored in the films upon cooling down from growth temperature as a result of the film/substrate thermal expansion mismatch. The thinner films exhibit the highest level of strain and degraded electrical properties while both the metal-insulator and structural phase transitions are shifted towards higher temperatures. Increasing the film thickness result in strain relaxation and improved electrical properties. Additionally we evidence the presence of a strain-stabilized intermediate phase appearing during the transition.