TaO_2 – the new kid on the 5*d* block

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For the realization of the next generation of fast, energy-efficient nanoelectronics, there is a great need for new materials whose electrical and optical conductivities can be sensitively tuned between high (on) and low (off) states by altering a thermodynamic control parameter, e.g., strain or temperature. Unfortunately, most materials are either metallic or insulating and their conductivities cannot be changed substantially. Materials exhibiting a metal-insulator transition (MIT) at or above room temperature are quite rare, limiting their applicability in devices. The archetypical compound displaying an MIT is VO_2 with a transition temperature of 65 °C. Shortly after the discovery of the MIT in $3d^1$ VO_2 [1], a similar effect was discovered in $4d^1$ NbO_2 albeit at a much higher temperature of 807 °C [2]. Thus far, the $5d^1$ analog TaO_2 has remained elusive.

In this talk, I will showcase the growth of untwinned epitaxial thin films of phase-pure $5d^1$ TaO_2 (the rutile-like polymorph) using suboxide MBE. This recently developed flavor of MBE utilizes a molecular beam of TaO_2 emanating from a crucible containing Ta_2O_5 in an effusion cell heated to temperatures around 1750 °C [3]. This approach avoids the notoriously unstable electron-beam evaporation of Ta metal and need for subsequent oxidation using a background gas or plasma. The latter is particularly challenging to control in the quest for TaO_2 as the stable bulk phase of tantalum oxide is the $5d^0$ compound Ta_2O_5, a band insulator without an MIT, similar to the case of $3d^0$ V_2O_5 and $4d^0$ Nb_2O_5. In the suboxide MBE approach, the Ta^{4+} is delivered to the substrate from a pre-oxidized molecular beam of TaO_2.

To achieve the targeted rutile structure of the thin film, growth must take place at very low oxygen partial pressures, e.g. $< 10^{-8}$ Torr in the case of TaO_2. Viable substrates to stabilize such rutile thin films must hence be able to withstand aggressively reducing conditions at temperatures frequently exceeding 1000 °C, dramatically limiting the number of candidate materials. We note that TiO_2 and MgF_2 –the only two commercially available rutile substrates– are very prone to reduction and evaporation, respectively, at such high temperatures, and can adversely react with these desired rutiles. Therefore, they are of limited use for the growth of many rutiles irrespective of their lattice mismatch.

Ongoing efforts entail the detailed investigation of the structural and spectroscopic properties of TaO_2 thin films on Al_2O_3 substrates and the exploration of exotic new candidate substrates. To this end, we are employing an ensemble of X-ray, optical, and electrical transport techniques, as well as scanning transmission electron microscopy, searching for signs of a structural and electronic phase transition in this candidate $5d^1$ MIT compound. **Looking forward, we have identified promising trirutile and columbite materials to be explored jointly with IKZ as novel substrates for rutile thin films.**

References:

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