

Colour characteristics of nanocrystalline WO_{3-x} thin films as a function of their stoichiometry



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ANTECEDENTS

Stoichiometric WO₃ crystallizes in tetragonal or hexagonal structures based on corner-sharing WO₆ octahedra. Each W ion is surrounded by six O ions, ideally forming an octahedron; whereas each O ion is bound to two W ions in a linear configuration, which can be represented as $W^{6+}-O^{2-}-W^{6+}$ [1]. One may assume that the basic building blocks are similar in the amorphous material, even though bond lengths and bond angles exhibit considerable disorder.

Although stoichiometric WO₃ is a transparent oxide, there exist a number of sub-stoichiometric forms (WO_{3-x}) that exhibit different colours, from blue in the case of a slight oxygen deficiency to brownish for WO₂ [2].

APPROACH

In the present work, WO_{3-x} thin films have been obtained by reactive sputtering of a metallic target (99.9% purity) on unheated glass substrates. The oxygen to argon partial pressure ratio (O_{pp}) has been changed to analyse its influence on the structural, optical and electrical properties.

RESULTS

All the tungsten oxide films were found amorphous to the X-ray diffraction.

Figure 1 shows the optical transmittance, as a function of the radiation wavelength, for the tungsten oxide films deposited at different oxygen partial pressures O_{pp}.

Figure 2 represents the dependence of the absorption coefficient on the radiation energy, used to calculate the bandgap energy for the tungsten oxide films prepared at different O_{pp}.

Figure 3 displays the visible transmittance (at λ = 550 nm) and the electrical conductivity for the tungsten oxide films prepared at different O_{pp}.

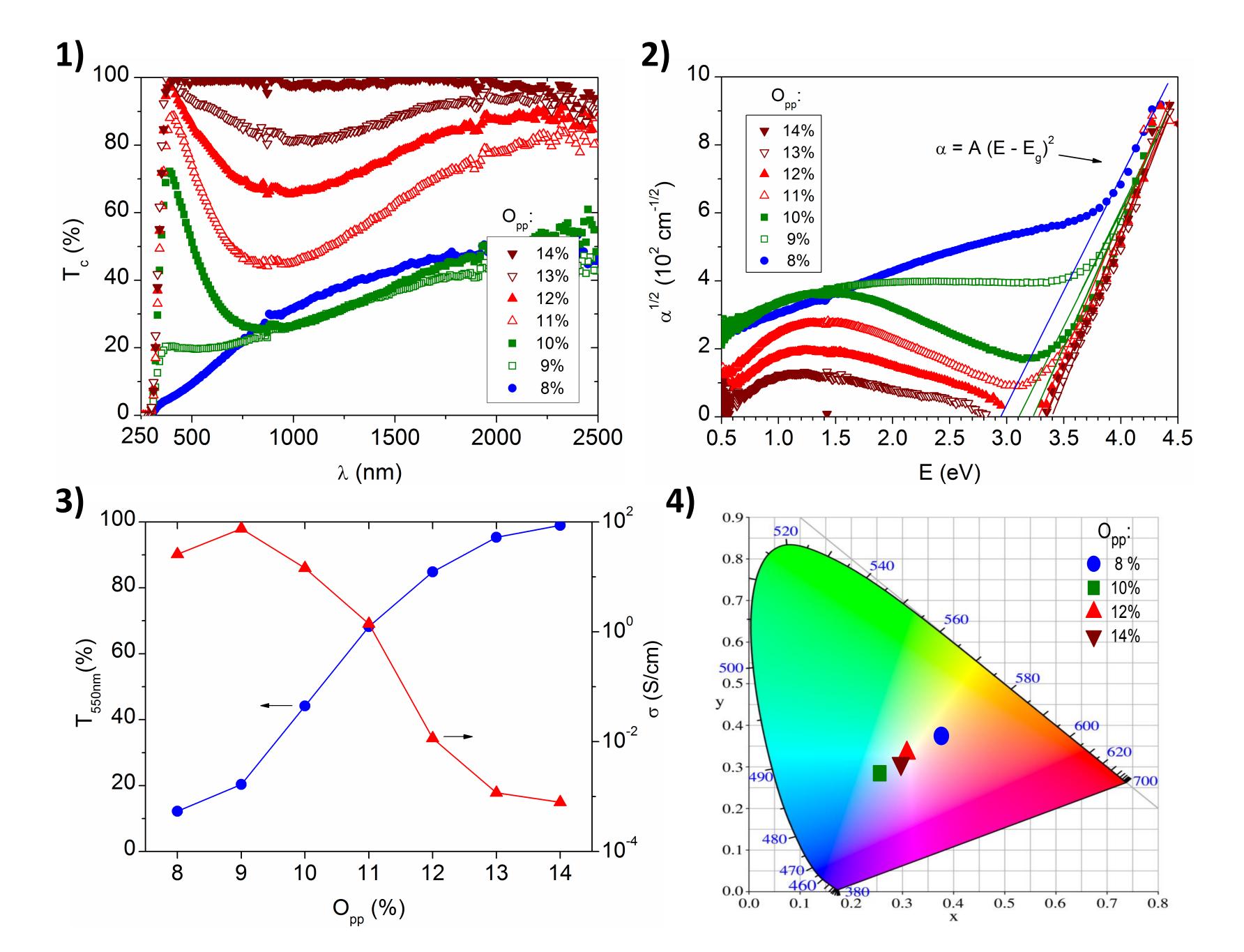


Figure 4 shows the colour characteristics (in the chromatic diagram CIE-1931) of tungsten oxide films deposited at different O_{pp} .

DISCUSSION

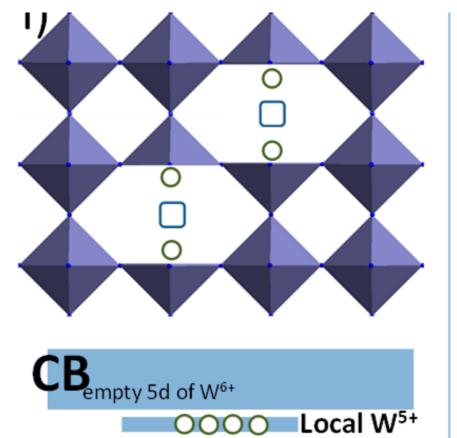
For the substoichiometric oxides, most common defects are the oxygen vacancies, which can be neutral (V_0^0) , singly charged (V_0^+) , or doubly charged (V_0^{2+}) with respect to the unperturbed lattice. The formation of a doubly charged vacancy and two W⁵⁺ ions seems to be energetically advantageous [3].

Absorption of light can arise from the phonon-mediated excitation of an electron in one such W⁵⁺ site to a neighbouring W⁶⁺ site [3, 4]. Such absorption in substoichiometric films has been controlled by the deposition conditions. This is useful for smart windows and

Sub-stoichiometric WO_{3-x} structure

← O layer - WO₂ layer ← O layer Oxygen Tungsten

Ideal cubic WO₃ structure and WO₆ octahedra



other related applications [4, 5].



CONCLUSIONS

WO_{3-x} thin films prepared by reactive sputtering on unheated substrates have different stoichiometries controlled by the oxygen partial pressure, which allows tuning their optical and electrical characteristics according to the specific application.



