

Cation-doped Cu₂O as a transparent p-type semiconducting oxide with enhanced performances: A comparison between strontium and magnesium incorporation

J. Resende^{1,2}, S. Brochen¹, L. Bergerot¹, C. Jiménez¹, N. D. Nguyen², J. L. Deschanvres¹

¹ Laboratoire des Matériaux et du Génie Physique, Univ. Grenoble Alpes, LMGP, F-38000 Grenoble, France; CNRS, LMGP, F-38000 Grenoble, France

² Solid State Physics, Interfaces and Nanostructures, Institut de Physique B5a, Allée du Six Août 19, B-4000 Liège, Belgique

joao.resende@grenoble-inp.fr

In the group of semiconducting metallic oxides, cuprous oxide (Cu₂O) presents promising electrical and manufacturing features for a variety of applications as p-type transparent material suitable in the domains of transparent electronics and photovoltaic cells. However Cu₂O suffers from optical and electrical limitations, due to a relatively small bandgap of 2.17 eV and a fairly high resistivity ($> 10^2 \Omega \cdot \text{cm}$) in intrinsic thin films at room temperature.

In this work, we successfully doped Cu₂O thin films with different divalent cations, namely Sr and Mg, by metal-organic chemical vapour deposition. We compared the effects of each element on crystallographic structure, films morphology, electronic transport and optical transmittance. In both cases, the presence of the cation contributed to a higher stability of the Cu₂O phase, reducing the appearance of CuO parasitic phase. Nevertheless, a SrCO₃ phase was detected in the Sr doped system. In terms of electrical properties, the incorporation of Sr, up to 16%, reduced the resistivity down to $1 \Omega \cdot \text{cm}$, with a mobility of $16 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$. Moreover, the incorporation of strontium also leads to the emergence of a deep acceptor level located around $E_A = 278 \pm 21 \text{ meV}$ above the top of the valence band. The concentration of this deep acceptor level, attributed to simple copper vacancies, drastically increases with the strontium content, due to a decrease of its formation energy. The effect on optical transmittance could not be detected. The Mg-doped Cu₂O thin films were monophasic and showed a higher resistivity of $6.6 \Omega \cdot \text{cm}$ at an Mg concentration of 17%, due to the lower mobility, $1 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$. Although, the presence of this dopant contributes for the highest charge-carrier density observed in this work, up to $8 \times 10^{17} \text{ cm}^{-3}$. As in the Sr case, this can be explained by a simple copper vacancy doping mechanism assisted by cation incorporation. Additionally, a slight increase of transparency is observed when compared to intrinsic Cu₂O.

The control of carrier concentration and mobility values by dopant concentration, as well as the improvements in phase stability and transparency are key factors for the application of this versatile p-type oxide in transparent electronics and solar cells applications.