The role of defects in Tuning the Properties of Highly Conductive Cuprous Oxide Thin Films revealed through Positron Annihilation Spectroscopy

Abderrahime Sekkat[1,2,3,*] Maciej Oskar Liedke[4], Viet Huong Nguyen[5], Maik Butterling[4], Federico Baiutti[6], Juan de Dios Sirvent Veru[6], Matthieu Weber[1], Laetitia Rapenne[1], Daniel Bellet[1], Guy Chichignoud[3], Anne Kaminski-Cachopo[2], Eric Hirschmann[4], Andreas Wagner[4], and David Muñoz-Rojas[1]

[1] Univ. Grenoble Alpes, CNRS, Grenoble INP, LMGP, F-38000 Grenoble, France
[2] Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, IMEP-LaHC, 38000 Grenoble, France
[3] Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMAP, 38000 Grenoble, France.
[4] Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328, Dresden, Germany
[5] Faculty of Materials Science and Engineering, Phenikaa University, Hanoi 12116, Vietnam
[6] Catalonia Institute for Energy Research (IREC), Jardins de Les Dones de Negre 1, Barcelona 08930, Spain

*abderrahime.sekkat@grenoble-inp.fr**

Cu_2O, being a non-toxic and abundant p-type semiconductor, is drawing a lot of attention for several energy applications. So far, the lowest resistivity values have been obtained for films deposited by physical methods and/or at high temperatures (~1000 °C), limiting their mass integration. In this work, Cu_2O thin films with record resistivity values of 0.4 Ω.cm were deposited at only 260 °C by atmospheric pressure spatial atomic layer deposition, a scalable chemical approach. The carrier concentration (7.10^{14}-2.10^{18} cm^{-3}), mobility (1- 86 $cm^2/V.s$), and optical bandgap (2.2-2.48 eV) can be simply tuned by varying the deposition parameters. Our results show that the transport properties of the films are correlated to the nature and concentration of defects, as revealed by positron annihilation spectroscopy (PAS) studies and density functional theory calculations. This study reveals the existence of large complex defects and the evolution of the overall defects concentration and transport properties evolving with varying deposition conditions, opening prospects for the adoption of Cu_2O.