Effect of oxygen pressure on optical and electrical properties of single-crystalline Cu_2O fabricated by pulsed laser deposition

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Copper oxide Cu_2O is an important and well known p-type transition metal oxide semiconductor material which has the advantages of direct band gap 2.1 eV and high absorption coefficient in the visible spectral range. This material has already been employed in the fabrication of electronic devices, thanks to its low cost, non-toxicity and fairly good carrier mobility. For example Cu_2O has been used in thin photovoltaic devices, resistive switching, transistors, gas sensors or catalysts.

In our work the epitaxial films Cu_2O (110) have been fabricated by Pulsed Laser Deposition on MgO(100) substrates maintained at temperature 700°C. Our attention was focused on the influence of the oxygen pressure, which was varied between 10^{-5} Pa and 10^{-1} Pa, on the structural and following on optical and electrical properties. The crystalline quality and out-of-plane orientation of the films were characterized by means of X-ray diffracton. The surface morphology and composition were characterized by Atomic Force Microscopy and XPS, respectively. The optical properties, complex dielectric constants, and optical gap, of the films were determined by spectral ellipsometry in the range of 250 - 1700 nm. Resistivity and Hall voltage measurements were carried out using the differential van der Pauw (vdP) method in a quasi-square arrangement at room temperature.

Because of Cu_2O is a natural p-type semiconductor, whose carrier concentration depends on copper and vacancies, our attention was focused on the examination of defects by means of Electron paramagnetic resonance (EPR) and Positron annihilation spectroscopy (PAS). EPR carried out in the temperature range from 5K to 700 K on Bruker ELEXSYS E580 at X-band. PAS measurement of Cu_2O films was carried out on a pulsed slow positron beam MePs at the Electron LINAC with high Brilliance and low Emittance (ELBE) facility at Helmholtz Zentrum Dresden-Rossendorf. The energy of incident positrons was varied in the range from 1 to 16 keV.

Two exponential components corresponding to positron annihilation in Cu_2O layer were resolved in lifetime spectra: (i) positrons trapped at vacancies and (ii) large vacancy clusters with lifetime τ_2 = 400 ps to 500 ps. The sample deposited under high oxygen pressure contains predominantly single copper vacancies V_{Cu} (τ_1 = 229 ps) while the sample deposited under low oxygen pressure contains complexes of copper vacancies coupled with oxygen vacancies (V_{Cu} + V_O and V_{Cu} + $2V_O$, τ_1 = 262 ps and 284 ps) due to the oxygen deficiency during the deposition. Since isolated oxygen vacancy is not able to trap positrons, it cannot be detected by positron annihilation spectroscopy. The sample deposited under low oxygen atmosphere contains bigger vacancy clusters compared to the sample deposited under high oxygen pressure.

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