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Non-equilibrium phase map, optical and electrical properties of Cu-Zn-O alloys ARCHANA SUBRAMANIYAN, Colorado School of Mines, Golden, CO, JOHN PERKINS, National Renewable Energy Laboratory, Golden, CO, RYAN O'HAYRE, Colorado School of Mines, Golden, CO, DAVID GINLEY, STEPHAN LANY, ANDRIY ZAKUTAYEV, National Renewable Energy Laboratory, Golden, CO — Cuprous oxide (Cu₂O) is a candidate p-type solar cell absorber material that has been spotlighted recently due to its low cost, earth abundant and non-toxic nature. The maximum reported efficiency of Cu_2O based solar cells is rather low (5. 38%) and it can in part be attributed its forbidden direct band gap (2.1 eV) and higher absorption threshold (2.6 eV). Here, we alloy Cu₂O with ZnO via combinatorial RF magnetron sputtering as a function of temperature (T) and composition at fixed 20 mTorr Ar pressure to modify the electronic band structure and reduce its absorption threshold, which can potentially enhance the solar cell performance. A non-equilibrium Cu-Zn-O phase map was generated in the T range 100 - 400 °C and Zn composition 0 - 37 at%. Highly crystalline Cu₂O structured Cu-Zn-O alloys with Zn content of 0 to 17 at% were synthesized in the T range 200 - 270 °C. With increasing Zn at%, the preferential orientation in Cu-Zn-O alloy changes from (200) to (111) direction. At lower T ($< 200 \, ^{\circ}\text{C}$), either amorphous or poor crystalline Cu₂O structured alloys were observed, whereas at higher T (>270 $^{\circ}$ C) and higher Zn composition (>25 at%), CuO or ZnO second phases were observed. The absorption coefficient of all Cu-Zn-O alloys was higher than that of phase pure Cu_2O . The absorption threshold () was also reduced significantly, for example, at = 2^{*10^4} cm⁻¹ the absorption threshold of Cu-Zn-O alloy with 10 at% Zn reduced from 2.4 eV to 2.1 eV. The electrical conductivity of all Cu-Zn-O alloys was measured to be within 2-5 mS/cm.

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