

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-principles study of oxygen enhanced wettability of copper on O-terminated ZnO surface EUN-AE CHOI, JUNG-HEUM YOON, SEUNG ZEON HAN, HAK-SUNG LEE, CHANG-SEOK OH, Korea Institute of Materials Science — Ultrathin films of metals such as copper have attracted much attention as a favorable candidate for flexible transparent electrodes due to high electrical conductivity and good ductility. However, the growth of islands results in high sheet resistance and low transmittance of metal ultrathin films. Here, we suggest that oxygen at the initial stage of Cu deposition can suppress the growth of Cu islands on O-terminated ZnO surface. We perform the density functional calculations for formation energies and electronic structures of Cu thin films on ZnO surface. Our calculations show that oxygen atoms stabilize both of the Cu/ZnO interface and the surface of Cu thin films. In addition, we extract the spreading parameter (S) of Cu films based on the simulations, showing the complete wetting of Cu at low concentration of oxygen. Finally, we confirm experimentally oxygen enhanced wettability of Cu on O-terminated ZnO substrate.

Byungki Ryu
Korea Electrotech Res Inst

Date submitted: 11 Nov 2016

Electronic form version 1.4