Interpreting O 1s XPS spectra: oxygen vacancies are invisible

Terry J. Frankcombe

School of Science, University of New South Wales, Canberra, ACT, Australia.
T.Frankcombe@adfa.edu.au

X-ray photoelectron spectroscopy (XPS) is a widely-used experimental technique for probing ionic environments in solids. Under X-ray bombardment, the kinetic energies of photoelectrons emitted from core states reveal information about the oxidation state of the parent ions as well as the surrounding material environment.

The lattice oxygen of metal oxides typically gives a strong XPS signal at 530 eV, being the binding energy of the O 1s electrons. For almost fifty years a weaker peak at 531 eV has been interpreted as being from "oxygen deficient regions", a.k.a. lattice oxygen vacancies. By explicitly calculating O 1s energy levels in ZnO crystals and crystalline surfaces we can demonstrate that this is a fiction. No (electrically neutral) bulk oxygen defects result in higher 1s binding energies. The observed 531 eV and 532 eV features correspond to O 1s electrons from surface species.