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MODIFICATION OF THE LOCAL STRUCTURE OF OXYGEN IN CdO UNDER IRRADIATION

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We have studied the effects of high concentration of point defects on the electronic structure of CdO. The defects were introduced by irradiation with high energy Ne ions. The "*as-grown*" and "*irradiated*" samples were investigated at the Advanced Light Source (ALS) Lawrence National Berkeley Laboratory at the beamline 11.0.2. Significant differences between experimental near edge x-ray absorption fine structure (NEXAFS) spectra gathered in total fluorescence yield (TFY, bulk sensitive) and total electron yield (TEY, rather surface sensitive) detection modes are observed. Such observation makes clear that irradiation process drastically modifies the surface layer of investigated films.

An interpretation of NEXAFS spectra at the *K*-edge of oxygen in "*as-grown*" and "*irradiated*" CdO films, within the *ab-initio* real space multi-scattering (RSMS) formalism applying the FEFF8 code, with many-body effects incorporated in terms of final-state potentials and complex energy-dependent self-energy, will be shown.

Different models with point defects (namely oxygen vacancy and cadmium interstitials) in the host CdO matrix were considered and respective theoretical spectra were calculated. Basing on the RSMS theory, we are able to interpret the experimental spectra in terms of changes in the local atomic (geometrical) and electronic structure around oxygen atoms.

Comparison of the experimental ("*irradiated*" versus "*as grown*") and theoretical data allows to conclude that electronic levels of defects push the Fermi level into the conductive band, thus modify the charge transfer around the oxygen atoms with the defected local atomic order what leads to the shift of the absorption threshold to a higher energy. The observed leading edge differences of TFY and TEY spectra could be likely explained basing on electron accumulation at the surface of n-type CdO due to the presence of positively charged donor-type surface states. Our conclusions are confirmed by optical absorption measurements.