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Local Structures Around S in CdS:O Thin Films Photovoltaic Materials Probed by S K-edge X-ray Absorption Fine Structures[1] Y. L. SOO, W. H. SUN, S. C. WENG, Y. S. LIN, S. L. CHANG, National Tsing Hua University, Taiwan, L. Y. JANG, NSRRC, Taiwan, X. WU, Y. YAN, NREL — Local Structures around S in thin films of CdS:O have been investigated using EXAFS and NEXAFS techniques at the S K absorption edge. Our S K-edge EXAFS results clearly indicate the presence of S-O bonds that coexist with S-Cd bonds in the oxygen-containing samples. The S K-edge NEXAFS data further identify SO_3 and SO_4 complexes in the samples. As indicated by our previous results on Cd K-edge EXAFS, Cd atoms are predominantly bonded with S. These x-ray results demonstrate that the oxygen atoms actually combine with S to form SO_3 and SO_4 complexes instead of being incorporated into the CdS host. In combination with the evidence of nanoparticles revealed by TEM, our results suggest that oxygen-free CdS nanocrystals are formed in the films due to the O content. The bandgap of the samples is therefore found to increase with O concentration as opposed to the bandgap decrease for O doping expected in the band anticrossing model.

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Yun-Liang Soo
National Tsing Hua University

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