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Cu K-edge XAFS in CdTe before and after treatment with $CdCl_2$

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ABSTRACT

We have used the fine structure in the Cu K-edge x-ray absorption spectrum to help elucidate the lattice location of Cu in polycrystalline, thin-film CdTe solar cells. In particular, we have studied how the typical $CdCl_2$ vapor treatment in dry air changes the local environment of the Cu in CdTe. We find the Cu absorption spectrum to be similar to that of Cu_2Te in the as-deposited CdTe film but to convert to a spectrum similar to Cu_2O environment after the vapor $CdCl_2$ treatment.

INTRODUCTION

High performance CdS/CdTe thin film solar cells are usually completed with a low resistance Cu back contact. The copper appears to be critical for achieving heavy p-type doping of the CdTe at the contact. It is also known that Cu doping can increase the open-circuit voltage. However, copper is also a fast diffuser, [1] which can accumulate at CdS/CdTe junction and is suspected of playing a role in cell performance deterioration under certain conditions.

High-temperature $CdCl_2$ treatment in the presence of oxygen is a critical step needed to improve the performance of CdTe thin-film cells, which can improve the cell efficiency a factor of two or more.[2,3] However the process is not well understood yet. Thus, for this study, samples were prepared through the same processes as completed cells except that the transparent conducting oxide (TCO) and CdS layers were omitted.

X-ray absorption fine structure (XAFS) is a powerful technique in materials science research for understanding the lattice environment around designated element atoms, which include two independent parts: the x-ray absorption near edge structure (XANES) and the extended x-ray absorption fine structure (EXAFS). The XANES is the absorption fine structure spectrum covering the range between the absorption edge of the element itself and the point usually considered to be 50 eV beyond the threshold. The EXAFS is the periodic oscillatory structure in the absorption spectrum above the edge due to the phase difference between back-scattered and out-going electron waves. The lattice environments are derivable from absorbance spectra by mathematically converting the EXAFS spectrum into a radial distribution function (RDF).

EXPERIMENTAL DETAILS

The 2-3 micron CdTe layers were magnetron sputtered at ~ 250 $^{\circ}$C, as described in paper B3.7 of this proceeding, onto either fused silica or Kapton polyimide sheet (from DuPont High Performance Materials) substrates [4]. All the samples were prepared with 40 ~ 200 Å