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Thin Solid Films 480–481 (2005) 95–98

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Cu K-edge X-ray fine structure changes in CdTe with $CdCl_2$ processing

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Abstract

We have used the MR-CAT beamline of the Advanced Photon Source at Argonne National Laboratory to study the fine structure in the Cu K-edge X-ray absorption in 3 μm thick polycrystalline films of CdTe on fused silica. About 4 nm of evaporated Cu is diffused either with or without prior vapor $CdCl_2$ treatments in dry air. Cu absorption is monitored through the Cu K_α fluorescence using a 13-element Ge detector. The absorption fine structure indicated predominantly Cu_2Te when Cu was diffused into the as-deposited CdTe film but a Cu_xO environment when Cu was diffused *after* the vapor $CdCl_2$ treatment. We believe most of the diffused Cu decorates grain boundaries as oxides, consistent with the low doping densities typically observed in CdTe solar cells. The significance for grain boundary passivation will be discussed.

Keywords: CdTe; $CdCl_2$ processing; Cu K-edge X-ray fine structure

1. Introduction

High performance CdS/CdTe thin film solar cells are usually completed with a low resistance back contact containing Cu. The copper appears to be critical for achieving heavy p-type doping of the CdTe at the contact. Since CdTe is a material with high electron affinity (χ_A=4.28 eV), a back contact to the p-type CdTe would require a material (usually metal) with a work function of $W=\chi_A+E_g\approx 5.78$ eV to achieve flat-band conditions appropriate for hole transport. Since there are no common metals that satisfy this criterion, the second approach is to fabricate a heavily doped CdTe layer at the back contact to allow for tunneling. Thus essentially all successful stable back contacts to CdTe have involved the use of copper to create a heavily doped layer next to the metal. In our relatively thin (2–2.5 μm CdTe) sputtered cells, we have successfully used very thin evaporated Cu (3 nm) followed by evaporated Au (10–20 nm) to achieve 14% efficiency cells at AM 1.5 [1]. If all of the Cu were evenly diffused through the CdTe, one could expect a Cu density of $\sim 10^{20}$ cm^{-3}. However, C–V measurements of CdTe cells from several laboratories indicate maximum acceptor densities in CdTe of $\sim 5\times 10^{14}$ cm^{-3} [2]. Thus most of the Cu is inactive. The goal of our measurements was to identify the lattice location of most of the Cu in CdTe.

X-ray absorption fine structure (XAFS) is a powerful technique for understanding the lattice environment around selected elements. The periodic oscillatory structure, known as extended X-ray absorption fine structure (EXAFS), in the absorption spectrum above the edge due to the phase difference between back-scattered and out-going electron waves is the key to this technique. The lattice environments are derivable from the Fourier transform of the EXAFS spectrum [3,4].

By using the fine structure in the Cu K-edge X-ray absorption spectrum we can elucidate the predominant 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 subsequently diffused into CdTe.

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

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doi:10.1016/j.tsf.2004.11.116