Cu K-edge EXAFS Studies Of $CdCl_2$ Effects On CdTe Solar Cells

Xiangxin Liu,[1] Alvin D. Compaan,[1] and Jeff Terry[2,3]
[1]*Department of Physics and Astronomy, The Univ. of Toledo, Toledo, OH 43606*
[2]*Department of Biological, Chemical, and Physical Sciences, Illinois Institute of Technology, Chicago IL 60616*
[3]*Department of Physics, University of Notre Dame, Notre Dame IN 46556*

ABSTRACT

The highest performance CdS/CdTe thin film solar cells are generally completed with a Cu-containing back contact. The copper appears to be critical for achieving heavy p-type doping of the CdTe at the contact to permit the formation of a low resistance contact. In previous extended x-ray absorption fine structure (EXAFS) work we have inferred that most of the Cu in CdTe films resides as Cu_2O at the boundaries of CdTe grains in films that have received a chloride treatment in the presence of oxygen, a critical step needed to improve the performance of all CdTe thin-film cells. This has suggested a mechanism for grain boundary passivation in thin-film CdTe solar cells. 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. We also find evidence that the grain-boundary Cu_2O in $CdCl_2$ treated CdTe films is unstable and tends to transform to CuO under some stress conditions.

INTRODUCTION

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.[1,2] Fitting with theoretical standards derived from the *ab initio* multiple-scattering code FEFF [3] is then performed to obtain more detailed information about the near-neighbor distance and the coordination numbers of the environment surrounding the interested atoms. 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.

$CdCl_2$ treatments near 400 °C in the presence of oxygen are a critical step needed to improve the performance of CdTe thin-film cells. This $CdCl_2$ activation can improve the cell efficiency a factor of two or more[4,5] However the process is not yet well understood. Oxygen in the air or in the He/O_2 or Ar/O_2 atmospheres during the chloride process is probably active in passivating the grain boundaries although some may also be active in forming doping complexes. Visoly-Fisher and Cahen [6] with scanning probe microscopy have observed potential barriers at the grain boundaries which are consistent with this grain boundary passivation model. Our XAFS measurements suggest that virgin sputtered films (without post-deposition $CdCl_2$ treatment) which receive typical amounts of Cu at the back contact, yield XAFS spectra indicating that Cu resides in a Cu_2Te environment; however, if films are prepared *with* the chloride treatment, most of the Cu ends up bound with oxygen as Cu_2O or CuO.[2] Details are given in our previous