Spectroscopic, topological, and electronic characterization of ultrathin *a*-CdTe:O tunnel barriers

Ivan Dolog, Robert R. Mallik,[a] Dan Malz, and Anthony Mozynski
Department of Physics, The University of Akron, Akron, Ohio 44325-4001

(Received 6 October 2003; accepted 17 December 2003)

Ultrathin oxygenated amorphous CdTe (*a*-CdTe:O) films are prepared by rf sputtering of CdTe in a background of argon or argon/nitrogen/oxygen mixtures. Atomic force microscopy (AFM) is used to characterize the films and shows that they have an island structure typical of most sputtered thin films. However, when sufficiently low powers and deposition rates are employed during sputtering, the resulting films are remarkably smooth and sufficiently thin for use as barrier layers in inelastic electron tunneling (IET) junctions. Four terminal current–voltage data are recorded for Al/*a*-CdTe:O/Pb tunnel junctions and conductance–voltage curves are derived numerically. WKB fits to the conductance–voltage curves are obtained using a two-component trapezoidal plus square (TRAPSQR) model barrier potential to determine values for the tunnel barrier parameters (height, shape, and width); these parameters are consistent with AFM topological measurements and values from similar devices reported in the literature. IET spectra are presented which confirm that electrons tunnel through ultrathin regions of the *a*-CdTe:O films, which contain aluminum oxide subregions in a manner consistent with the TRAPSQR barrier model. Because tunneling occurs predominantly through these ultrathin regions, IET spectroscopic data obtained are representative of states at, or within a few tenths of nanometers from, the surface and confirm that the *a*-CdTe:O surface stoichiometry is very sensitive to changes in the argon/oxygen/nitrogen concentration ratios during film growth. Full IET spectra, current–voltage, and conductance–voltage data are presented together with tunnel barrier parameters derived from (WKB) fits to the data. The results presented here indicate that inelastic electron tunneling spectroscopy is a useful tool for characterizing the surface states of *a*-CdTe:O and possibly other photovoltaic materials. [DOI: 10.1063/1.1647259]

I. INTRODUCTION

CdTe is one of the most promising semiconductor materials for high-efficiency thin-film photovoltaic cells. It has a direct band gap in the range 1.4–1.5 eV, which is near the maximum solar energy conversion point. Other advantages spectroscopy,[10] and deep level transient spectroscopy.[11] In this article, we use inelastic electron tunneling spectroscopy (IETS), which been used previously to study the vibrational spectra of ultrathin sputtered films of germanium oxide,[12] silicon and its oxides,[13,14] and evaporated silicon and its oxides.[15] In this technique, inelastic scattering of electrons tunneling through a thin-film barrier in a metal/barrier/metal tunnel junction is employed to excite vibrational, optical, and electronic modes in the barrier material. Using IETS to study thin films has an advantage over Raman and IR spectroscopy because the signal to noise ratio for IETS increases for thinner adsorbed layers, whereas it decreases for Raman and IR. This enhances the ability of IETS to detect surface states. Also, optically forbidden modes can be observed as strong peaks. IETS can detect fractional monolayer coverage and has been used to study many complex systems.[16]

The IET barrier parameters (height and width) have a great influence on the elastic and inelastic components of the tunnel current. This influence can be investigated by modeling the metal/barrier/metal system using the WKB approximation. This has been done for alumina tunnel barriers with and without adsorbed molecular layers.[17–19] However, the literature indicates this has not been done for CdTe IET barriers. In this article, we present results of a study of thin, *a*-CdTe:O films using IETS. We also determine model tunnel barrier parameters such as height, width, and shap277.3(of).

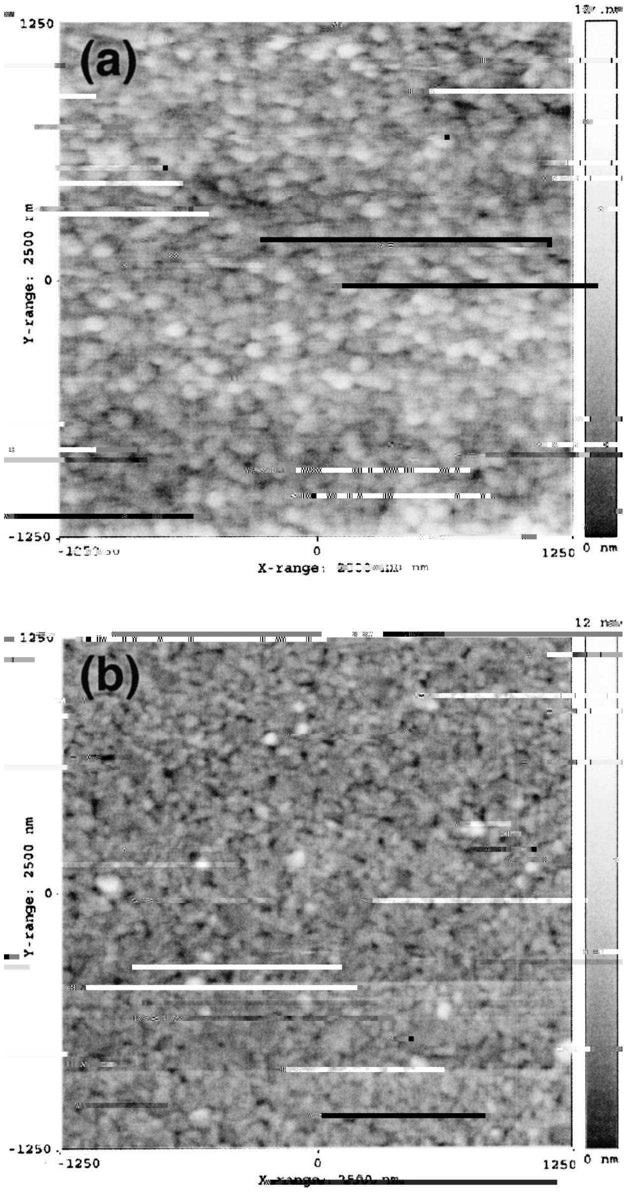

FIG. 1. (a) AFM image of a 16-nm-thick *a*-CdTe:O film sputtered onto a thin-film aluminum electrode supported on a glass microscope slide. The *a*-CdTe:O film shows structure typical of island growth. The islands are approximately 11-nm-thick (z direction) and 40–70 nm diameter ($x-y$ plane). (b) AFM image of a ~100 nm aluminum film, of the type used for the present IETS measurements, evaporated onto a glass microscope slide. This is representative of the structure below that of Fig. 1(a).

onto a clean glass microscope slide. As can be seen, a much finer granular structure is observed. From this we can be sure that the larger islands observed in Fig. 1(a) are indeed *a*-CdTe:O.

In order to record tunnel currents sufficiently large for IETS, it is necessary for the effective barrier thickness to be of the order of <3 nm. Since we are able to record IET spectra (see Sec. III C later) it is evident that tunneling does not take place uniformly through the entire barrier, which has an average thickness of approximately 10 nm. Rather, tunneling occurs preferentially through thinner regions of the tunnel barrier. Based upon the AFM characterization of our films (earlier), and subsequent IET measurements, we believe an idealized cross-section of the IET junctions can be represented schematically as shown in Fig. 2. We believe thin regions of aluminum oxide exist on the aluminum electrode, while clusters of *a*-CdTe:O form to create a quasicontinuous granular film. For subsequent modeling of the tunnel barrier (see Sec. III B later) we assume that tunneling occurs predominantly through regions containing both alumina and *a*-CdTe:O as indicated by the arrows in Fig. 2.

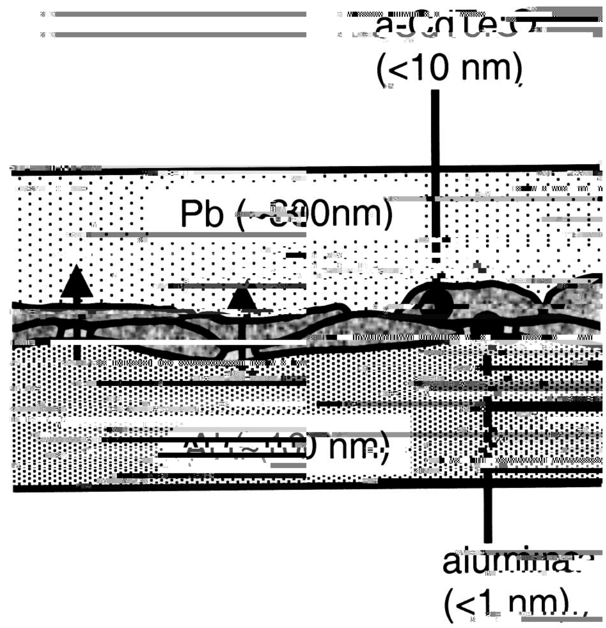

FIG. 2. Schematic cross section of an Al/*a*-CdTe:O/Pb tunnel junction (not to scale) indicating nominal film thicknesses. Thicknesses for the aluminum and lead electrode films are not critical. The average thickness of the *a*-CdTe:O island layer is determined by a quartz crystal monitor. IET spectral data and WKB fits to tunneling conductance–voltage measurements indicate that nanoscale subregions of alumina are interspersed as shown.

B. Model barrier parameter calculations

A typical $I-V$ curve for an Al/*a*-CdTe:O/Pb tunnel junction is shown in Fig. 3. The junctions are remarkably linear up to about ± 0.6 V with an approximately 10%–30% change in the conductance (the magnitude of the change depends on whether the junction is under forward or reverse

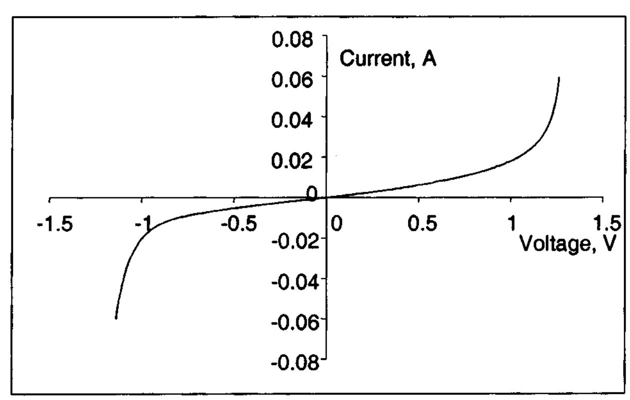

FIG. 3. Typical $I-V$ curve for an Al/*a*-CdTe:O/Pb tunnel junction. The slope change from 0 V to approximately ± 0.6 V is typically 10%–30% and is asymmetric with bias polarity.

bias). However, at higher voltages exponential behavior is observed. The derivative of the curve was obtained numerically to give the $G-$

3628 cm^{-1} are more noticeable in the second spectra, Fig. 7(b), since more oxygen is present in the chamber during preparation.

IV. CONCLUSIONS

Remarkably smooth ultrathin films, suitable for IET spectroscopy, can be produced by sputtering commercially available CdTe source material in a background of either argon or argon/nitrogen/oxygen. AFM measurements presented here have shown that the films exhibit an island structure, with typical island dimensions of 40–70 nm in the $(x-y)$ plane of the IET junction, and ~10 nm in the z direction. Electron tunneling $G-V$ measurements provide evidence that electrons tunnel predominantly through thinner regions of the films, as one would expect. IET spectroscopic measurements indicate that these regions, which are representative of the surface of the sputtered films, are composed of a-CdTe:O and incorporate interspersed nanoscale subregions of aluminum oxide. IETS confirms that the stoichiometry of these regions is very sensitive to small fluctuations in the argon/nitrogen/oxygen concentrations during film growth. Notwithstanding the complexities of determining the exact composition of the barrier material, it is possible to obtain reasonable WKB fits to the experimental $G-V$ curves by assuming a simple two-component TRAPSQR barrier model comprising of the a-CdTe:O islands and alumina subregions. WKB fits are achieved by using values for the effective tunnel barrier region thicknesses, based on AFM topological measurements, and heights based on plausible values from the literature suitably modified to take into account surface effects and compositional changes. To summarize, we have shown that the combination of AFM, IETS, and tunneling $G-V$ measurements provide self-consistent results which are very useful for determining the composition and topology of ultrathin sputtered a-CdTe:O films, and, by extension, possibly other photovoltaic materials.

ACKNOWLEDGMENTS

The authors would like to thank Research Corporation for a Cottrell College Science Award, which provided two of the authors (D.M., A.M.) with studentships and a research fellowship for another (R.R.M.). They are also grateful to Professor Sergei Lyuksyutov, for the use of his class-100 clean-room facilities for the AFM measurements.

[1] H. Uda, A. Nakano, K. Kuribayashi, Y. Komatsu, H. Matsumoto, and S. Ikegami, Jpn. J. Appl. Phys., Part 1 **22**, 1822 (1983