A Scanning Probe Microscopy Study of Cd$_{1-x}$Zn$_x$Te

C.K. EGAN,1,3 P. DABROWSKI,2 Z. KLUSEK,2 and A.W. BRINKMAN1

1.—Department of Physics, Durham University, South Road, Durham DH1 3LE, UK. 2.—Division of Physics and Technology of Nanometer Structures, Department of Solid State Physics, University of Lodz, Pomorska 149/153, 90-236 Lodz, Poland. 3.—e-mail: c.k.egan@durham.ac.uk

The effects of several ex vacuo methods used in the surface preparation of Cd$_{1-x}$Zn$_x$Te (CZT) have been studied using noncontact atomic force microscopy, scanning tunneling microscopy, and scanning tunneling spectroscopy. Preparation techniques include mechanical lapping, hydroplane bromine-methanol polishing, and in vacuo annealing. The morphology, electrical homogeneity, and local density of states (LDOS) have been studied for each preparation method. Impurities and oxides quickly form on the surface after each preparation method. Annealing in ultrahigh vacuum causes the surface electronic structure to become inhomogeneous whilst the LDOS suggests a compositional change from an oxide surface to p-type CZT.

Key words: Cd$_{1-x}$Zn$_x$Te, surface, STM, STS, CITS

INTRODUCTION

Cd$_{1-x}$Zn$_x$Te (CZT) is a material that has some very useful properties, making it applicable to a wide variety of applications. Currently, the most prominent application is the use of CZT as a detector material in x-ray and gamma-ray solid-state pixilated detectors.1,2 The construction of such devices requires the deposition of good-quality metallic contacts.3 Polishing and etching of CZT in Br$_2$/MeOH solution is a common surface preparation method for producing damage-free surfaces after mechanical lapping. It has been reported that this produces a Te-rich surface which quickly oxidizes, forming TeO$_2$.4 The formation of a surface oxide directly controls the surface leakage current and contact ohmicity both rely upon the nanoscale topography and composition of surfaces.5 Polishing and etching of CZT in Br$_2$/MeOH solution is a common surface preparation method for producing damage-free surfaces after mechanical lapping. It has been reported that this produces a Te-rich surface which quickly oxidizes, forming TeO$_2$. The formation of a surface oxide directly controls the surface leakage current and contact ohmicity. Here scanning probe microscopy techniques [noncontact AFM, scanning tunneling microscopy (STM), and scanning tunneling spectroscopy (STS)] have been used to study the effects of common surface preparation methods used on CZT for electrode deposition. In particular, STS is an effective probe of the surface electronic structure, giving information about the local density of states (LDOS) and surface states, and can also be used as a compositional analysis tool.5,6

EXPERIMENTAL PROCEDURE

All experiments were performed in an ultrahigh vacuum (base pressure ~2 × 10$^{-10}$ mbar) Omicron SPM equipped with in vacuo cleaning facilities. STM/STS measurements were made using mechanically sectioned platinum–iridium wire. Noncontact AFM measurements were made using Omicron Needle Sensor tips operating at a resonant frequency of ~1 MHz.8,9 Samples were grown by the multitube physical vapor transport (MTPVT) method with a zinc concentration of ~3%.10 Various surface preparation methods were investigated: mechanical lapping followed by hydroplane polishing in Br$_2$/MeOH solution, chemical passivation in H$_2$O$_2$, and in vacuo annealing. All samples were cleaned with methanol and dried with nitrogen prior to loading into vacuum via a fast-entry load lock. STM/STS measurements
were performed in constant-current mode with a bias of \(-4\) V and a tunnel current of 0.2 nA. Spectroscopy measurements were made using a resolution of 128 points per curve. From this current imaging tunneling spectroscopy (CITS) images were produced. The normalization procedure proposed by Feenstra where differential conductance is divided by total conductance \([dI/dV]/(I/V)\) was applied to \(I-V\) curves using a broadening of 1.5 V to overcome the divergence problem. The normalization is generally considered to yield values that are proportional to the LDOS around the Fermi energy.\(^5\) Surface roughness analysis was made by taking the average over multiple nc-AFM topographic images using a number of different tips.

**RESULTS AND DISCUSSIONS**

**Mechanical Lapping**

Figure 1 shows the surface morphology over large and small areas taken using nc-AFM for a mechanically lapped and polished sample, using a final grit size of 0.1 \(\mu\)m. Scratches are clearly visible and are a common feature after such a process.\(^{11,12}\) By taking line profiles the scratches were found to be typically 5 nm deep and 100 nm wide. The surface roughness is summarized in Fig. 2. It can be seen that lapping produces the smoothest surfaces over small areas (\(<500\) nm \(\times\) \(500\) nm), the increase in roughness for larger areas can be explained by the scratches on the surface since the typical distance between them is \(>500\) nm. CITS images (not shown) reveal that the surface electronic structure is homogeneous, however normalized conductance spectra (Fig. 3) show that the surface is insulating since conduction-band states can only be probed at biases greater than 7 V. This suggests that the surface has absorbed a large number of impurities either during or after the lapping process.

**Br\(_2/MeOH\) Hydroplane Polishing**

Figure 4 shows the surface morphology after hydroplane polishing in 1% Br\(_2/MeOH\) solution. The scratches observed after lapping have been removed, leaving a more uniform surface. The surface morphology has changed, producing smaller features, and the roughness over small areas (Fig. 2) has increased. However because the surface scratches have been removed the large-area roughness has been reduced. CITS images (not shown) again reveal that the electronic structure is homogeneous, whilst normalized conductance spectra show that the surface band gap has been reduced to around 4 eV. It has been suggested in the past that Br\(_2/MeOH\) etching produces a Te-rich surface, a suggestion which is not supported by the present study since the Te band gap is around 0.35 eV.\(^{12}\) On the other hand, the band gap observed here is consistent with TeO\(_2\), perhaps suggesting that the surface quickly oxidized between polishing, cleaning, and loading into vacuum.\(^{13}\)

**Annealing in UHV**

A lapped and hydroplane polished sample was annealed in ultrahigh vacuum (UHV) for 2 h at 400°C. The STM topographic image is shown in Fig. 5 and demonstrates that the topography has been altered, producing more elongated features. The directional correlation seen in Fig. 5 is representative of the whole surface and could be due to the crystal orientation; however the exact origin is unknown and requires further investigation. The annealing process has caused the overall surface roughness to increase, whilst the roughness over large and small areas has approached one another (Fig. 2). This is probably due to vaporization of