Formation of $Cd_2Te_2O_7$ Phase Induced by Chemical Etching and its Influence on the Electrical Properties of Au/CdTe Contact

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Supplementary Materials

I Supplementary Figures

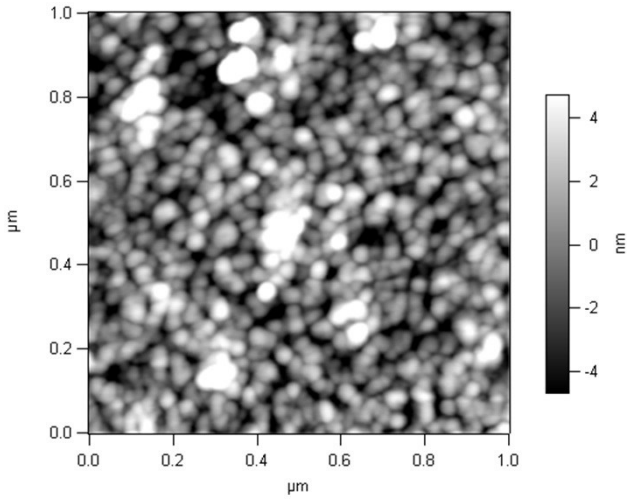

Figure S1 AFM image of CdTe surface after 20 min chemical etching in 2% Br_2-MeOH solution shows no significant change in both surface morphology and roughness when compares with the sample etched for 10 min.

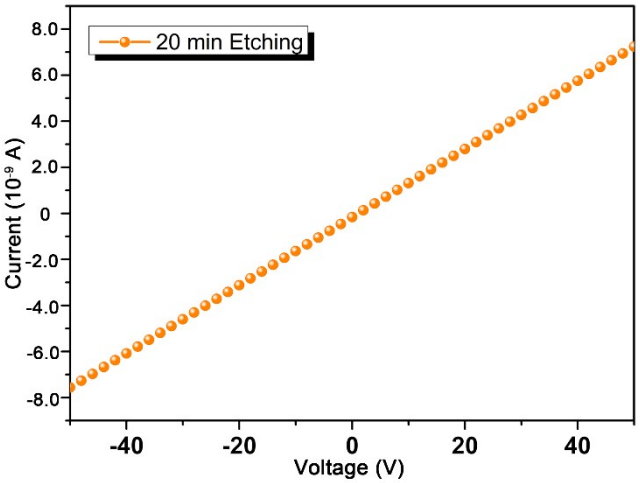

Figure S2 I-V curve of Au/CdTe contact structure after 20 min chemical etching.

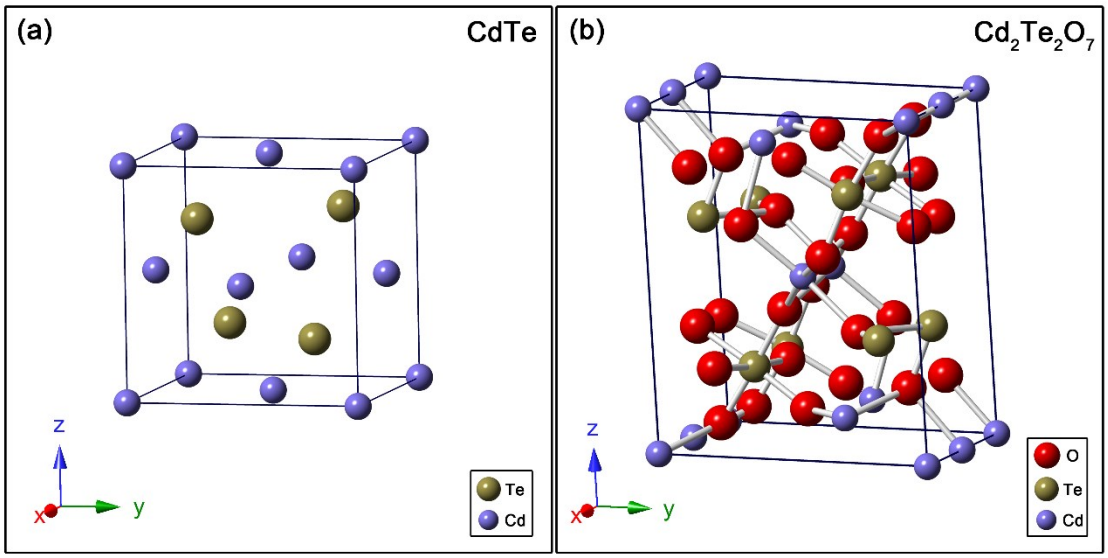

Figure S3 Structure unit cells of CdTe (a) and $Cd_2Te_2O_7$ (b).

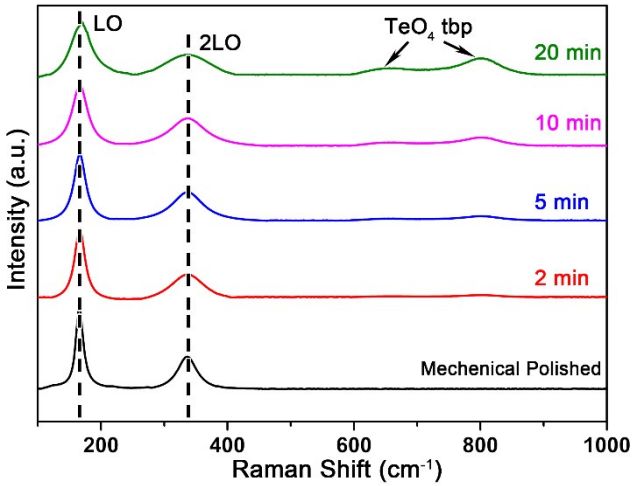

Figure S4 Raman spectroscopy of CdTe wafers under different surface treatments.

II Determination of orientation relationships between CTO and CdTe

The determination of orientation relationships between CTO and CdTe is completed with the help of Stereographic Projection 2.0.1 software in this work. Specifically, the lattice parameters of CTO and CdTe have been firstly inputted to the software. The pole center is set to be $(110)_{CdTe}//(0.4245, 0.7817, 2.0394)_{CTO}$ based on the TEM results. Here, all the indices are expressed by lattice plane indexing. Therefore, $(110)_{CdTe}$ is also the normal plane of $[110]_{CdTe}$, while $(0.4245, 0.7817, 2.0394)_{CTO}$ is calculated to be the normal plane of $[012]_{CTO}$. The first parallel relationship just corresponds to the viewing direction in TEM observation. According to the Weiss zone law, all the diffraction planes appears under the viewing direction along a certain zone axis must contain a vector parallel to such zone axis. In the stereographic projections, the spots representing these diffraction planes must fall on the large circle when the public zone axis has been set as the pole center. In this case, a mutual rotation of 36° and 145° can be applied to obtain the second parallel relationships of $(100)_{CTO-I}//(1\bar{1}1)_{CdTe}$ and $(100)_{CTO-II}//(\bar{1}11)_{CdTe}$ for variant 1 and 2 respectively. Finally, the last parallel relationships can be determined by finding the indices of lattice planes perpendicular to the second parallel relationships on the large circle. Such relationships can be confirmed to be $(\bar{1}\bar{8}4)_{CTO-I}//(\bar{1}12)_{CdTe}$ and $(18\bar{4})_{CTO-II}//(1\bar{1}2)_{CdTe}$ for variant 1 and 2 respectively. Figure S5 illustrates the stereographic projections of the two orientation relationships between CdTe and CTO-$_{V1/V2}$ respectively. The red and blue spots represent the lattice planes of CTO and CdTe respectively.

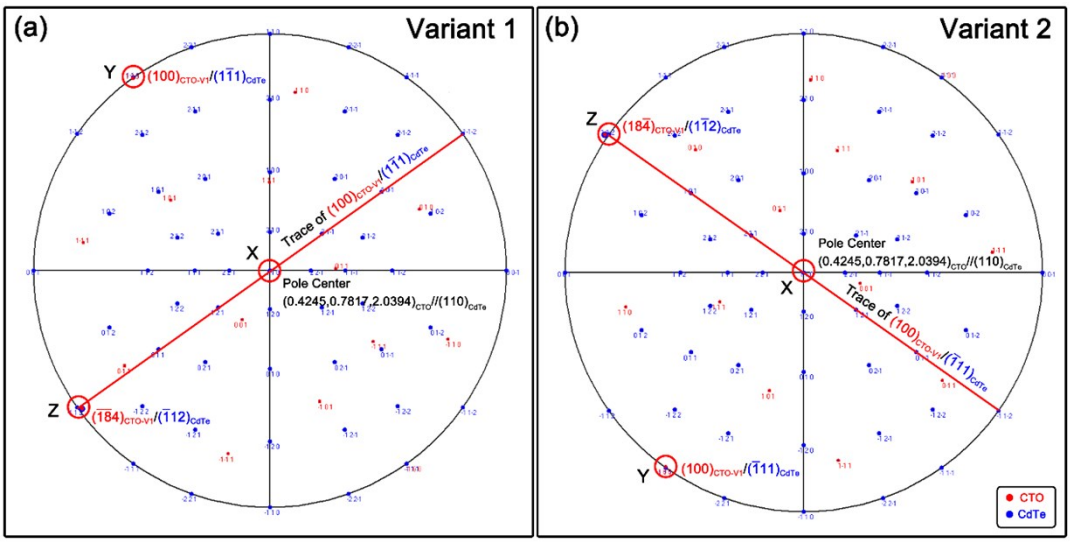

Figure S5 Stereographic projection of planes for the established orientation relationships between CTO and CdTe: (a) variant 1; (b) variant 2.