

Changes of Fermi Surface Topology due to the Rhombohedral Distortion in SnTe

This data repository is organised as follows:

All figures are included as pdfs.

Files containing data for Figure 1;

Energetic landscape of rhombohedral distortion Fig 1(b); EN_SURF_fig_1b.txt.

Fm3m band structure Fig1 (c)(i); Fig1_c_i_bands-Fm-3m-L-G-X-W-K-G-L.dat.

R3m band structure Fig 1(c) (ii); Fig_1_c_ii_bands-R3m-L-G-F-B-P-G-Z.dat.

Density of states Fm3m structure Fig 1(e); DOS_Fm-3m_fig_1e.txt.

Density of states R3m structure Fig 1(e); DOS_R3m_fig_1e.txt.

Files containing data for Figure 2;

Measured ARPES data Figure 2(a); Fig2a.txt.

Measured ARPES data Figure 2(c); Fig2c.txt.

Measured ARPES data Figure 2(d); Fig2d.txt.

Graphic DFT calculated ARPES Fig 2(c); DFT_ARPES_kz=0_fig2c.png.

Graphic DFT calculated ARPES Fig 2(d); DFT_ARPES_kz=pi/a_fig2d.png.

Details of graphics; DFT_ARPES_README.txt.

Files containing data for Figure 3;

Resistivity curve Fig 3(a); Resistivity_Fig3a.txt.

Magnetoresistance data for applied field angle in Fig 3(b) are; MR_\$\$deg_Fig3b.txt. Here \$\$ is given in the file name and corresponds to the applied field angle.

Oscillations at 0 degrees in Figure 3(c); Delta_MR_0deg_Fig_3c.txt.

Oscillations at 45 degrees in Figure 3(c); Delta_MR_45deg_Fig_3c.txt.

Fourier transforms of oscillations at 0 deg in Figure 3(d); Delta_MR_FFT_0deg_Fig3d.txt.

Fourier transforms of oscillations at 45 deg in Figure 3(d); Delta_MR_FFT_45deg_Fig3d.txt.

Extracted oscillation frequencies vs angle in Figure 3(e); Frequencies_vs_angle_Fig_3e.txt.

Contour plot in Figure 3(f); Contour_plot_Fig_3f.txt.

DFT calculated frequencies in Figure 3(f);

DFT_ANGSWEEP_FPF_interp6_0.0045_ALL_fig3f.txt.

DFT_ANGSWEEP_FPF_interp6_0.0045_L_band1_fig3f.txt.

DFT_ANGSWEEP_FPF_interp6_0.0045_L_band2_fig3f.txt.

DFT_ANGSWEEP_FXF_interp6_0.0045_ALL_fig3f.txt.

DFT_ANGSWEEP_FXF_interp6_0.0045_L_band1_fig3f.txt.

DFT_ANGSWEEP_FXF_interp6_0.0045_L_band2_fig3f.txt.

Frequencies as a function of distortion size in Figure 3(h);

FREQSinterp_B001_0.0045_band1_ALL_fig3h.txt.

FREQSinterp_B001_0.0045_band1_L_fig3h.txt.

FREQSinterp_B001_0.0045_band2_ALL_fig3h.

FREQSinterp_B001_0.0045_band2_L_fig3h.txt.

Files containing data for Figure 4;

Normalised resistivity 6 kbar Fig 4(a); normalised_resistivity_6kbar_Fig4a.txt.

Normalised resistivity 10 kbar Fig 4(a); normalised_resistivity_10kbar_Fig4a.txt.

Normalised resistivity 18 kbar Fig 4(a); normalised_resistivity_18kbar_Fig4a.txt.

Differentiated resistivity 6 kbar inset Figure 4(a);

normalised_resistivity_6kbar_diff_Fig4a_inset.txt.

Differentiated resistivity 10 kbar inset Figure 4(a);

normalised_resistivity_10kbar_diff_Fig4a_inset.txt.

Magnetoresistance 6 kbar Figure 4(b); MR_6kbar_Fig4b.txt.

Magnetoresistance 10 kbar Figure 4(b); MR_10kbar_Fig4b.txt.

Magnetoresistance 10 kbar Figure 4(b); MR_10kbar_Fig4b.txt.

Hall resistivity 6 kbar Figure 4(c); Hall_6kbar_Fig4c.txt.

Hall resistivity 10 kbar Figure 4(c); Hall_10kbar_Fig4c.txt.

Hall resistivity 18 kbar Figure 4(c); Hall_18kbar_Fig4c.txt.

Hall conductivity 6 kbar Figure 4(d); Hall_conductivity_6kbar_Fig4d.txt.

Hall conductivity 10 kbar Figure 4(d); Hall_conductivity_10kbar_Fig4d.txt.

Hall conductivity fit 6 kbar Figure 4(d); fit_Hall_conductivity_6kbar_Fig4d.txt.

Hall conductivity fit 10 kbar Figure 4(d); fit_Hall_conductivity_10kbar_Fig4d.txt.

Distortion against pressure calculated from DFT in Figure 4(e);
Alpha_tau_pressure_Fig4e.txt.

Files containing data for Figure 5;

Hall resistivity 6 kbar in Figure 5(a); Hall_6kbar_Fig5a.txt.

Hall resistivity 10 kbar in Figure 5(a); Hall_10kbar_Fig5a.txt.

Magnetoresistance 6 kbar in Figure 5(b); MR_6kbar_Fig5b.txt.

Magnetoresistance 10 kbar in Figure 5(b); MR_10kbar_Fig5b.txt.

Oscillations in Hall at 6kbar in Figure 5(c) (i); Delta_Hall_6kbar_Fig5_c_i.txt.

Oscillations in Magnetoresistance at 6kbar in Figure 5(c) (ii);
Delta_MR_6kbar_Fig5_c_ii.txt.

Oscillations in Hall at 10kbar in Figure 5(c) (iii); Delta_Hall_10kbar_Fig5_c_iii.txt.

Oscillations in Magnetoresistance at 10kbar in Figure 5(c) (iv);
Delta_MR_10kbar_Fig5_c_iv.txt.

Dingle fit Figure 3(c)(iii); dingle_fit_Fig5_c_iii.txt

Fourier transform Hall oscillations 6 kbar Figure 5(d)(i); Hall_6kbar_FFT_Fig5d_i.txt

Fourier transform Magnetoresistance oscillations 6 kbar Figure 5 (d)(ii);
MR_6kbar_FFT_Fig5d_ii.txt

Fourier transform Hall oscillations 10 kbar Figure 5 (d)(iii); Hall_10kbar_FFT_Fig5d_iii.txt

Fourier transform Magnetoresistance oscillations 10 kbar Figure 5 (d)(iv);
MR_10kbar_FFT_Fig5d_iv.txt

Oscillations amplitude in Figure 5(e); Amplitude_Fig5e.txt.

Fits to oscillation amplitude in Figure 5(e); Fit_Amplitude_Fig5e.txt.

Oscillation amplitude in Dingle plot Figure 5(f); dingle_amplitude_Fig5f.txt.

Dingle fit Figure 5(f); fit_dingle_amplitude_Fig5f.txt.

The BXSF files used for Fermi surface calculations in the cubic and the optimised rhombohedral structure are also included. Additionally, the BXSF files for the interpolation of the distortion size between the cubic and optimised rhombohedral structure;

optimised_Fm-3m.bxsf.
optimised_R3m.bxsf.
interp_1.bxsf.
interp_2.bxsf.
interp_3.bxsf.
interp_4.bxsf.
interp_5.bxsf.
interp_6.bxsf.
interp_7.bxsf.
interp_8.bxsf.
interp_9.bxsf.

Also included are example input files for the VASP package used in bandstructure calculations;

INCAR.bands-so.
INCAR.energy-so.
KPOINTS.bands-select.
KPOINTS.mp
POSCAR
POTCAR