A.12: Probing electronic density of states in CrSi using photoemission

Magnetic materials with topological electronic states at the surface have shown potential technological applications in spintronics and thermoelectricity. CrSi is a metallic thermoelectric material and also has magnetoresistive memory applications. CrSi has noncentrosymmetric B20 crystal structure with broken space inversion symmetry. We have observed a large positive magnetoresistance of 25% in CrSi at 5 K and 5 T magnetic field. It is paramagnetic at room temperature (RT) with competing ferromagnetic and antiferromagnetic correlations at low temperature (LT) due to the presence of Dzyaloshinskii-Moriya interaction. We have performed temperature dependent electronic structure studies on CrSi to understand the role of Cr 3d electrons in the origin of complex magnetism and thermoelectric properties.

Polycrystalline ingot of CrSi was prepared by arc melting technique. Resonant photoemission (RPES) measurements with synchrotron source at LT (15 K) and RT (300 K) were performed at the angle resolved photoelectron spectroscopy beamline at Indus-1. RPES spectra were recorded in the energy range between 35 eV to 60 eV across the Cr 3p-3d transition with typical energy resolution of 135 meV. High resolution photoemission (HRPES) measurements with energy resolution of 10 meV at LT and 100 meV at RT were performed with He-1 source at the angle resolved photoelectron spectrometer at Indus-2.

RPES data at 300 K and 15 K in Figure A.12.1(a) and (b) show drastic changes across the Cr 3p-3d resonance. Six features observed in the valence band spectra at 0.15, 0.95, 4.0, 6.5, 8.5 and 10.8 eV marked as A, B, C, D, E and F, respectively in the Figure A.12.1(a) and (b). The features A, B and C have dominant contribution from the Cr 3d states, while the features D, E and F have mixed contribution from Cr 3d, Si 3s and Si 3p states. Comparing the RT and LT RPES data, we find that the intensities of D, E and F enhance at LT while the intensity of A and B reduces. Constant initial state (CIS) spectra for feature A, B, C and D are plotted from the RPES data in Figure A.12.1(c) using the standard method. The CIS spectra are fitted with Fano line profile and the parameter q determined at RT and LT (shown in Figure A.12.1(c)). The Fano parameter q gives the information about the nature of the valence electrons. Small value of q for feature A and B indicates more itinerant character of the Cr 3d electrons near Fermi edge while large value of q for feature C and D indicates more localized character. Moreover, the value of q is found to be positive at RT but negative at LT indicates that there is change in the conduction electron screening.

Drastic variations observed in HRPES data (Figure A.12.2(a)) of the valence states along with band broadening at LT indicate the increase in Cr 3d and Si 3p hybridization. Spectral density of states (SDOS) derived using standard method from HRPES spectra near EF clearly show a maximum intensity at RT and minimum intensity at LT at 80 meV (marked by vertical line in Figure A.12.2(b)) which is a signature of pseudogap. Moreover, a peak developed at 30 meV at LT (marked by arrow in Figure A.12.2(b)) is a signature of topological state present at LT. Similar peak corresponding to topological state has also been observed in the difference spectrum (marked by arrow in Figure A.12.2(c)).

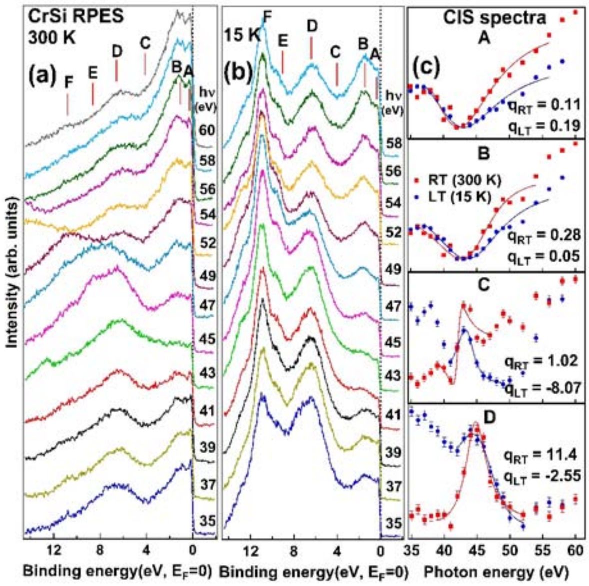

Fig. A.12.1: RPES data across Cr 3p-3d resonance at (a) 300 K (RT) and (b) 15 K (LT). (c) CIS spectra for A, B, C and D features with fitted Fano profile (solid line). The values of q at RT and LT mentioned in (c).

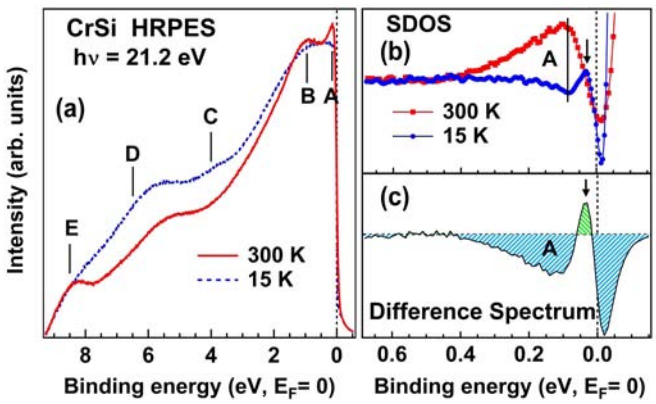

Fig. A.12.2: Temperature dependent (a) HRPES spectra and (b) SDOS at 300 K (RT) and 15 K (LT). (c) Difference spectrum obtained by subtracting RT from LT spectrum shown in (a).

In conclusion, we find that there is a strong d − p hybridization in CrSi which leads to both localized and delocalized electronic states. Enhanced localization effects and evidence of topological transition observed at LT. Large density of itinerant Cr 3d electrons with topological phase transition and large positive magnetoresistance at LT suggests CrSi as a potential candidate for both the thermoelectric and spintronics applications. For more details, please refer to Scientific Reports 10, 12030 (2020).

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