A.10: Electronic structure and crystal structure of PrGe studied using Indus SRS

Rare-earth compounds are important for fundamental and technological applications because of their unique magnetic properties. These properties are governed due to the interplay between localized (*4f*) and delocalized (*spd*) electronic states. Magnetic studies on PrGe showed two different magnetic transitions from paramagnetic (PM) to antiferromagnetic (AFM) at 44 K and from AFM to ferromagnetic (FM) at 41.5 K. PrGe [010] surface showed a giant Rashba effect (α_R= 5 eVÅ) in the PM phase, giant negative MR (43% at 8 Tesla) in the AFM phase and tunable Rashba parameter with temperature across the magnetic transitions. Rashba effect is the momentum dependent splitting of spin bands at zero magnetic field. It has important applications in spintronics where the spin currents can be generated and controlled with an electric field or voltage. Hence, PrGe is proposed to be a promising candidate for AFM spintronics application. Using beamlines at Indus synchrotron, the electronic and crystal structure of PrGe are studied to understand the nature of Pr *4f* states and the spin polarization, which gives rise to Rashba effect and different magnetic phases present in this system.

PrGe single crystal was grown by the Czochralski method. Electronic structure of PrGe is studied using resonant photoemission (RPES) experiments at AIPES beamline (BL-2), Indus-1. Low temperature XRD measurements were performed at ADXRD beamline (BL-12),Indus-2. Magnetization, resistivity, susceptibility and specific heat measurements were also carried out.

X-ray diffraction (XRD) studies showed CrB type crystal structure with *Cmcm* space group. RPES has been performed across Pr *4d−4f* resonance in the photon energy range from 110 to 140 eV. The RPES data are plotted in the contour plot as shown in Fig. A.10.1(a), where 4 prominent features marked as *A, B, C* and *D* are observed. Across the Pr *4d* to *4f* resonance, only feature *A* shows significant enhancement in intensity. Hence, the constant initial state (CIS) spectrum for the feature *A* has been plotted in the Fig. A.10.1(b) using the standard method. To understand the character of this feature Fano line profile of the form $f = (q+\varepsilon)^2/(1+\varepsilon^2)$ and $\varepsilon = (h\nu - E_0)/\Gamma$ has been fitted and shown in Fig. A.10.1(b) with a solid line. Here, the parameters E_0, q and Γ represents the resonance energy, discrete/continuum mixing strength and the half-width of the line. The values of the parameters are shown in Fig. A.10.1(b). The larger value of q indicates that the feature *A* is localized in nature. The resonance energy observed at 125 eV is much above the Pr *4d* threshold energy of 114 eV which indicates that the *4f* states are hybridized in this system. Hybridization related feature is also observed in Pr *3d* core level. Since, Pr *4f* states carries the local moment in PrGe hence, the strong hybridization of the Pr *4f* states with the conduction electrons leads to the spin polarization, which give rise to the Rashba effect in this system.

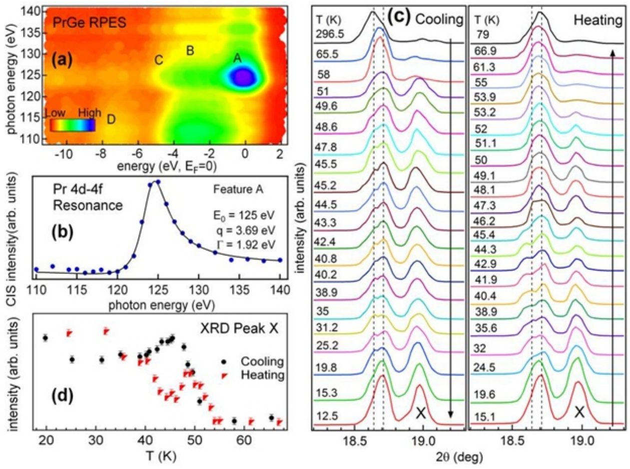

Fig. A.10.1:(a) RPES data across Pr 4d-4f resonance shown in the contour plot. (b) CIS spectrum for feature A (as in (a)), where the blue dots and solid line are the experimental data and the fitted Fano profile respectively. (c) temperature dependent XRD at 13 keV energy shown for both heating and cooling cycles. (d) The intensity of peak X marked in (c) is plotted as a function of temperature which shows a hysteresis in both PM to AFM and AFM to FM phase transitions

Temperature dependent XRD measurements using linearly polarized 13 keV X-ray have been performed to explore the possibility of the spins being coupled to the lattice. XRD patterns from the polarized synchrotron source showed some additional peaks as compared to those recorded from lab source. In Fig. A.10.1(c) the most intense peak shows signature of splitting in both heating and cooling cycles (shown by dotted lines in the Fig. A.10.1(c)). The intensity of peak X as in Fig. A.10.1(c) is plotted as a function of temperature in Fig. A.10.1(d). Hysteresis is observed around the magnetic transitions, which indicate the first order nature of these transitions and hence, the spins are strongly coupled to the lattice.

The conclusions drawn from the RPES and the XRD studies performed are: 1) Pr *4f* electrons are hybridized with the conduction electrons which give rise to the spin polarization and the Rashba effect in this system, 2) there is a strong coupling between the spins and the lattice and 3) magnetic ordering causes change in the spin polarization, that gives rise to tunable Rashba parameter in PrGe which has technological importance. For details please refer to Soma Banik et al., *Scientific Reports* 7, 4120 (2017).

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