Commensurate vs Incommensurate Charge Ordering near the Superconducting Dome in Ir$_1$Pt$_x$Te$_2$ Revealed by Resonant X-Ray Scattering

The electronic-structural modulations of Ir$_1$Pt$_x$Te$_2$ have been examined both by resonant elastic and inelastic X-ray scattering (REXS and RIXS) techniques. Charge-density-wave-like superstructures with wave vectors of Q = (0.2 0 4.2) for Ir$_1-x$PtxTe$_2$ (0 ≤ x ≤ 0.15) are observed on the same sample of IrTe$_2$ at the lowest temperature. In contrast, superstructures around Q = (1/5 0 −1/5) are observed for doped samples. The superstructure reflections persist to higher Pt substitution than previously assumed. REXS and RIXS results indicate the importance of the Te 5p states rather than the Ir 5d states in the formation of the spatial modulation of these systems.

A charge-density-wave (CDW)-like structural transition was reported in the 5d transition-metal chalcogenide IrTe$_2$ at T$_c$ = 280 K. This has attracted great interest because of the recent discovery of superconductivity in Pt- and Pd-substituted compounds [1–3]. With increasing Pt-substitution, the structural transition is suppressed, and a superconducting dome appears in the region of 0.04 ≤ x ≤ 0.12, indicating similar diagrams to those of other unconventional superconductors. Although numerous studies have followed these initial works, there is still no consensus on the mechanism of this structural transition. The phase transition of IrTe$_2$ is accompanied by the emergence of a superstructure modulation, with wave vector Q$_0$ = (1/5 0 −1/5) as expressed in reciprocal lattice units in trigonal notation. The main elements are the Ir-Ir dimerization along the a-axis with period 5a, and the consequent distortion of the triangular Ir sublattice in the a-b plane, occurring together with a trigonal-to-triclinic symmetry reduction. Since in IrTe$_2$, the formal valence of Ir is +4, the Ir 5d electrons with t$_{2g}$ configuration are the closest to the chemical potential, and they are thus expected to play a central role in the CDW. However, some previous studies indicated that the charge-transfer energy between Ir and Te is close to zero, and that the Te 5p states are also important for the low-energy physics, especially for their surface region. To revisit the superstructures in Ir$_1-x$PtxTe$_2$, and to clarify the relation between superconductivity and superstructural modulation, we studied the spatial ordering of electronic states by means of resonant elastic and inelastic X-ray scattering (REXS and RIXS) at both edges of Ir and Te. Single-crystal samples of Ir$_1-x$PtxTe$_2$ (0 ≤ x ≤ 0.12) were prepared using a self-flux method. Resonant elastic X-ray scattering (REXS) at the Ir L$_3$ edge for the Ir$_1$Te$_2$(2p to 5d) absorption edge in the hard X-ray region was performed at the Photon Factory’s BL-4C. REXS at the Te L$_2$ (2s to 5p) absorption edge was conducted at BL-22U-XU of SPring-8. On the other hand, resonant inelastic X-ray scattering (RIXS) at the Ir L$_3$ edges was conducted at BL-11U-XU of SPring-8. REXS at the Te M$_{4,5}$ (3d to 5p) edge in the soft X-ray region was performed at the REXS beamline of the Canadian Light Source.

Figure 1(A) shows X-ray diffraction along (0 0 −4) to (1 0 −5) through the superstructure peaks for IrTe$_2$ (x = 0.0). The Q = (1/5 0 −1/5), (1/8 0 −1/8), and (1/6 0 −1/6)-type superstructures are observed for IrTe$_2$ at the lowest temperature of T = 10 K, whereas only the Q$_0$-type superstructures were reported in previous studies for these samples [4, 5]. The periods of the superstructures at low temperature strongly depend on the experimental protocol, or cooling rate. In contrast, incommensurate ordering peaks around Q = (1/5 0 −1/5) are observed for the doped samples of 0.02 ≤ x ≤ 0.05 at any cooling rate [Fig. 1(B)]. The superstructures coexist with the superconducting phase for Ir$_1-x$PtxTe$_2$ (x = 0.05) as shown in Fig. 1(C), suggesting that CDW persists to higher Pt substitution than previously thought. In addition, incommensurability of CDW is observed for x = 0.04 and 0.05 samples which coincide with the onset of superconductivity.

Surprisingly, the REXS and RIXS spectra for the Ir L$_3$ edge scarcely depend on the wavevectors, while the REXS line shape at the Te edges strongly depends on the Q position (Fig. 2), indicating that the spatial charge modulation only exists on the Te sites. Therefore, the charge modulation in the bulk resides in the Te orbitals rather than the Ir orbitals. The phase diagram re-examined in this work suggests that the CDW incommensurability in the Te sites will correlate with the emergence of superconducting states. Ir$_1-x$PtxTe$_2$ may harbor similar exotic phases for unconventional superconductors.

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