[MS32-P02] The X-ray study of phase transion in Sc doped TiOCl

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As one of the low dimensional quantum magnetic systems, the compound TiOCl has the same structure as FeOCl with the orthorhombic space group *Pmmn*, Ti-O double layers sandwiched by Cl layers.[1] Its dimerized, spin-Peierls state at low temperatures has attracted huge interest. [2,3] With the temperature dropping, a phase transition occurs at Tc2 = 90K which drive the structure into an incommensurate phase. Below Tc1 = 67K, a twofold superstructure develops. Accompanying with the incommensurate phase, a temperature-dependent *c*-axis unique monoclinic distortion of the crystal lattice is observed between *Tc2* and *Tc1*.[4] Detailed temperature-dependent X-ray diffraction measurements on a single crystal of 0.5% Sc doped TiOCl have been performed in order to study the critical properties of the phase transitions. According to the q scans along **a*** centered on (0,-2.5,-3) and (1,-0.5,-9), obvious peak splitting was found with two peaks appeared at positions (±q1,-2.5,-3) and (1±q1,-0.5,-9) respectively in each q scan between 62.5K and 85K, and values of q1 were determined by fitting these peaks with pseudo-voigt function at all measured temperatures. Tc1 of doped TiOCl was found to be 61.64(27)K with a critical exponent of γ =0.305(27), which is lower than the transition temperature of TiOCl. Meanwhile, *c*-axis unique monoclinic distortion of the crystal lattice vanishes between Tc1 and Tc2. Data collections for both main reflections and satellite reflections at 8K were performed to refine the modulated structure. Here we discuss the results of these experiments and provide a model for the modified transition behavior of doped TiOCl.

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