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ACCEPTED MANUSCRIPT

Effects of S-Se substitution and magnetic field on magnetic order in $Fe_{0.5}Ti(S,Se)_2$ layered compounds

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Abstract

Powder neutron diffraction and specific heat measurements have been employed to study the evolution of an antiferromagnetic (AFM) structure in the intercalated $Fe_{0.5}TiS_{2-y}Se_y$ compounds with S-Se substitution and under application of a magnetic field. In $Fe_{0.5}TiS_2$ ($y = 0$), the magnetic structure just below $T_N \simeq 140\,K$ is incommensurate while it becomes commensurate with further cooling below $T_t \simeq 125\,K$. The presence of two magnetic phase transitions at T_t and T_N in $Fe_{0.5}TiS_2$ is confirmed by specific heat measurements. The field-induced AFM–FM transitions occurring in $Fe_{0.5}TiS_2$ within temperature interval $T_t < T < T_N$ and below T_t are evidenced by neutron diffraction measurements under application of a magnetic field. Unlike $Fe_{0.5}TiS_2$ having a quadruplicated AFM structure, the compounds with the Se concentrations $y > 0.5$ are observed to exhibit an AFM structure with the doubled magnetic unit cell along a and c crystallographic directions of the monoclinic crystal lattice ($I12/m1$ space group). In the transition region around the critical Se concentration $y_c \approx 0.5$, the magnetic structure of $Fe_{0.5}TiS_{2-y}Se_y$ is found to be incommensurate. The appearance of the AFM order with decreasing temperature in $Fe_{0.5}TiS_{2-y}Se_y$ is accompanied by anisotropic deformations of the crystal lattice. At low temperatures, the

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