Short-Range and Long-Range Ferrimagnetic Order in Fe(Te1.5Se0.5)O5Cl

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Abstract : Considerable attention has been paid recently to FeTe₂O₅Cl due to reduced dimensionality and frustration in the magnetic subsystem, succession of phase transitions, and multiferroicity. The efforts to grow its selenite sibling resulted in mixed halide compound, Fe(Te_{1.5}Se_{0.5})O₅Cl, which was found crystallizing in a new structural type and possessing properties drastically different from those of a parent system. Hereby we report the studies of magnetization M and specific heat C_P, combined with Raman spectroscopy and density functional theory calculations in Fe(Te_{1.5}Se_{0.5})O₅Cl. Its magnetic subsystem features weakly coupled Fe³⁺ - Fe³⁺ dimers showing the regime of short-range correlations at TM ~ 70 K and long-range order at TN = 22 K. In a magnetically ordered state, sizable spin-orbital interactions lead to a small canting of Fe³⁺ moments. The density functional theory calculations of leading exchange interactions were found in agreement with measurements of thermodynamic properties and Raman spectroscopy. Besides, because of the relatively large magnetic moment of the Fe³⁺ ion, we found that magnetic dipole-dipole interactions contribute significantly to experimentally observed orientation of magnetization easy axis in ac-plane. As a conclusion, we suggest a model of magnetic subsystem in magnetically ordered state of Fe(Te_{1.5}Se_{0.5})O₅Cl based on a model of interacting dimers.

Keywords : dipole-dipole interactions, low dimensional magnetism, selenite, spin canting

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