

Resolving the origin of the low temperature phase transition T_X in 1-dimensional $BaVS_3$

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Transition metal oxides exhibiting low-dimensional strongly electron correlated systems presents phenomena like, metal-insulator (MI) transition, charge, spin and orbital ordering and superconductivity [1]. In contrast to oxides, sulfides are much less explored. They present reduced ionicity of the metal-sulphur bond, thereby increasing the effect of hybridization. That allows to study interesting electronic phenomena from a different base. The compound $BaVS_3$ crystallizes in a hexagonal structure, with two formula units per unit cell and the the formation of VS_6 chains running along the c axis. The V-V distance in the chain (2.84\AA) is much shorter than the distance V-V interchain (6.72\AA) what gives to this compound quasi-1D properties. This compound undergoes three transitions as a function of temperature. First a structural transition at 240K to an orthorhombic structure [2]. No significant change on the electronic properties has been observed at this temperature. Then a MI transition at $T_{MI}=70\text{K}$ [1], below which a charge density wave with superstructure corresponding to a doubling along the chain direction develops [3]. And finally a transition at $T_X=30\text{K}$, whose origin is still a matter of controversy. At this temperature an anomaly is observed at the magnetic susceptibility. Neutron powder diffraction studies provided evidence for incommensurate reflection below this temperature [4]. Based on the assumption of no inter chain coupling, the modulation vector of $(0.226\ 0.226\ 0)$, in the hexagonal structure, of the possible magnetic order was suggested. However, NMR studies [5] suggest the presence of orbital order to occur at this temperature. The exact nature of the transition at T_X is not yet clear, and the ground state of $BaVS_3$ is unknown.

Here we used resonant soft x-ray diffraction on the V $L_{2,3}$ absorption edges to study this low temperature phase ($T < T_X$). This technique has been proved very powerful in the study of charge, orbital and magnetic order in many systems [ref], since it probes directly the 3d electrons. Our study of the superlattice reflections at the low temperature phase shows that the modulation vector is not along the direction proposed by the neutron study, and that its origin is mainly magnetic.

References

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