THE PRESSURE EFFECT ON THE CRYSTAL AND MAGNETIC STRUCTURE OF $ScMnO_3$

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It is well known that hexagonal $RMnO_3$ manganites (R = Ho-Lu, Y, In, and Sc) are the part of a class of promising multiferroic materials for spintronic application, where an antiferromagnetic transition of Mn^{3+} occurs between 70 K and 130 K, and a ferroelectric transition occurs between 570 K and 990 K due to a structural distortion. The strong coupling between the antiferromagnetic ordering and ferroelectric ordering allows the possibility of controlling magnetism with an electric field (and vice versa).
Hexagonal $ScMnO_3$ consists of stacked Mn-O and Sc layers, the Mn ions forming a nearly ideal two-dimensional triangular lattice [1], crystalizing in the $P6_3cm$ space group. The Mn-Mn interactions between adjacent Mn planes are due to superexchange paths, via the apical oxygen ions of MnO_5 bipyramids, exhibiting AFM orderings below around 100 K. Interestingly, spin-reorientation phase transitions were reported at $T_R < T_N$ for $ScMnO_3$ [2]. Furthermore, the observed rich variety of the magnetic properties of hexagonal manganites reflects a delicate balance between magnetic interactions, which can be easily modified by the changing in interatomic distances and angles by the application of high external pressure, that can lead to the discovery of new effects.
Neutron powder diffraction investigations of $ScMnO_3$ at pressures up to 2 GPa and low temperatures 10-300 K were performed at the DISC diffractometer at the neutron research reactor IR-8 (NRC "Kurchatov Institute"), using sapphire anvil high pressure cells. In the whole temperature and pressure ranges studied, the hexagonal crystal structure of $P6_3cm$ symmetry remains unchanged. There is also a noticeable change in the relative intensity of the peaks associated with the reorientation of the magnetic moments Mn with respect to the hexagonal crystallographic axes (a,b). At temperatures below 130 K at ambient pressure, the appearance of magnetic peaks (100) and (101) was observed, indicating the formation of an antiferromagnetic state within a triangular lattice. The calculated magnetic moment is 3.33 μ_B at 10 K and decreases to 1.8 μ_B at 2 GPa. The baric evolution of the crystal structure parameters of $ScMnO_3$ as well as their temperature dependences were obtained.

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[2] A. Muñoz, J. A. Alonso, M. J. Martínez-Lope, et al. (2000). Magnetic structure of hexagonal RMnO3(R=Y,Sc):Thermal evolution from neutron powder diffraction data. Phys. Rev. B. 62. 9498