Crystal and Magnetic Structure of the Defect Perovskite $Sr_2Fe_{1.5}Cr_{0.5}O_5$.

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$Sr_2Fe_{1.5}Cr_{0.5}O_{5.0}$ crystallizes in the defect perovskite structure with no oxygen vacancy ordering unlike the related $Ca_2Fe_{1.5}Cr_{0.5}O_{5.0}$ phase which shows brownmillerite ordering.[1,2] Also, unlike the similar material $Sr_2FeMnO_{5.0}$ [3] the compound undergoes long range antiferromagnetic order at a surprisingly high temperature. Figure 1 shows a refinement of the powder neutron diffraction pattern along with x-ray data at 290 K where the two strongest magnetic reflections are indicated.

The ordering wave vector of **k** = ½ ½ ½ is consistent with a G-type antiferromagnetic structure. To determine the critical temperature, T_c, data were taken up to 580 K. A plot of the intensity of the strongest magnetic reflection (Figure 2) showed a plateau above about 560 K so T_c was estimated by observing the divergence of the peak width which is estimated to occur at 565(5) K.

References

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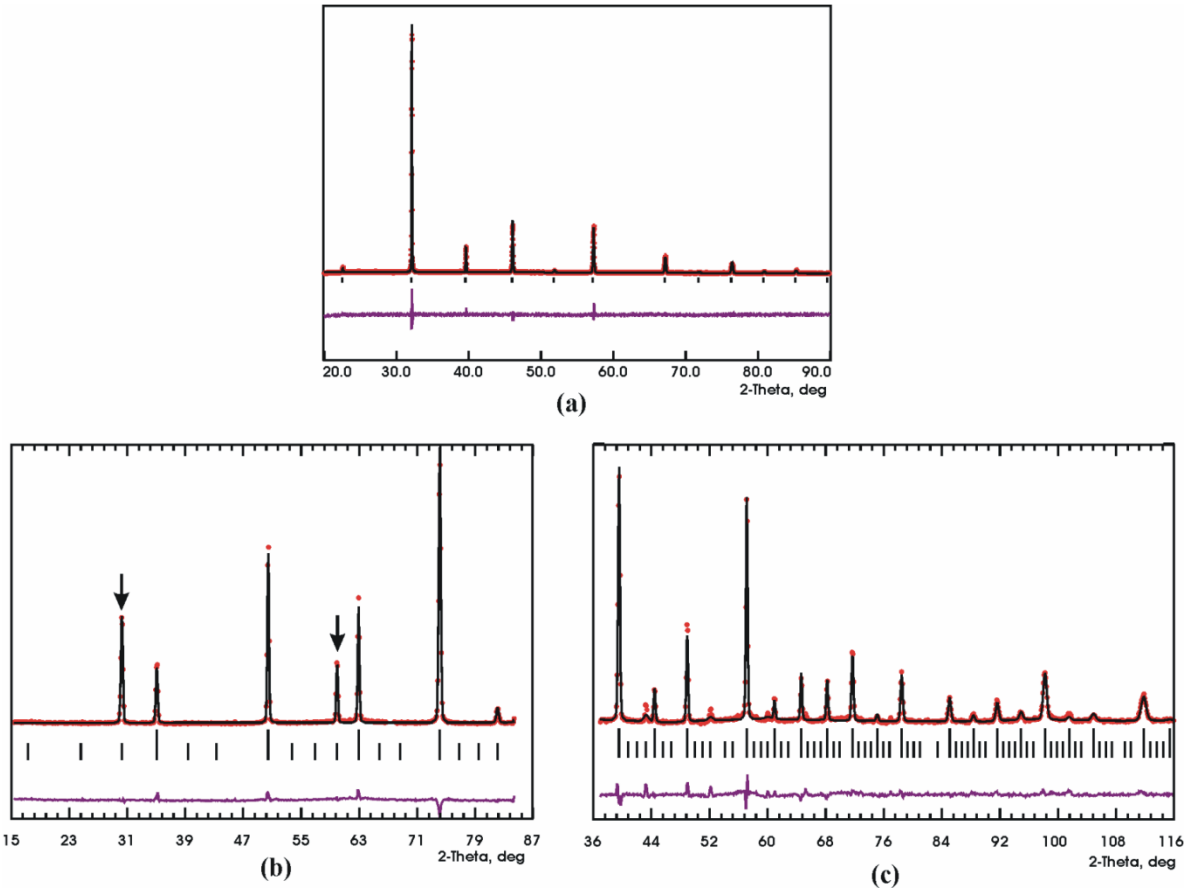

Fig. 1 Rietveld refinement of (a) x-ray and (b) and (c) neutron powder diffraction data at 290 K for $Sr_2Fe_{1.5}Cr_{0.5}O_{5.0}$. In (b) and (c) the lower row of tic marks indicate the magnetic reflections which index with **k** = ½ ½ ½. The space group is Pm-3m, the cell constant is *a* = 3.94491(14) Å and the moment at the Fe/Cr site (at 4 K) is 3.7(4) μ_B.

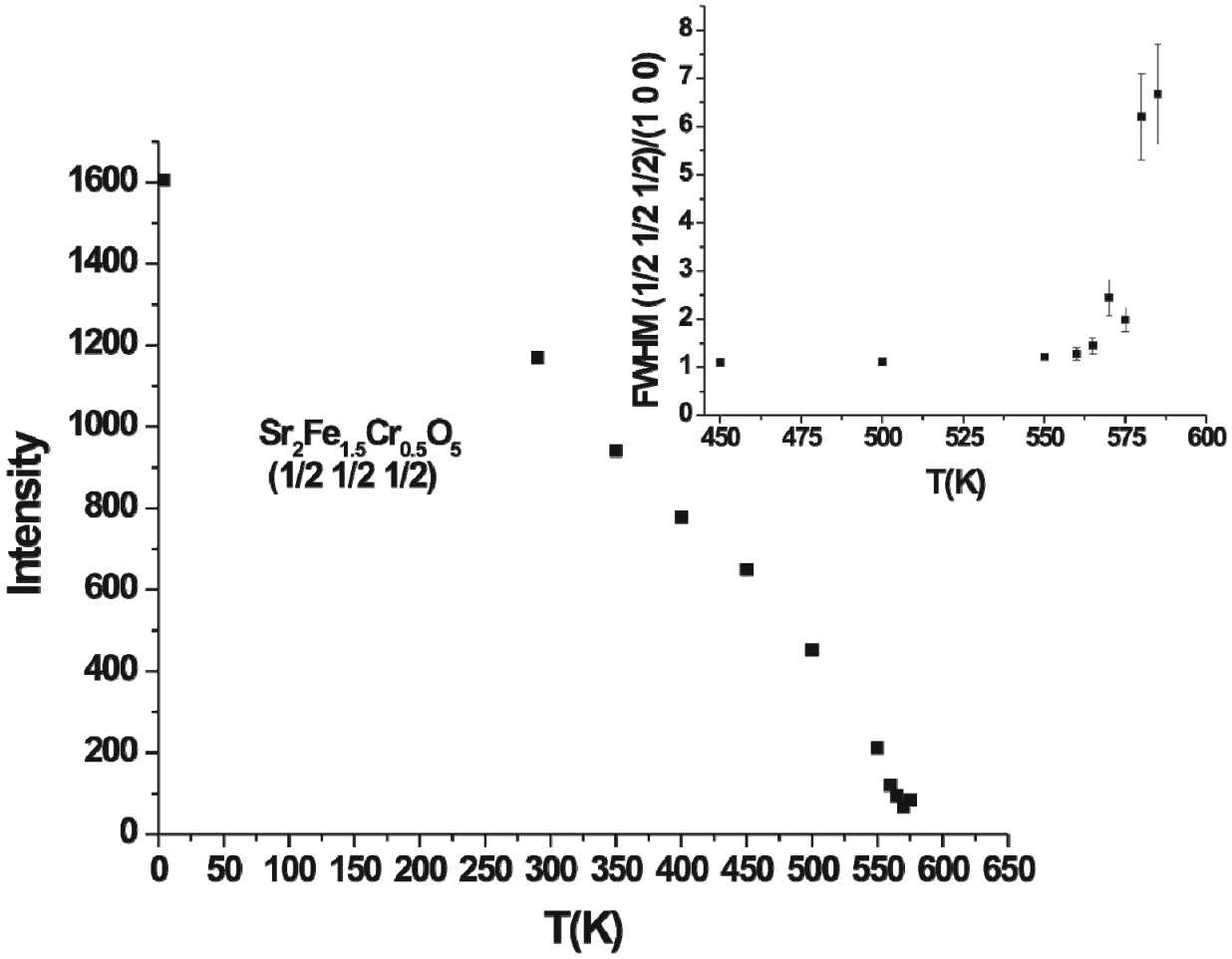

Fig. 2 The temperature dependence of the intensity and peak width (inset) of the (½ ½ ½) magnetic reflection. Note the sharp divergence of the peak width above 565 K.