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Neutron diffraction studies of Pr ordering in $PrBa_2Cu_4O_8$

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Abstract

Neutron diffraction and AC susceptibility measurements have been performed to study the magnetic ordering of the Pr spins in $PrBa_2Cu_4O_8$. An anomaly at 15 K, which we believe is associated with the ordering of the Pr spins, is clearly seen in the temperature dependence of the AC susceptibility, $\chi'(T)$. The coupling between the Pr spins, as revealed by neutrons, is antiferromagnetic in nature, with a spin structure may be characterized by the $\{\frac{1}{2}\,\frac{1}{2}\,1\}$ wave vector. Three-dimensional coupling between the Pr spins is observed, despite the appearance of exact cancellations of the coupling between the adjacent layers along the c-axis due to geometric symmetry.

Keywords: High-T_c compound; Neutron diffraction; Magnetic structure

The Pr-based 123-cuprate has distinguished itself from other high-T_c cuprates by its special properties [1,2]. In continuously exploring the mysteries of Pr cuprates, we report neutron diffraction and AC susceptibility studies of the magnetic ordering of the Pr spins in a $PrBa_2Cu_4O_8$ (Pr124) compound. The compound is synthesized at ambient oxygen pressure by the nitric pyrolysis method [3,4].

Fig. 1 shows the temperature dependence of the in-phase component of the AC susceptibility. The solid line shown is a fit of the data obtained between 25 and 80 K to the Curie–Weiss law. Clearly, below 15 K, the data depart from the fitted line. The origin of this anomaly is believed to be associated with the Pr spin ordering.

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Neutron diffraction measurements were performed on the US NIST BT-2 triple-axis spectrometer, operated in double-axis mode with pyrolytic graphite monochromator and filter, with an incident wavelength of 2.351 Å and angular collimations 40′–48′–48′. The magnetic peaks observed at 6 K are shown in Fig. 2, where the data taken at 25 K have been subtracted to isolate the magnetic signal. Two magnetic peaks were observed, with widths broader than the instrumental resolution. Due to a long lattice constant for the c-axis, the expected separation in 2θ between the $\{\frac{1}{2}\,\frac{1}{2}\,0\}$ and $\{\frac{1}{2}\,\frac{1}{2}\,1\}$ peaks is only 0.8°, which is beyond our instrumental resolution. If we fit the data assuming the peak at 25° contains two peaks, the fitted peak positions are at the expected positions for the $\{\frac{1}{2}\,\frac{1}{2}\,0\}$, $\{\frac{1}{2}\,\frac{1}{2}\,1\}$ and $\{\frac{1}{2}\,\frac{1}{2}\,2\}$ reflections and all three peaks are resolution limited. We hence believe that

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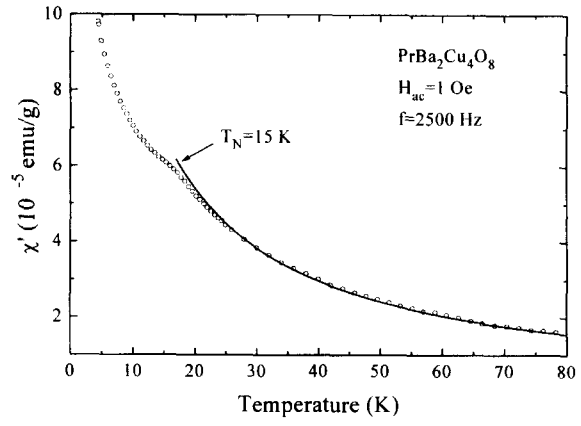

Fig. 1. Temperature dependence of the AC susceptibility revealing an anomaly at 15 K.

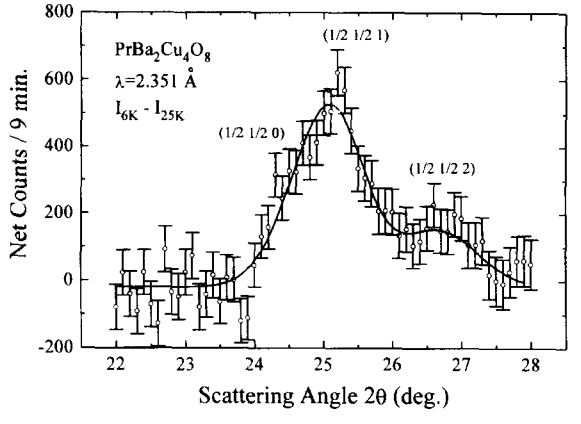

Fig. 2. The magnetic diffraction peaks observed at 6 K.

three magnetic peaks, which may be indexed as the $\{\frac{1}{2}\frac{1}{2}0\}$, $\{\frac{1}{2}\frac{1}{2}1\}$, and $\{\frac{1}{2}\frac{1}{2}2\}$ reflections, were observed. The solid curve shown in Fig. 2 is a fit of the data to three Gaussian resolution functions. By comparing the $\{\frac{1}{2}\frac{1}{2}1\}$ magnetic intensity observed at 6 K with that of $\{0\,0\,6\}$, we obtain a saturated

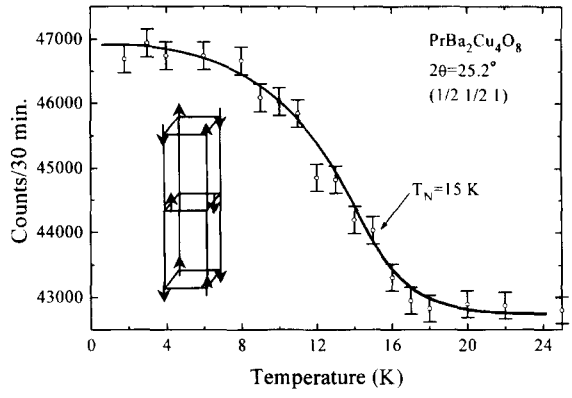

Fig. 3. Variation of the $\{\frac{1}{2}\frac{1}{2}1\}$ peak intensity. The inset shows the proposed spin structure.

moment of $\langle\mu_Z\rangle = 0.61(4)\mu_B$ where the moment points in the c-axis direction.

In Fig. 3, we show the variation of the $\{\frac{1}{2}\frac{1}{2}1\}$ peak intensity with temperature. The ordering temperature, as determined by the inflection point, is $T_N = 15$ K, which matches the temperature at which $\chi'(T)$ shows an anomaly. Shown as an inset in Fig. 3 is the proposed Pr spin structure, in which the adjacent spins in the a–b plane are antiparallel and the coupling between the adjacent layers along the c-axis are canceled due to geometric symmetry.

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