Comment on "Local Magnetism and Crystal Fields of Pr in $PrBa_2Cu_3O_7$ Studied by ^{141}Pr NMR"

Nehrke and Pieper presented a ^{141}Pr NMR study [1] in which they report a tiny ordered magnetic moment of Pr in $PrBa_2Cu_3O_7$ at low temperature. In addition, they determined the crystal field (CF) splitting (potential) of the Pr ions. They propose that the magnetic transition at 17 K is due to a ferromagnetic coupling between the CuO_2 planes of a bilayer induced by Pr. These conclusions are ambiguous and in total disagreement with most of the other experimental techniques.

The proposed reorientation of the Cu spins would indeed increase the magnetic $\frac{1}{2},\frac{1}{2},\frac{1}{2}(0)$ reflection but would strongly decrease the $\frac{1}{2},\frac{1}{2},\frac{3}{2}(1)$ and $\frac{1}{2},\frac{1}{2},\frac{5}{2}(2)$ reflections, which are not observed for $PrBa_2Cu_3O_7$ [2] ($T_N = 17$ K), $PrBa_2Cu_3O_6$ [3] ($T_N = 10$ K), nor for $Pb_2Sr_2PrCu_3O_8$ [4] ($T_N = 7$ K). There are only positive Bragg intensities observed in the neutron diffraction patterns, indicating an additional magnetic moment in the system.

Figure 1 shows inelastic neutron scattering (INS) data from $Pb_2Sr_2PrCu_3O_8$ [5], which are very similar compared to $PrBa_2Cu_3O_7$ [6] because of the same local structure around the Pr ions. The magnetic scattering is obviously peaked around 3 meV, which is directly related to the splitting of the quasitriplet. The proposed energy level scheme of Nehrke and Pieper (11 meV) is in strong contrast to this result. We note that INS is the most direct probe for a determination of the CF in these optically opaque systems. In addition, the tabulated CF parameters are totally different from those presented for the other $RBa_2Cu_3O_7$ systems (e.g., R = Ho [7]). The ratio of the fourth and sixth order CF parameters do not even have the same sign compared with the results retrieved with INS or structural modeling [7]. However, what is even more strange is that we were not able to reproduce the tabulated splittings with the presented parameters.

The proposed susceptibility (χ) is in strong disagreement with the observations for temperature below 20 K [6]. χ is not constant below 20 K (due to the large energy separation of the proposed quasitriplet), but increases further despite the small hump due to the ordering of the Pr sublattice, which is consistent with the INS results.

The experimental results of specific heat studies [6] are in good agreement with the CF proposed from the INS and the magnetic ordering of the Pr sublattice, but are in contradiction to the presented interpretation of this Letter.

The cited Mössbauer study [8] found a magnetic field of 0.5–1 T at the rare earth site which can never be explained by the proposed Cu spin ordering (it cancels due to symmetry) but is well understood by the magnetic ordering of the Pr sublattice below 17 K.

A possible explanation for these results may be related to the different time scale probed by the different techniques. Neutron scattering is a fast probe, which means it sees slowly fluctuating spins as static, whereas NMR is much slower. Pr Mössbauer, which lies in between these techniques, reports an ordered moment of $0.32\mu_B$ [9], still much higher compared to those reported in the Letter [1] but half of the value obtained by neutron diffraction.

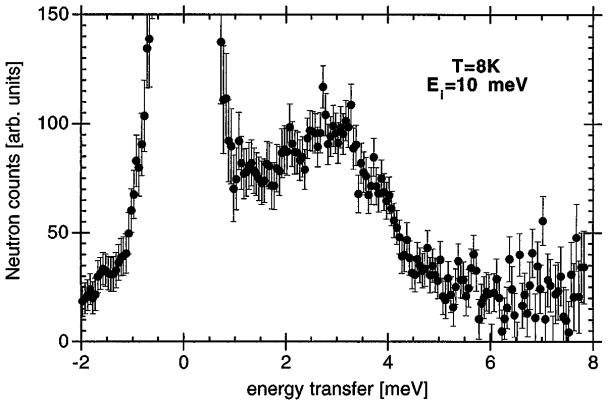

FIG. 1. Neutron energy spectra of $Pb_2Sr_2PrCu_3O_8$, a double layer cuprate similar as $PrBa_2Cu_3O_7$.

In summary, the presented conclusions in this Letter are very ambiguous because they are in disagreement with all the results obtained by other experimental techniques.

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