Comment on "Superconducting $PrBa_2Cu_3O_x$"

Recently, Zou *et al.* [1] reported the observation of bulk superconductivity (SC) for a $PrBa_2Cu_3O_x$ (Pr123) single crystal grown by the traveling-solvent floating-zone (TSFZ) method. The SC of Pr123 itself and also the increase of the T_c from 85 to $\approx$105 K under pressure are of general interest. These unexpected results (see also [2]) are in sharp contrast with the generally accepted view that Pr123 is the only nonsuperconducting compound among the orthorhombic $RBa_2Cu_3O_{7-y}$ (R = Y, rare earth) cuprates. More detailed knowledge of TSFZ crystal properties is required to resolve this discrepancy.

Zou *et al.* reported only slight differences in the crystal structure between TSFZ Pr123 and crystals grown by the flux method: An elongation of the c-axis parameter connected with the expansion of the distance between two CuO_2 planes was found. We agree with Zou *et al.* that it is hard to attribute the hole delocalization and the occurrence of SC in the TSFZ crystal to the small elongation of the Pr-O(2) distance. Because of the "strong sample inhomogeneity" the substitution of Ba for Pr might create mobile superconducting holes [1]. However, the effective magnetic moment of Pr μ_{eff} was found to be $2.92\mu_B$ [1], i.e., close to that of their flux crystal. Thus, given this value of μ_{eff} it is difficult to imagine a substantial substitution of nonmagnetic Ba for Pr.

The aim of this Comment is to show the *inconsistency* of the value of μ_{eff} reported by Zou *et al.* with their magnetic susceptibility $\chi(T)$ data (Fig. 3 of Ref. [1]). For clarity the data of Ref. [1] are shown here together with recent results of our group for a high quality Al-free Pr123 single crystal grown in a Pt crucible [3]. For this Pr123 crystal the $\chi^{-1}(T)$ curves are shown in Fig. 1 for the field parallel ($H \parallel c$) and perpendicular ($H \parallel ab$) to the c-axis. (The field direction for the TSFZ crystal was not mentioned in [1].) The values of $\mu_{\text{eff}} = 2.9\mu_B$ and $3.1\mu_B$ were obtained for our crystal for $H \parallel ab$-plane and $H \parallel c$-axis, respectively, from the best fits of points at $50 \leq T \leq 300$ K to the modified Curie-Weiss law including a temperature independent χ_0 (shown in Fig. 1 by solid lines). These values are in good agreement with previously reported ones; see, e.g., [4]. Since it is impossible to have very closely similar values of μ_{eff} from quite different "flux" and "TSFZ" curves, we reestimated the value of μ_{eff} from the TSFZ data shown in Fig. 1.

The first estimate from the *linear* approximation by Zou *et al.* to the $\chi^{-1}(T)$ data (dotted line in Fig. 1 here) gives $\mu_{\text{eff}} = 2.32\mu_B$. According to [1] their fit was obtained with $\chi_0 = 4.5 \times 10^{-4}$ emu/mol. But the *straight* line in Fig. 3 of [1] representing the fit *cannot* be reproduced with that χ_0 value. The second estimate made directly from their data points fitted to the modified Curie-Weiss law including χ_0 gives an even smaller value of $\mu_{\text{eff}} = 2.09\mu_B$ and a Curie constant $C = 0.546$ emu K/mol. The C value for the TSFZ crystal is about one-half of that for our flux crystal (1.04 and 1.19 emu K/mol for $H \parallel ab$ and $H \parallel c$, respectively). This suggests that Pr occupies only about a half of the R sites (assuming for the TSFZ crystal nearly the same Pr local moment as for the flux grown one). The other half of the R sites is occupied most probably by the nonmagnetic Ba. Noteworthy, SC with $T_c \approx 43$ K was observed for $Pr_{0.5}Ca_{0.5}Ba_2Cu_3O_{7-y}$ thin films [5]. Ba^{2+} as well as Ca^{2+} on R site dopes additional mobile holes and compensates for the localization of holes by the Pr-O(2, 3) hybridization. Ba^{2+} has a larger ionic radius than Pr^{3+} and so the substitution of Ba for Pr could give a natural explanation not only for the SC in TSFZ Pr123 but also for the elongation of the distance between the CuO_2 planes observed in [1].

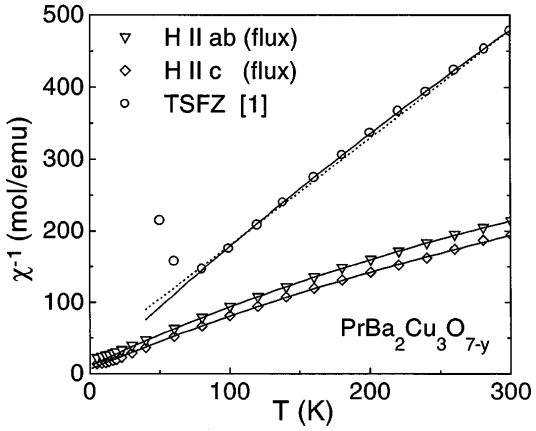

FIG. 1. χ^{-1} vs T for flux grown [3] and TSFZ [1] Pr123 single crystals. Solid lines: fits to the Curie-Weiss law. Only some representative points are shown. For details, see text.

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