Knight shift vs hole concentration in Hg1201 and Hg1212

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We studied the hole concentration dependences of $^{63}$Cu Knight shifts in single-CuO$_2$-layer high-$T_c$ cuprate superconductors HgBa$_2$CuO$_{4+\delta}$ and double-layer HgBa$_2$CaCu$_2$O$_{6+\delta}$. We found that the spin Knight shift at room temperature as a function of the hole concentration in the single-layer superconductor is different from that in the double-layer superconductor. Two type relations between the spin Knight shift and the hole doping level serve to estimate the individual hole concentrations of the non-equivalent CuO$_2$ planes in a unit cell.

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I. INTRODUCTION

The doped hole carriers have been believed to distribute nonuniformly in the multi-layer cuprate superconductors. How to estimate the individual carrier doping levels of the non-equivalent CuO$_2$ planes in the multi-layer superconductors has been an issue. The bond valence sum associated with a local ionic valence has been adopted for the multi-layer systems. However, the uniform spin susceptibility per Cu spin in single-layer systems is known to be larger than those in double-layer systems. It should be noted that the difference in $^{63}K_{ab}$ of single-CuO$_2$-layer superconductor HgBa$_2$CuO$_{4+\delta}$ (Hg1201) and double-layer HgBa$_2$CaCu$_2$O$_{6+\delta}$ (Hg1212) has been overlooked. Thus, an issue how relevant the application of the single universal relation between $^{63}K_{ab}$ and $p$ is for the multi-layer systems should be addressed.

The optimal $T_c$s of Hg1201 and Hg1212 are the highest among the single-layer and the double-layer systems. The structural flatness of the CuO$_2$ plane characterizes Hg1201 and Hg1212. Figure 1 shows the schematic crystal structures of Hg1201 (left) and Hg1212 (right). Figure 2 shows the $^{63}$Cu Knight shifts $^{63}K_{ab}$'s of Hg1201 (open symbols) and Hg1212 (closed symbols) in an external magnetic field along the ab planes, which are reproduced from [9, 11]. The doping levels are catego-
relations of $S_1$:

In [9–11]. From the least squares fits, we obtained two overdoped doping (c).

The $63^{\text{Cu}}$ Knight shift $K_{ab}$ is given by $K_{ab} = K_s + K_{orb}$, where $K_s$ is the spin Knight shift and $K_{orb}$ is the orbital shift. $K_s$ is proportional to the uniform spin susceptibility multiplied by the hyperfine coupling constant. $K_{orb}$ is proportional to the Van Vleck orbital susceptibility. The temperature dependence of $63^{\text{K}}$ in the cuprate superconductors comes from that of the spin shift $K_s$. We have estimated $K_{orb} \sim 0.25\%$ for Hg1201 and $\sim 0.20\%$ for Hg1212 [9–11]. As seen in Fig. 2, $K_s$ of Hg1201 is larger than that of Hg1212 at each doping regime.

Figure 3 shows the hole concentration $p_h$ in [12] against $K_{ab}$ (%) at room temperature of Hg1201 and Hg1212 in [3,11]. From the least squares fits, we obtained two relations of S1: $p_h = 0.63^{\text{K}}(RT) - 0.13$ (Hg1201) and D1, $p_h = 0.74^{\text{K}}(RT) - 0.04$ (Hg1212). The solid lines in Fig. 3 indicate the fit functions of S1 and D1. The extrapolations of S1 and D1 to $p_h = 0$ lead to $K_{ab} = 0.21\%$ (Hg1201) and $0.05\%$ (Hg1212) at the phase boundary. The empirical functions of S1 and D1 are different from the previous fit functions F1 and F2. $K_s < 0.5\%$ adopted for the multi-layer systems in [3].

III. DISCUSSIONS

We discuss the hole concentration dependence upon the spin Knight shift for the other cuprate superconductors and the alternative estimation of the hole concentration.

Figure 4(a) shows $p_h$ against $K_{ab}$ (%) of Hg1201, LSCO [13]; Hg1212, Y1237 [14,15] and Y1248 [16,18]. We estimated $K_{ab}$ at room temperature for LSCO by linear extrapolation from the existing data in [13]. The single-layer system LSCO is located close to S1. The double-layer systems of Y1237 and Y1248 are located close to the line D1.

In Fig. 4(b), we estimated the hole concentrations $p_h$ by the parabolic curve of $T_c/T_{c,\text{max}} = 1 - 82.6(p - 0.16)^2$ in [19] after [5]. Figure 4(b) shows $p$ against $K_{ab}$ (%) of Hg1201, LSCO [13], Tl$_2$Ba$_2$CuO$_{6+\delta}$ (Tl2201) [20]; Hg1212, and Ba$_2$CaCu$_2$O$_{6-\delta}$ (0212F) [6]. In spite of the alternative estimation of the hole concentration, the $p$ vs $K_{ab}$ dependence of Hg1201 is different from that of Hg1212. The reason why $K_{ab}$ of Hg1212 are smaller than those of Hg1201 at the respective doping levels in Figs. 2 and 3 may be due to the effect of the magnetic bi-

FIG. 2: $63^{\text{Cu}}$ Knight shifts $K_{ab}$ for Hg1201 (open symbols) and Hg1212 (closed symbols) in the underdoped (a), the optimally doped (b), and the overdoped regimes (c), which are reproduced from [9–11]. The dashed lines indicate the individual $T_c$’s. The solid lines in (c) are visual guides.

FIG. 3: Hole concentration $p_h$ against spin Knight shift $K_{ab}$ (RT) (%) in Hg1201 and Hg1212. The solid lines are the fit functions of S1 and D1. The single-layer system LSCO is located close to S1. The double-layer systems of Y1237 and Y1248 are located close to the line D1.
layer coupling. The effect of the bilayer coupling has also been studied for the triple-layer superconductors. Thus, one should take into consideration which type relation is relevant $S_1$ or $D_1$ to estimate the individual hole concentrations of the non-equivalent CuO$_2$ planes in the multilayer superconductors.

IV. CONCLUSION

We found that the spin Knight shift $^{63}K_s^{ab}$ as a function of the hole concentration $p_h$ in the single-layer superconductors Hg1201 is different from that in the double-layer superconductors Hg1212. Since we believe that Hg1201 and Hg1212 are the canonical systems, the $p_h$ dependences upon $^{63}K_s^{ab}$ at room temperature in Hg1201 and Hg1212 should be standard to estimate the individual hole concentrations of the non-equivalent CuO$_2$ planes in a unit cell.

V. REFERENCES

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