Buckling of the CuO2 Plane in Single Crystals of La-Based High-TC Cuprates Observed by NMR

Buckling of the CuO$_2$ Plane in Single Crystals of La-Based High-T_C Cuprates Observed by NMR

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Abstract. The buckling of CuO$_2$ plane in single crystals of La-based high-T_C cuprates LSCO (x=0.15) and LBCO (x=0.08) was directly observed by Cu-NMR. In both the cases, buckling patterns obtained by NMR disagree with those expected in the averaged structure at the vicinity of the structural phase transitions.

Keywords: NMR, local structure, La-based cuprate.
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INTRODUCTION

La-based high-T_C cuprates show the structural phase transition from $I4/mmm$ phase to $Cmca$ at the temperature T_{d1}. Among them, La$_{2-x}$Ba$_x$CuO$_4$ (LBCO) and Nd-doped La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) show the successive transition to $P4_2/ncm$ at still lower temperature T_{d2}[1]. These two structural phase transitions are associated with the change in the flatness of CuO$_2$ plane. In $I4/mmm$ phase, the plane is flat, and CuO$_6$ octahedra stand vertically. In low temperature phases, there appear a characteristic buckling pattern in the plane. Especially, the pattern in the $P4_2/ncm$ phase is believed to pin the dynamically fluctuating stripe and stabilize it. This static stripe order suppresses the superconductivity as is well known in Nd-doped LSCO and LBCO[2,3].

However, there is a disagreement in reported experimental results on the bucking in the CuO$_2$ plane. Billinge *et al.* reported by the study on the pair distribution function of the neutron scattering that the CuO$_6$ octahedra in LBCO tilt randomly even in the $I4/mmm$ phase[4]. They claim that the local structure is quite different from the averaged one. Some other reports by techniques of XAFS, XANES *etc.*, also support the existence of the local structure, while still others do not [5~9]. The purpose of this work is to investigate the existence of the local structure in single crystals by Cu-NMR, which is a local probe, and is expected to detect local structures. We also expect

that this study will give a further insight to the role of the structure of CuO$_2$ plane in the stripe order.

EXPERIMENTAL

The single crystals of LSCO (x=0.15, T_C=37K) and LBCO (x=0.08, T_C=24K) were prepared by the conventional floating zone method [3,10]. Cu-NMR "angle-swept spectra" were obtained by recording the spin-echo amplitude while rotating a single crystal in a constant magnetic field.
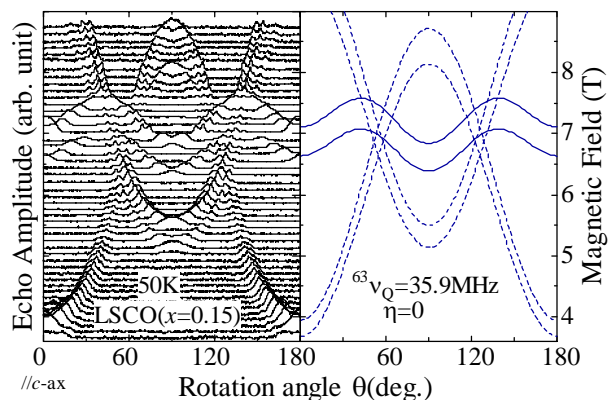

FIGURE 1. Angle-swept spectra of $^{63/65}$Cu-NMR in LSCO (left), and calculated curves with parameters of $^{63}\nu_Q$ = 35.9MHz, $K \approx 0.5\%$ and $\eta = 0$ (right). The field is tilted from c-axis to $(\cos 29°, \sin 29°, 0)_t$ in the tetragonal notation.
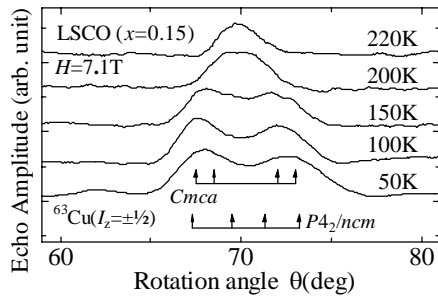
FIGURE 2. The temperature dependence of profile of angle-swept spectra in LSCO. Arrows show peak positions calculated assuming that the principal axis of the EFG tensor is tilted from c-axis by 3.5°.

RESULTS AND DISCUSSION

Figure 1 shows the rotational pattern of Cu-NMR spectra in LSCO. Each peak shows a slight split when the direction of the applied field is tilted from c-axis. We made a calculation of the quadrupolar shift with a second order perturbation assuming that the principal axis of the electric field gradient is parallel with the direction of the apical oxygen. In *Cmca* phase, there are the four tilting directions of the octahedron $(\pm1,\pm1,0)_t$, for the sample has a twin structure. In $P4_2/ncm$ phase, the tilting directions are $(\pm1,0,0)_t$ or $(0,\pm1,0)_t$. The calculated peak positions are shown by arrows in Fig. 2. One can see that *Cmca* with the tilting angle 3.5° reproduces the observed splitting at 50K. This indicates that the local structure observed by NMR is identical with the averaged structure which is reported to be *Cmca*.

When the temperature is raised, the split shrinks in the high temperature phase *I4/mmm*. Figure 3 shows the temperature dependence of the splitting width and the ultrasonic velocity. The latter is a good probe for the structural phase transition. In general, the lattice shows the softening around the transition temperature. In La-based cuprates, T_{d1} is determined from the
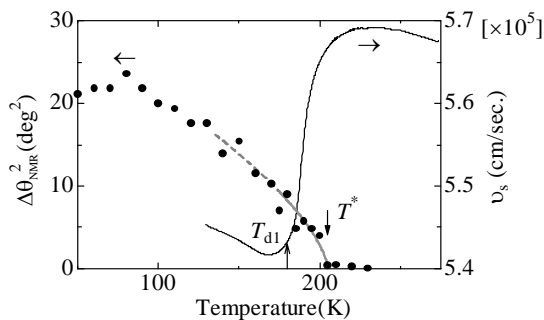
velocity data as the crossing point of linear extrapolations from the both sides of the transition[11]. Thus determined T_{d1} agrees with the onset of the orthorhombicity observed by X-ray diffraction. Note that onset of the NMR peak split is $T^*=205$K much higher than $T_{d1}=180$K. In the temperature region between T_{d1} and T^*, where the averaged structure is *I4/mmm*, what NMR sees is the local structure of *Cmca*. This local structure is static in time, because the characteristic time scale of NMR is very slow. As the temperature is decreased to T_{d1}, the static but non-periodic buckling pattern is first formed at T^*, and then it is aligned periodically at T_{d1}.

Finally, we show in Fig. 4 the rotational profile of ^{63}Cu-NMR in LBCO ($x=0.08$), T_{d2} of which is reported to be around 10K[12]. Calculated peak positions based on the local structure of $P4_2/ncm$ and *Cmca* are shown by arrows. The observed profile of a single spired peak suggests that the local structure is likely to be the former up to 100K, while the averaged one is the latter. The existence of the buckling pattern of $P4_2/ncm$ can be related with the recently reported field-induced stripe order in LBCO with x slightly apart from 1/8[10].
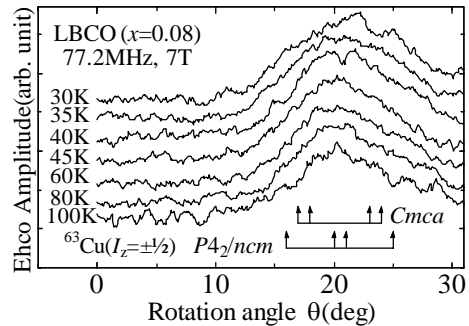

FIGURE 4. The temperature dependence of profile of angle-swept spectra in LBCO. The field is tilted from c-axis to $(\cos35°,\sin35°,0)_t$. Arrows show the calculated position of peaks expected for local structures of *Cmca* and $P4_2/ncm$ with a tilting angle of 4.5°

FIGURE 3. Temperature dependence of NMR-splitting width (solid-symbols), and the ultrasound velocity measured by longitudinal wave of 9MHz, C_{11} mode. The definition of T_{d1} is stated in the text. T^* is the onset of the peak splitting. The gray curve is a guide to eyes.

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