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# Local magnetic fields in antiferromagnetic $Bi_2CuO_4$: as seen from $^{63,65}$Cu and $^{209}$Bi nuclear resonance

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**Abstract**

A complex spin-echo spectrum of $^{63,65}$Cu and $^{209}$Bi has been observed in antiferromagnetic $Bi_2CuO_4$ at 4.2 K. The spectrum consists of $^{63,65}$Cu AFNR and $^{209}$Bi NQR. The Cu AFNR is characterized by the internal field $H_{\mathrm{int}} = 99$ kOe at Cu nuclei and by the $^{63}\nu_Q = 10$ MHz. It is argued that the low-limit of the internal field at the $^{209}$Bi nuclei is 4.3 kOe. The occurrence of $H_{\mathrm{hf}}$ at $^{209}$Bi nuclei shows that $Bi^{3+}$ anions take part in the superexchange interaction between Cu atoms along the Cu–O–Bi–O–Cu bonds. 

*Keywords:* AFNR; NQR

The structure of $Bi_2CuO_4$ does not allow an ordinary Cu–O–Cu superexchange interaction between $Cu^{2+}$ cations. The AF order is maintained by strongly anisotropic inter- and intra-sublattice interactions involving at least several anions by two possible ways: Cu–O–Bi–O–Cu [1] or Cu–O–O–Cu [2]. There is still no understanding of the role of Bi ions in these interactions. Here we present spin-echo studies in pure AF samples of $Bi_2CuO_4$.

Cu NQR spectra were obtained using a point-by-point technique at 4.2 K. In order to separate the $^{63,65}$Cu part of the observed complex spectrum from $^{209}$Bi we measured the zero-field spectrum of $Bi_2CuO_4$ enriched by the $^{65}$Cu isotope (Figs. 1–3). This allows to conclude, that all the observed resonance lines below 80 MHz belong to $^{209}$Bi nuclei.

We have assigned the upper frequency triplet with the intense central line at 112.5 MHz in Fig. 3 to a quadrupole splitted spectrum of $^{63}$Cu isotope. Using the experimental frequencies of the left- and right-side peaks (107.0(1) and 117.0(1) MHz) of the triplet, the second-order perturbation treatment for $\eta = 0$ and $\theta = 90^\circ$ yields $^{63}\nu_L = 112.0(1)$ MHz and $^{63}\nu_Q = 10.0(1)$ MHz. The calculated frequency for the central line, 112.2 MHz, lies within the limits of experimental error of peak position.

The obtained Larmor frequency $^{63}\nu_L = 112.0(1)$ MHz corresponds to a hyperfine field of 99.0(1) kOe. Using the hyperfine coupling constant for $Cu^{2+}$ equal to 120 kOe/$\mu_B$ and ignoring the dipolar contribution, we obtain a magnetic moment of $0.82\mu_B$ which is close to the value of $0.85\mu_B$ deduced from neutron diffractometry [3].

From the principal axes directions of the electric field gradient tensor it is evident that in the elementary cell of $Bi_2CuO_4$ there are four pairs of crystallographic sites of Bi atoms which become inequivalent when a magnetic field appears at Bi sites. Such a magnetic inequivalency might be the reason for the abundance of resonance lines observed in $Bi_2CuO_4$ (Figs. 1–3), which considerably hampers the interpretation of the spectrum.

In the presence of a high internal magnetic field $H_{\mathrm{int}}$ and the asymmetry parameter $\eta$ close to unity, the Bi nuclei could exhibit Zeeman transitions ($-m \Leftrightarrow m$) with

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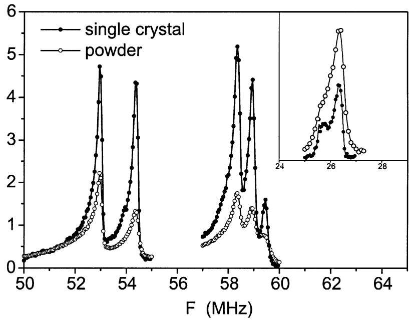


Fig. 1. Low-frequency part of the zero-field spectra of $Bi_2CuO_4$. Ceramic sample enriched by $^{65}Cu$. Inset: the low-frequency line of this spectrum in the same frequency scaling.

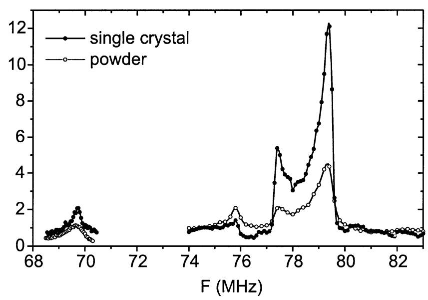


Fig. 2. Middle-frequency part of the zero-field spectra of $Bi_2CuO_4$. Ceramic sample enriched by $^{65}Cu$.

the highest probability for $(-\frac{1}{2} \Leftrightarrow \frac{1}{2})$ [4]. Since the low-frequency spectrum cannot fit Bi NQR, we assume that the resonance line at 26.35 MHz corresponds to the $(-\frac{1}{2} \Leftrightarrow \frac{1}{2})$ transition. We estimate the minimum value of $H_{int}$ necessary to create this transition to be $H_{int}(\min) =$ 4.3 kOe.

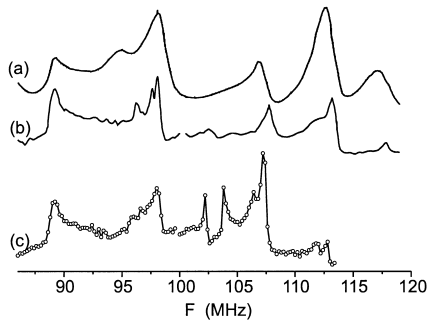


Fig. 3. High-frequency part of the zero-field spectra of different $Bi_2CuO_4$ samples: (a,b) different single crystals and (c) ceramic sample enriched by $^{65}Cu$.

This value is almost one order of magnitude larger than $H_{dip}$, which supports our assumption about a comparatively large $H_{hf}$ contribution to $H_{int}$ at Bi atoms.

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