Supertransferred Hyperfine Interactions in $LaSrGa_{0.995}Cu_{0.005}O_4$ Single Crystal and Isostructural Cuprates

Yu.V. Yablokov[a], **O.A. Anikeenok**[b], **M.A. Augustyniak-Jabłokow**[a] **and T.A. Ivanova**[c].

[a]Institute of Molecular Physics PAS, Smoluchowskiego 17, 60-179 Pozna, Poland
[b]Kazan State University, Kremljevskaja 18, 420 008 Kazan, Russia
[c]Kazan Physical Technical Institute RAN, Sibirskii Trakt 10/7, 420 029 Kazan, Russia

9.7 cm

A nearly isotropic supertransferred hyperfine coupling of Cu^{2+} electron spin with the four neighboring Ga^{3+} nuclei in $LaSrGa_{0.995}Cu_{0.005}O_4$single crystal are discovered. EPR spectra parameters $A_{Cu\|} = 143\pm.5$; $A_{Cu\perp} = 3\pm0.5$; $A_{Ga\|} = 18.4\pm0.3$; $A_{Ga\perp}$ 22.1 ± 0.3 (in 10^{-4}cm^{-1}); $g_{\|} = 2.320 \pm0.005$; $g_{\perp} = 2.058 \pm.005$ are temperature independent in the 4.2 – 300 K range. An analysis of the obtained data is fulfilled in a framework of the configurational interaction theory. The cascade transfers of gallium $3s$-and $3p$-electron onto the copper orbitals through the $2s-$ and $2p-$orbitals of the intermediate oxygens, due to the overlapping and covalence effects, are shown to explain the experimental parameters. The transfer integrals $3s$, $3p$ (Ga) $\rightarrow$ unfilled orbital of oxygen are equal λ_s = 0.15, $\lambda_\sigma = 0.18$ and consistent with literature data for the iron group ions. Assuming identity of the on-set and supertransferred hyperfine fields in $LaSrGa_{0.995}Cu_{0.005}O_4$and in La_2CuO_4 and using the results of NMR in the antiferromagnet La_2CuO_4 [T.Tsuda et al., J.Phys.Soc.Jpn. **57**, 2908(1989)] we estimate a zero-point spin deviation of $\approx$0 % in this compound. The shown comparability obtained local fields in $LaSrGa_{0.995}Cu_{0.005}O_4$ with the corresponding fields in La_2CuO_4 determined in the study of anisotropies of the Knight shifts and relaxation rates of the Cu nuclei and calculated by P. Hüsser et al. [Phys.Rev.**61**, 1567(2000)] is discussed.

13.4 cm

Subject category :

4. Rare Earths and Actinides, Alloys and Compounds

Presentation mode :
poster

Corresponding author :
Yu.V. Yablokov

Address for correspondence :
Institute of Molecular Physics, PAS// ul. Smoluchowskiego 17//60-179 Poznań, POLAND

Email address :
yablokov@ifmpan.poznan.pl