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EPR of $YBa_2Cu_3O_{6+y}$: models of paramagnetic centers with $g \approx 4.2$

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Abstract

A systematic investigation of the EPR line with $g \approx 4.2$ in $YBa_2Cu_3O_{6+y}$ has been carried out. From the temperature dependence of the line integrated intensity we have deduced that the line is due to paramagnetic centers with integer spin. The energy interval between the ground singlet state and the excited state with $S = 1$ was estimated as 8–10 K. Energy levels of the cluster $Cu^{2+}(S = \frac{1}{2})$–"$Cu^{3+}(S = 0)$"–$Cu^{2+}(S = \frac{1}{2})$ were calculated for different sets of parameters.

Keywords: Copper–oxygen cluster; Electron paramagnetic resonance; YBaCuO

It is supposed that EPR signals in $YBa_2Cu_3O_{6+y}$ compounds for $0.09 < y < 0.7$ can be attributed mainly to paramagnetic chain fragments (see Ref. [1] and references therein). The electronic structure of those fragments has not been completely understood. Systematic investigations have been performed on the EPR line with $g \approx 2$. In the present communication we report our results about the additional EPR signal in $YBa_2Cu_3O_{6+y}$ with $g \approx 4.2$.

A short summary of our experimental observations can be given as follows: the line is detected for a different doping index y. Part of our results for $YBa_2Cu_3O_{6.35}$ are given in Figs. 1 and 2. No superconducting transition was detected by our susceptibility measurements. The signal in half-magnetic field is detected both in nonoriented and oriented samples at $H \| c$ and $H \perp c$. The lines with $g \approx 4.2$ and 2 are not correlated with each other and therefore belong to different chain fragments. The temperature dependence of the integrated intensity of the line with $g \approx 4.2$ in contrast to the integrated intensity of EPR line with $g \approx 2$ in $YBa_2Cu_3O_{6.35}$ does not obey the Curie law. It can be described by $I \approx \text{const.}/[T(3 + \exp(\Delta/T))]$ were Δ is the energy interval to the excited state $S = 1$.

Under incomplete filling of the chains by oxygen ions in $YBa_2Cu_3O_{6+y}$ we can expect the formation of two- or

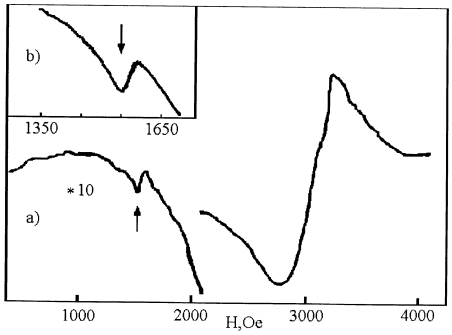

Fig. 1. EPR spectrum of nonoriented $YBa_2Cu_3O_{6.35}$, X-band. (a) $T \approx 14$ K, (b) fragment in range 1300–1700 Oe, $T \approx 4$ K. Arrows indicate the line with $g \approx 4.2$.

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