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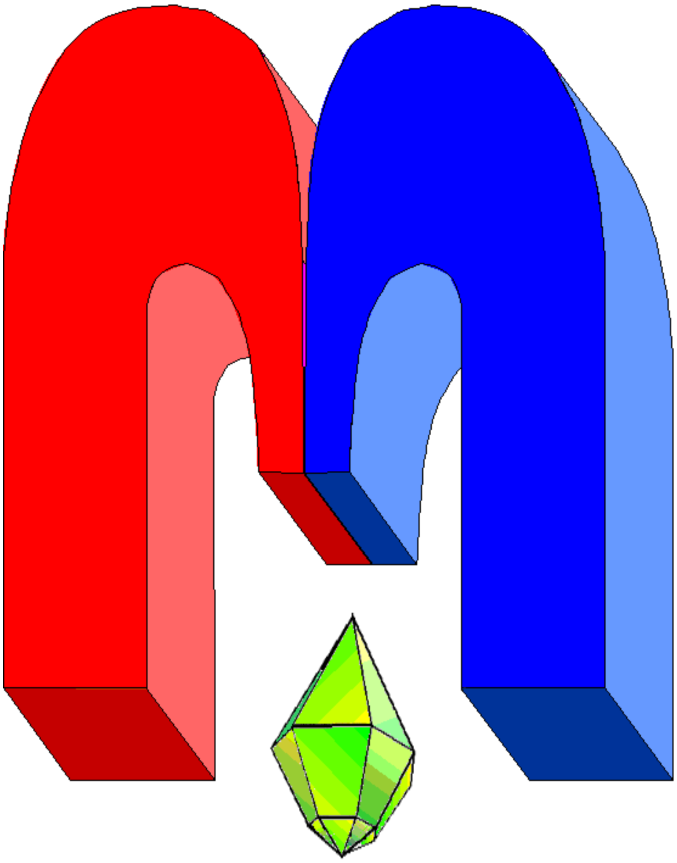

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[*] In Kazan University the Electron Paramagnetic Resonance (EPR) was discovered by Zavoisky E.K. in 1944.

Inhomogeneous broadening of the EPR signal of Yb^{3+} ions in domain walls of lightly doped antiferromagnetic cuprates

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Distortion of the long-range antiferromagnetic order in the $YBa_2Cu_3O_{6+y}$ is investigated by the electron paramagnetic resonance (EPR) measurements for $y = 0.1 - 0.4$. In the case of the doping level $y = 0.2, 0.3$ the EPR signal consists of narrow and broad lines, which we relate to formation of the charged domain walls. Our theoretical analysis of the inhomogeneous EPR broadening due to the local antiferromagnetic order distortion in domain walls is well consistent with experimental results for the case of coplanar elliptical domain walls.

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Keywords: YBCO, elliptical domain wall, EPR

1. Introduction

The electron paramagnetic resonance (EPR) proved to be a powerful method of studying electronic properties of the high-temperatures superconductors (see review [1]). The low-frequency spin kinetics of the parent compound $YBa_2Cu_3O_{6+y}$ with $y = 0.1$ was investigated recently using the Yb^{3+} ion as the EPR-probe [2, 3]. At this level of oxygen doping the *p*-holes do not yet appear in the CuO_2 planes, and the ideal antiferromagnetic (AF) order is not affected [4]. The broadening of the Yb^{3+} EPR signal was explained by the spin-spin indirect interaction via magnons and the usual magnetic dipole-dipole interactions [2-3]. It is widely accepted that at $y > 0.15$ the holes in the CuO_2 planes start to destroy the long-range magnetic order by creating polarons, domain walls, vortices and skyrmions [5-8]. This evolution of the AF state could be detected by the additional broadening of the EPR linewidth.

In this paper we report the results of our EPR signal investigations in $Y_{0.98}Yb_{0.02}Ba_2Cu_3O_{6+y}$ with $y = 0.2, 0.3, 0.4$. We have found that the Yb^{3+} EPR signal can be described by the sum of two lorentzians with sufficiently different linewidths. Figure 1 shows the temperature dependence of the narrow and the broad lines for different levels of oxygen doping. The intensity of the broad line increases with doping and disappears at $y = 0.4$. In the case $y = 0.3$ almost only the broad line is seen.

We assume that this EPR signal behavior can be explained by the electronic phase separation into the rich and poor in holes regions in the CuO_2 planes. The separation can be related naturally to creation of charged domain walls (stripes). The local distortions of the antiferromagnetic order in the domain walls should give an additional inhomogeneous broadening to the Yb^{3+} EPR signal due to exchange coupling between the ytterbium and copper ions. We will consider separately the collinear and coplanar antiphase domain walls, which are created by the *p*-holes localized in the CuO_2 planes on the oxygen ions around the Cu^{2+} ions.

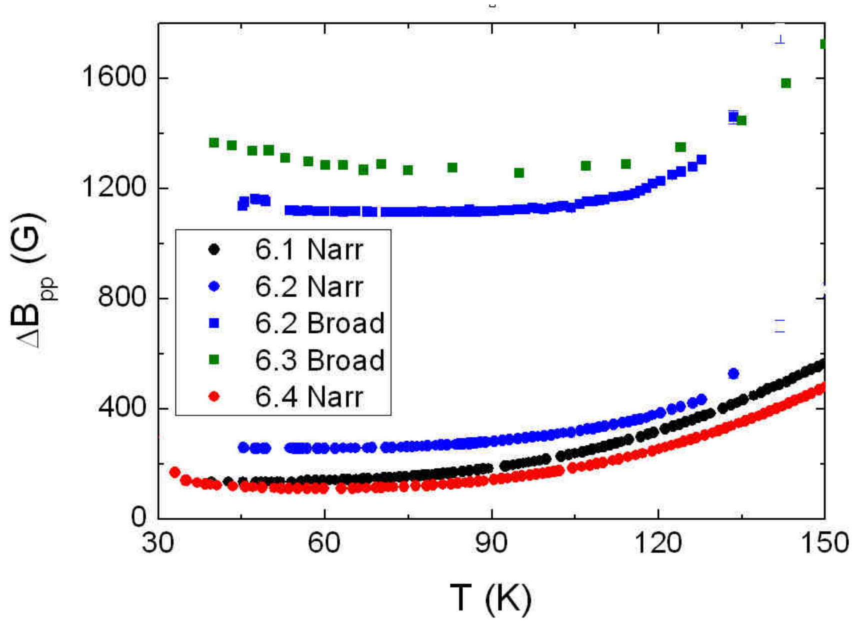

Figure 1. EPR linewidths for the broad and narrow lines fitted with Lorentzian lineshape.

2. Collinear domain walls

The detailed investigation of this type of charged domains was performed by Giamarchi and Lhuillier based on the two-dimensional Hubbard model [9]

$$H = -t\sum_{\langle ij\rangle,\sigma} c^{+}_{i\sigma} c_{j\sigma} + U\sum_{i} n_{i\uparrow} n_{i\downarrow}. \qquad (1)$$

Here $c_{i\sigma}\left(c^{+}_{i\sigma}\right)$ are annihilation (creation) operators for an electron with spin σ at the site i, and $n_{i\sigma} = c^{+}_{i\sigma} c_{i\sigma}$. U is the on-site Hubbard repulsion ($U > 0$), and t is the hopping parameter. The numerical solutions were investigated by the Monte Carlo variational technique using the Hartree-Fock trial function. For the strong enough Hubbard repulsion ($U/t \geq 4$) the stable collinear domain-wall solutions were found, where the doped *p*-holes are localized within a stripe around the each Cu^{2+} site. This stripe separates two AF ordered regions with opposite signs in the AF order parameter. In the $U/t = 10$ case the calculated spin texture of the collinear domain wall along the *y*-axis could be well reproduced by the phenomenological model for the *x*-component of the order parameter for two sublattices:

$$\left\langle S^{xa}_{n}\right\rangle = S_0 \tanh\left(x_n/\xi\right), \quad \left\langle S^{xb}_{n}\right\rangle = -S_0 \tanh\left(x_n/\xi\right). \qquad (2)$$

Here x_n is the position of the site with respect to the stripe, ξ gives a width of the domain wall and S_0 is the order parameter on a long distance from the stripe. These results were confirmed later by Seidbold, Sigmund and Hizhnyakov by numerical calculations within the slave-boson mean-field approximation for the two-dimensional Hubbard model [10].

In the presence of the external magnetic field directed along the stripe the order parameter component along the magnetic field appears [2]:

$$\left\langle S^{ya}_{n}\right\rangle = \left\langle S^{yb}_{n}\right\rangle = S_0 \sin\varphi \tanh\left(x_n/\xi\right); \qquad (3)$$
$$\sin\varphi = g_{\mathrm{Cu}}\mu_B H_0 / 4J.$$

An angle φ between the sublattices' magnetizations and the *x*-axis is defined by the relation between the Zeeman energy of the Cu^{2+} ions $g_{\mathrm{Cu}}\mu_B H_0$ and the exchange coupling *J* between them [2]. This magnetizations components of the AF sublattices give a contribution to the Yb^{3+} ions Zeeman energy due to their exchange coupling with the neighboring Cu^{2+} ions:

$$H_{\mathrm{YbCu}}^{\mathrm{col}} = 8A\sin\varphi\, S_0 \sum_n Y_n^y \tanh\left(x_n / \xi\right). \tag{4}$$

Here *A* is the exchange coupling between the ytterbium and copper ions, Y_n^y is the *y*-component of the Yb^{3+} ion spin operator. This interaction is the source of the additional inhomogeneous EPR signal broadening due to the Yb^{3+} ions located in the domain walls. The corresponding contribution to the EPR linewidth can be estimated by the moments method. The second moment has the form

$$M_2 = \mathrm{Sp}\left\{\left[Y_0^x, H_{\mathrm{YbCu}}^{\mathrm{col}}\right]\left[Y_0^x, H_{\mathrm{YbCu}}^{\mathrm{col}}\right]\right\}\left\{\mathrm{Sp}\left(Y_0^x Y_0^x\right)\right\}^{-1} = \sum_n \left(4A\sin\varphi\right)^2 \left[\tanh\left(x_n\right)\right]^2. \tag{5}$$

We here put $S_0 = 1/2$. In the similar way the forth moment can be calculated. Transforming the sum over the sites inside the domain wall into the integral ($-2\xi \le x \le 2\xi$) we can find the EPR linewidth:

$$\begin{gathered} M_2 = 0.5\left(4A\sin\varphi\right)^2, \quad M_4 = 0.35\left(4A\sin\varphi\right)^4; \\ \Delta H_{\mathrm{theor}}^{\mathrm{col}} \sim 2\left(M_2^3 / M_4\right)^{1/2} \approx 4.8\left|A\right|\sin\varphi \approx 90\ \mathrm{G}. \end{gathered} \tag{6}$$

The obtained value is much less than the experimental value of the broad EPR line $\Delta H_{\mathrm{exp}}^{\mathrm{broad}} \approx 1200$ G. The smallness of the contribution calculated appears due to a very small value of $\sin\varphi$ which is defined by the relation of Zeeman energy to the exchange coupling between the nearest Cu^{2+} ions, which is $\sin\varphi \approx 6\cdot 10^{-5}$ in our case. This argument stimulates the investigation of a possible role of the coplanar domain walls.

3. The elliptical domain wall

An existence of the coplanar domain walls in the AF order of the CuO_2 planes was predicted by Zachar, Kivelson, and Emery on the basis of the Landau theory of phase transitions [11]. Particular spin and charge textures for elliptical domain walls were calculated by Seibold within the two-dimensional Hubbard model [12]. It was shown that for the completely filled domain wall (i.e. one hole per site along the stripe) only the collinear solutions exist whereas the coplanar structures become stable for half-filled walls for small hole concentrations. Figure 2a shows the spin texture for the case when two holes occupy alternatively the neighboring sites along the charged stripe. In this case the spin texture is similar to the coupled vortex-antivortex structure [12]. We suggest the following phenomenological model to reproduce the calculated spin texture.

a) The hole is present in the stripe:

$$S_n^{ya} = S_0 \sin\alpha \frac{\tanh\left(x_n / \xi\right)}{\cosh\left(x_n / \xi\right)}, \quad S_n^{yb} = -S_0 \sin\alpha \frac{\tanh\left(x_n / \xi\right)}{\cosh\left(x_n / \xi\right)}. \tag{7}$$

b) The hole is absent in the stripe:

$$S_n^{ya} = S_0 \sin\alpha \frac{1}{\cosh\left(x_n / \xi\right)}, \quad S_n^{yb} = -S_0 \sin\alpha \frac{1}{\cosh\left(x_n / \xi\right)}. \tag{8}$$

Here $\sin\alpha$ defines the eccentricity of the elliptical domain wall; the case $\alpha = \pi/4$ describes an ideal spiral solution, whereas $\alpha = 0$ reduces the spin structure to a collinear domain wall.

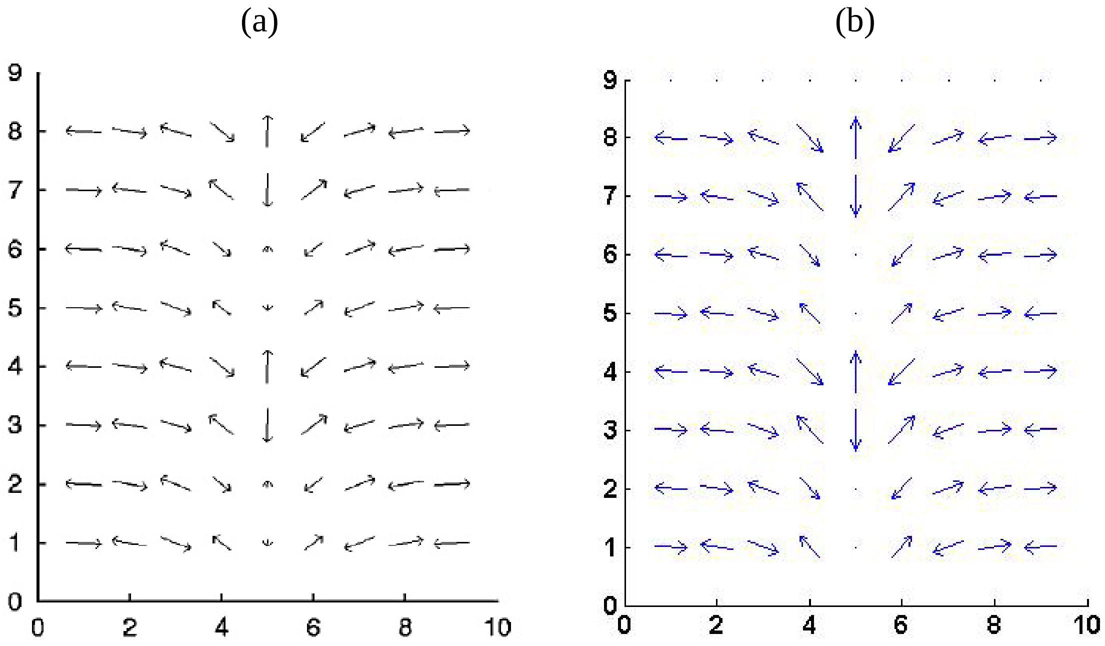

Figure 2. Spin structures for the elliptical domain wall: the pattern (a) was calculated numerically by Seibold [12]; the pattern (b) shows our phenomenological model, calculated using formulas (7) and (8).

Hereafter we neglect an additional rotation of the magnetic moments caused by the external magnetic field. One can see (Figure 2b) that this model reproduces the calculated spin texture quite well.

The secular part of the corresponding Hamiltonian for the exchange interaction between the ytterbium ion and the elliptical domain wall takes the following form

$$H_{\mathrm{YbCu}}^{\mathrm{ell}} = \frac{A}{2}\sin\alpha \sum_n Y_n^y F\left(x_n/\xi\right),$$
$$F\left(\frac{x_n}{\xi}\right) = \left\{\frac{\tanh\left(x_n/\xi\right)}{\cosh\left(x_n/\xi\right)} - \frac{1}{\cosh\left(x_n/\xi\right)} - \frac{\tanh\left[(x_n+a)/\xi\right]}{\cosh\left[(x_n+a)/\xi\right]} + \frac{1}{\cosh\left[(x_n+a)/\xi\right]}\right\}. \tag{9}$$

Calculations similar to the case of the collinear domain wall give

$$M_2 = 8.5\cdot10^{-3}\left(A\sin\alpha\right)^2, \quad M_4 = 1.9\cdot10^{-4}\left(A\sin\alpha\right)^4;$$
$$\Delta H_{\mathrm{theor}}^{\mathrm{ell}} = 0.132|A|\sin\alpha. \tag{10}$$

Taking again the value $|A| = 120\,\mathrm{K}$ [2], we can achieve the experimental value for the broad EPR line $\Delta H_{\mathrm{exp}}^{\mathrm{broad}} \approx 1200\,\mathrm{G}$ with a rather small eccentricity of the elliptical domain wall: $\sin\alpha = 2.9\cdot10^{-2}$. One could expect that at the level of oxygen doping approaching $y = 0.4$ the AF order will be destroyed, the holes in the CuO_2 planes delocalized, and the inhomogeneous broadening of the Yb^{3+} EPR line will vanish. Such a behavior was actually observed in our case.

To conclude, we have investigated both experimentally and theoretically the evolution of the AF order in the $Y_{0.98}Yb_{0.02}Ba_2Cu_3O_{6+y}$ system on the basis of the EPR measurements. We have found that the EPR results can be explained on the basis of the electronic phase separation in the CuO_2 planes due to a formation of the antiphase elliptical domain walls by the doped oxygen *p*-holes.

Acknowledgments

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