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Mössbauer effect applications to the investigation of Cu(1) sublattice dynamics in oxide HTS at temperatures around T_c

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An attempt has been made to study the changes caused in the dynamics of local atomic vibrations in CuO chains by a Bose condensation of local pairs of holes which have formed in valence shells of oxygen atoms.

1. Introduction

Direct evidence that displacements of oxygen atoms in O4 sites play an important role in the superconductivity [1] and in the pronounced anharmonicity of the oxygen vibrations [2] has emerged from an EXAFS study of $YBa_2Cu_3O_{7-\delta}$ compounds. Anomalies in the vibrations in CuO_2 layers near T_c have been found in previous experiments on ion channeling [3].

Further proof that there is a relationship between the dynamics of the ions of the copper–oxygen subsystem and superconducting correlations comes from the decrease in the probability for the Mössbauer effect (f') near T_c. This decrease has been observed in several doped superconducting metal oxides [4–6]. It stems from an increase in the mean square vibration amplitude of the Mössbauer atoms occupying the copper sites at low concentrations.

An approach of interest for studying this relationship has been formulated by various investigations on the basis of ref. [7]. The idea involves a lifting of the degeneracy of the electron spectrum by means of an interaction with displaced ions (a band Jahn–Teller effect). This idea would lend support to the idea that a strongly correlated state forms in a high T_c superconductor [8] and would make it possible to study the "softening" of the oxygen-ion vibrations (including the formation of a two-well ion potential) at low temperatures [9]. Guided by the results of refs. [7–9], we have attempted in the present study to learn about the changes caused in the dynamics of local atomic vibrations in CuO chains by a Bose condensation of local pairs of holes which have formed in valence shells of oxygen atoms. The superconducting correlations are described on the basis of the exciton mechanism developed in the ref. [10]. That mechanism leads to an attraction of the holes of oxygen ions in CuO chains. A calculation carried out here on the basis of a local-pair superconductivity can be used, with appropriate generalizations, to study the effect of superconducting correlations and correlations of other types on the ion dynamics in CuO chains.

It is well known that at low concentrations of the Mössbauer nuclei (^{57}Fe and ^{119}Sn) replacing copper, primarily in Cu(1) sites, in the metal oxides, no significant changes occur in T_c [6]. This assertion does of course not mean that the oxygen surroundings, the energetics of the valence states, and the elastic coupling constants of the substituted atoms do not differ from the corresponding properties of copper in Cu(1) sites. The superconducting properties in the one or two nearest coordination spheres around the substituent atoms are undoubtedly disrupted to a substantial extent, and these regions no longer take

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