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Supertransferred hyperfine interactions in layer $\text{LaSrGa}_{0.995}\text{Cu}_{0.005}\text{O}_4$

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Abstract

The EPR allowing a direct observation of supertransferred hyperfine fields on the nuclei of the next-nearest cations to copper ion in the structure of $\text{LaSrGa}_{0.995}\text{Cu}_{0.005}\text{O}_4$ isomorphous to the superconducting cuprates prove the far delocalisation of the spin density. The theoretical analysis of the value and mechanisms of this process by the method of configurational interaction leads to a good agreement with the experiment. It is shown that the cascade processes involving simultaneous electron transfers from the oxygen to the copper atom and from the neighbouring cation to the same oxygen, in the fragment considered bring a substantial contribution into polarisation of 3s-shell of gallium ion.

A comparison of the supertransferred hyperfine fields and g -tensor values in the studied, diluted $\text{LaSrGa}_{0.995}\text{Cu}_{0.005}\text{O}_4$ crystal and in the La_2CuO_4 cuprate confirms the validity of the local centre approach in the analysis of cuprate properties.

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1. Introduction

We have recently reported [1] an observation of the magnetic superhyperfine structure due to the interaction of the unpaired electron of Cu^{2+} ion

with nuclear magnetic moments of Ga^{3+} ions, which are the next nearest cations of Cu^{2+} ions in the $\text{LaSrGa}_{0.995}\text{Cu}_{0.005}\text{O}_4$ crystal belonging to the K_2NiF_4 structure type. The study of the local magnetic fields at the nuclei of diamagnetic cations in the crystals doped with magnetic ions allows elucidation of the mechanisms of the electron density transfer from the metal ion into the orbitals of the neighbouring ions in the crystals. Such a transfer is usually realised indirectly

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