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LOCAL STRUCTURE, DISTORTIONS AND DISORDER IN ADVANCED PEROVSKITE MATERIALS

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Abstract

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Both high-temperature superconductors and the lanthanum-manganate-based giant magnetoresistors have a perovskite-like structure and interesting electronic properties. In each case, the deviations from the perovskite structure may be the key to understanding the novel behavior of these materials. These deviations can take the form of a distortion of the crystal structure, such as a Jahn-Teller distortion, or distortions that only occur on the local scale and thus do not affect the average crystal structure as determined by diffraction experiments. Disorder of the individual atomic sites can also have an effect on the electronic properties. For instance, various phonon modes may be very important for understanding change transfer if an electron-phonon coupling exists. Correlation measurements provide an important indicator for certain kinds of disorder, such as optical phonons and polaron distortions. In this dissertation I present x-ray-absorption fine-structure (XAFS) data that demonstrates such disorder in the $La_{1-x}A_xMnO_3$ materials and consider the possibility in the high-T_c superconductors $YBa_2Cu_3O_7$ and $HgBa_2CuO_4$. I also consider the effect of static distortions in these materials, and in particular, I explore the effect of substituting praseodymium for yttrium in $YBa_2Cu_3O_7$ in light of the anomalous suppression of T_c for this substitution. A monotonic decrease of the Pr-O XAFS amplitude with increasing Pr concentration is best fit by including a short Pr-O bond. Such a bond is evidence for a localized hole.

During the course of these studies, some improvements to the XAFS analysis technique were necessary. These include an improved self-absorption correction for measuring fluorescence yields, an understanding of the use of solid-state detectors and dead-time, and accurate background-absorption removal from the data. The latter often generated background-absorption curves with spurious features. With the help of Prof. J. J. Rehr, we considered the possibility that these features were not the result of multiple electron excitations (as was previously thought), but were actually the manifestation of the outgoing photoelectron backscattering off the absorbing atom's potential in a manner analogous to the Ramsauer-Townsend effect.

Contents

List of Figures

List of Tables

To my wife,

Margaret Coffey Booth

and

my parents, Corwin and Caroline

and

my siblings, Chris, Doug, Julie and Lyn.

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