Current Applied Physics 17 (2017) 1271–1278

Contents lists available at ScienceDirect

Current Applied Physics

journal homepage: www.elsevier.com/locate/cap

Theoretical investigation of electronic, magnetic, transport and optical properties of the pure and doped cuprate superconductor $HgBa_2CuO_{4+\delta}$

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ARTICLE INFO

Article history:
Received 27 June 2016
Received in revised form
11 June 2017
Accepted 13 June 2017
Available online 15 June 2017

Keywords:
Cuprate superconductor
DFT
Monte Carlo simulation
Ceramic materials

ABSTRACT

We report detailed DFT calculations and Monte Carlo simulations on the pure and doped cuprate superconductor $HgBa_2CuO_{4+\delta}$. For the pure compound ($\delta = 0$), we have obtained an insulating behavior with strong antiferromagnetic copper spin correlations in the CuO_2 plane. The high value of the calculated Néel temperature $T_N = 333$ K reflects the large in-plane exchange interaction $J = -145$ meV. The obtained optical properties and critical exponents demonstrate the anisotropic quasi-2D character of this type of materials. As for the doped compound the electronic structure and the transport properties have been investigated for various values of doping. Based on these data, we suggest a prediction of the value of optimum doping for $HgBa_2CuO_{4+\delta}$ ($\delta_{optimal} = 0.125$).

1. Introduction

In the year 1986 the scientific community was surprised with the measurements of Müller and Bednorz who discovered superconductivity with T_c of ~30 K in ceramic material $La_{2-x}Ba_xCuO$, having planes of copper oxide (cuprate) [1]. The event was noted as starting point of the discovery of High Temperature Superconductivity (HTSC). Till date there has been no agreement on a complete theory capable of explaining the unusual physical properties of these materials [2]. Not only the theory behind superconductivity for many HTSC is a mystery, but also the idea to realize this phenomenon at room temperature is one of the biggest challenges, which has led to an intense activity in this field including researchers and technologists working all around the world [3].

Since the first mercury based HTSC materials were synthesized by Putilin [4], extensive research have focused on these materials. $HgBa_2CuO_{4+\delta}$ is the first compound of the mercurocuprate series, one of the simplest oxide superconductors with only one CuO_2 plane between layers in the unit cell. The superconducting temperature T_c of $HgBa_2CuO_{4+\delta}$ can vary between 0 K and 98 K depending on the excess oxygen content δ [5]. This compound is also of interest for the reason that his copper–oxygen plan has the most ideal tetragonal structure compared with other cuprate materials which does not change when doping. It would therefore seem to be a perfect system to study the fundamental phenomena and the mechanism of HTSC.

In this work, two approaches ab initio calculations and Monte Carlo simulations (MCS) are used to shed light on some of the physical properties of $HgBa_2CuO_{4+\delta}$. All the results are compared to other theoretical and experimental data.

The paper is organized as follows: the crystal structure of the material of interest is described in section 2. Detailed theoretical techniques are given in section 3. The obtained results are presented and discussed in section 4. Finally, we present the conclusions of our work in section 5.

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http://dx.doi.org/10.1016/j.cap.2017.06.005
1567-1739/

2. Crystal structure

The crystal structure of $HgBa_2CuO_{4+\delta}$ (Hg-1201) is tetragonal with space group *P4/mmm*. The lattice constant $a = 3.875$ Å and the *c* over *a* ratio, $c/a = 2.455$ with a volume $V = 142.65$ Å^3. The unit cell and the positions of the atoms are shown in Fig. 1 and Table 1. The simple tetragonal unit cell of $HgBa_2CuO_{4+\delta}$ contains a single layer CuO_2, with apical oxygens above and below the Cu ions. The plane oxygen is represented by O(1) and the apical oxygen by O(2). The partial oxygen occupancy is denoted O(3). Barium ions (Ba) are placed above and below the centers of the cuprate squares. The physical properties and the superconducting transition temperature are strongly influenced by the concentration of the interstitial defect O(3). As a rule, the superconducting transition temperature T_c for copper-oxide superconductors has a parabolic variation with a maximum at optimal doping δ_{opt} [6].

3. Theoretical method

3.1. First principles calculations

3.1.1. Computational details

First principles calculations are performed using the FP-LAPW method based on spin polarized density functional theory, as implemented in the WIEN2k code [8]. The muffin tin radii (RMT) were assumed to be 2.05 a.u (atomic units) for Hg and 2.5 a.u for Ba and 1.96, 1.68 for Cu and O respectively. A mesh of $10 \times 10 \times 10$ k-points in the irreducible part of the first Brillouin zone (IBZ) has been used in the calculation. The convergence was achieved by considering the cut-off energy up to $R_{MT}{}^{*}K_{max} = 7$. The self-consistent calculations are considered to converge when the total energy of the system is stable within 0.00001 Ry. For the pure compound $HgBa_2CuO_4$ the exchange correlation potential was treated by the generalized gradient approximation including the Hubbard interaction *U* (GGA + *U*) for the total energy calculations where the value of *U* is taken from the previous studies as $U = 8.5$ eV [9]. The main intention of the GGA + *U* potential is to characterize the electronic interactions of strongly correlated materials. To investigate the ordered magnetic structure of our material, we considered a $2 \times 2 \times 1$ supercell model, which is composed of 32 atoms. As for the doped compound $HgBa_2CuO_{4+\delta}$, in order to simulate the doping-dependent electronic structure, we treat the doping by using a series of supercells containing excess of oxygen. Oxygen concentrations of $\delta = 0.083, 0.125, 0.167, 0.222$, and 0.25 with supercells size up to $6 \times 6 \times 1$ (97atoms), $4 \times 2 \times 1$ (65 atoms), $3 \times 2 \times 1$ (49 atoms), $3 \times 3 \times 1$ (74 atoms), $2 \times 2 \times 1$ (33 atoms), respectively. The exchange and correlation effects are treated within the local-density approximation (GGA) [10].

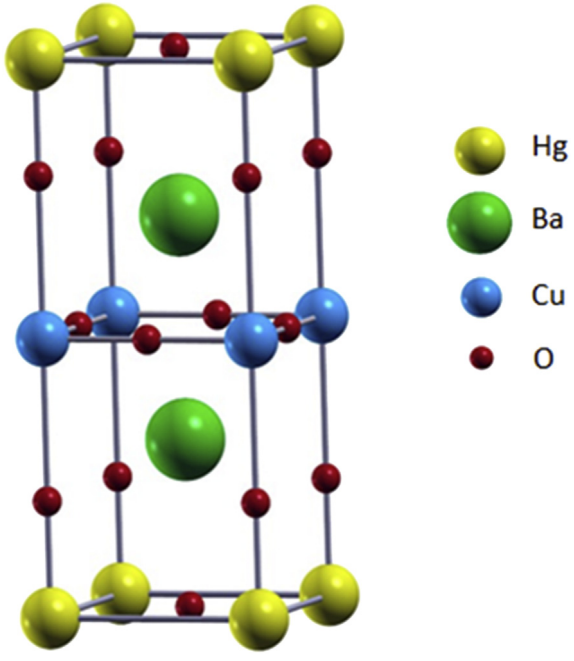

Fig. 1. Crystal structure of Hg-1201.

Table 1
Structural parameters of Hg-1201.Data from Ref. [7].

Elements	Occupancy	X	Y	Z
Hg	1.0	0.0	0.0	0.0
Ba	1.0	0.5	0.5	0.2991
Cu	1.0	0.0	0.0	0.5
O1	1.0	0.5	0.0	0.5
O2	1.0	0.0	0.0	0.2092
O3	δ	0.5	0.5	0.0

The optical properties of matter can be described by the complex dielectric function $\varepsilon(\omega)$ which represents the system response to an external electromagnetic field:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \tag{1}$$

where, $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are the real and imaginary parts of the dielectric function. Imaginary part of dielectric function $\varepsilon_2(\omega)$ is giving by:

$$\varepsilon_2(\omega) = \left(\frac{4\pi e^2}{\omega^2 m^2}\right) \sum_{i,j} \int i|M|j^2 f_i(1 - f_i) * \delta\left(E_f - E_i - \omega\right) d^3k \tag{2}$$

The real part of the dielectric function can be extracted from the imaginary part of the dielectric function by using the Kramers-Kronig relation:

$$\varepsilon_1(\omega) = 1 + \left(\frac{2}{\pi}\right) \int_0^{\infty} \omega' \varepsilon_2\left(\omega'\right) \Big/ \left(\omega'^2 - \omega^2\right) d\omega' \tag{3}$$

The Absorption coefficient and the Refractive index are given by:

$$\alpha(\omega) = \frac{\sqrt{2}}{c}\omega\sqrt{-\varepsilon_1(\omega) + \sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}} \tag{4}$$

$$n(\omega) = \left(\frac{\varepsilon_1(\omega)}{2} + \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}}{2}\right)^{1/2} \tag{5}$$

For more details about these properties, we refer the reader to [11,12].

The semi-classical Boltzmann theory as implemented in the BoltzTraP code is used to investigate the influence of doping in the $HgBa_2CuO_{4+\delta}$ for the transport properties. The electrical conductivity (σ/τ) and the Seebeck coefficient (S) as functions of temperature are calculated. We should point out that in the BoltzTraP code the relaxation time τ is taken as a constant. The BoltzTraP code has proven to be a very efficient technique for calculating the electronic transport properties [13]. The electrical conductivity is given by: