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Electrical resistivity of the $Mg(B_{1-x}C_x)_2$ superconductors: Role of electron-electron, and electron-phonon interactions

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ABSTRACT

In this paper, we undertake a quantitative analysis of temperature dependent resistivity Mg(B1-xCx)2 superconductors. Due to inherent two energy gaps, the elastic scatterings of electron from impurities have first been estimated and within a two-band picture, the impurity-limited resistivity due to □ band carriers □0□ is larger as compared to the contribution from □ band carriers. An effective inter-ionic interaction potential (EIoIP) with the long-range Coulomb, van der Waals interaction and the short-range repulsive interaction within the Hafemeister and Flygare approach have allowed us to determine the Debye and Einstein temperature. An investigation exhibit the mechanism of Mg(B1-xCx)2 (0.0 □ x □ 0.125) was accomplished by comparing to the resistivity estimated by considering both phonons, with that of reported metallic resistivity, accordingly ρdiff. = [ρexp.− {ρ0 + ρe-ph (= ρac + ρop)}] have been analysed through electron-electron scattering. The quadratic temperature dependence of ρdiff = [ρexp. – {ρ0 + ρe-ph (=ρ□e-ph + ρ□e-ph)}] is understood in terms of inelastic electron-electron scattering. The comparison of transport parameter with single crystal data appears consistent within the two-band scheme for resistivity that we have presented.

Keywords: energy harvesting, mix-generation, super capacitor.

1. Introduction

MgB2 as binary metallic compound has been extensively studied since its discovery with a superconducting transition Tc of 39 K [1]. Significant efforts have been made to enhance the *Tc* by chemical doping either at Mg or B site leading to a suppression of *Tc* [2, 3]. Precisely, adding an electron to MgB_2, by doping with Al or C, reduces the bond length, which lowers the density of states (DOS). Another unique property MgB_2 is the two gap structures in the electronic excitation spectrum with significantly different width [4- 8]. The larger energy gap develops on quasi-two-dimensional (2D) sheets of the Fermi surface referred as σ band. However, a reduced gap Δπ is formed on three-dimensional (3D) parts of the Fermi surface and is related with theπ band.

The temperature dependence of the electrical resistivity of the MgB_2 superconductors is an interesting probe in elucidating the mechanism and gap structures involved. Although progress in material processing has been achieved quite fairly, the temperature dependent resistivity behaviour of MgB_2 in the majority of both single- and poly-crystalline samples is highly unusual as the resistivity values are frequently extremely high. Also, *Tc* remains almost unchanged for samples comprising a strong variation of the magnitude of their normal state resistivity. Furthermore, even with huge resistivity, the temperature dependence from *Tc* to room temperature still exhibits power or cubic temperature dependence. Henceforth, the investigations of the electrical resistivity of MgB_2 and Al (C) doped could, therefore, contribute significantly to the understanding of the possible correlations between the zero temperature limited resistivity and the superconducting parameters, inter- and intra band scattering process and also of role of phonons and so on.

2. Method of calculations

We start by giving a brief description of the layered structure MgB_2 .The crystal structure of MgB_2 is the so-called AlB_2 structure. Honeycomb layers of boron atom alternate with hexagonal layer of Mg atoms. B atoms in different planes are on top of each other, and the B atoms at the centre of the hexagonal define the Mg atoms. It is now known that in metal diboride the boron atoms accept electrons from the metal, and the boron planes become negatively charged. The simplest ionic picture would suggest that in MgB_2 the Mg donates two electrons to the B planes, and the ionic compound $Mg^{++}(B^-)_2$ results which will be metallic due to boron band overlap.

The understanding of the dynamical properties of materials requires the formulation of an effective interionic potential. This is particularly important, as there is much disagreement as to whether long- or short-range interactions are at the origin of the substantial properties manganites. To begin with, we made the following assumptions: the change in force constants is small; the short-range interactions are effective up to the second-neighbour ions; and the atoms are held together by harmonic elastic forces without any internal strains within the crystal. We thus express the crystal energy for a particular lattice separation (r) as:

$$\Phi = \Phi^{C}_{kk'}(r) + \Phi^{R}_{k'}(r) + \Phi^{vdW}_{k'}(r)$$

where Coulomb contribution ϕ (r) is given by

$$\Phi^{C}_{kk'}(r) = \frac{-e^2}{2}\sum_{k'} Z_k Z_{k'} r^{-1}_{kk'}$$

with $r_{kk'}$ is the separation between the two atoms *k* and *k'*.

The overlap repulsive energy $\phi^{R}_{kk'}(r)$ according to Hafemeister–Flygare type interaction extended up to the second neighbour ions, is expressed as

$$\beta_{kk'} = 1 + \left(\frac{Z_k}{N_k}\right) + \left(\frac{Z_{k'}}{N_{k'}}\right)$$

where Z_k ($Z_{k'}$) and N_k ($N_{k'}$) are the valence and number of electrons in the outermost orbit.

The contributions from the van der Waals (vdW) attractions due to the dipole–dipole (*d–d)* and dipole– quadrupole *(d–q)* interactions are written as

$$\Phi_{kk'}^{vdW} = -\sum_{k'} c_{k,k'} r_{k'}^{-6} - \sum_{k'} c_{k,k'} r_{k'}^{-8}$$

where ckk' and dkk' are the vdW coefficients due to *d–d* and *d–q* interactions, respectively. The vdW values are determined using the Slater–Kirkwood variational method:

$$c_{kk'} = \frac{3e\hbar}{3m}\alpha_k\alpha_{k'}\left[\left(\frac{\alpha_k}{N_k}\right)^{1/2} + \left(\frac{\alpha_{k'}}{N_{k'}}\right)^{1/2}\right]^{-1}$$

$$d_{kk'} = \frac{21}{8}\frac{e\hbar^2}{m}\alpha_k\alpha_{k'}\left[\left(\frac{\alpha_k}{N_k}\right)^{1/2} + \left(\frac{\alpha_{k'}}{N_{k'}}\right)^{1/2}\right]^2\left[\left(\frac{\alpha_k}{N_k}\right)^{1/2} + \frac{10}{3}\left(\frac{\alpha_k\alpha_{k'}}{N_kN_{k'}}\right) + \left(\frac{\alpha_{k'}}{N_{k'}}\right)\right]^{-1}$$

where e and m are the charge and mass of the electron, respectively. α_k ($\alpha_{k'}$) are the polarizabilities of k (k') atoms. Nk (Nk') are the effective number of electrons responsible for polarization of k (k') ions.

The model parameters, hardness (b) and range (ρ) parameters are determined from the equilibrium condition

$$\left[\frac{d\phi}{dr}\right]_{r=r_0} = 0$$

and the Bulk modulus

$$B = \frac{1}{9\kappa r_0}\left[\frac{d^2\phi}{dr^2}\right]$$

The model parameters obtained from Eq's. (8) and (9) have been used to compute the second order elastic constants (C11, C12 and C44) as

$$C_{11} = \frac{e^2}{4r_0^4}\left[-5.112Z_m^2 + A_1 + \frac{(A_2+B_2)}{2}\right]$$

$$C_{12} = \frac{e^2}{4r_0^4}\left[0.226Z_m^2 - B_1 + \frac{(A_2-5B_2)}{2}\right]$$

$$C_{44} = \frac{e^2}{4r_0^4}\left[2.556Z_m^2 + B_1 + \frac{(A_2+3B_2)}{4}\right]$$

where (A1, B1) and (A2, B2) are the short-range parameters for the nearest and the next nearest neighbors, respectively. These parameters are defined as

$$A_1 = \frac{4r_0^3}{e^2}\left[\frac{d^2}{dr^2}V_{ij}(r)\right]_{r=r_0}$$

$$A_2 = \frac{4(r_0\sqrt{2})^3}{e^2}\left[\frac{d^2}{dr^2}V_{ii}(r) + \frac{d^2}{dr^2}V_{jj}(r)\right]_{r=r_0\sqrt{2}}$$

$$B_1 = \frac{4r_0^3}{e^2}\left[\frac{d}{dr}V_{ij}(r)\right]_{r=r_0}$$

$$B_2 = \frac{4(r_0\sqrt{2})^2}{e^2}\left[\frac{d}{dr}V_{ii}(r) + \frac{d}{dr}V_{jj}(r)\right]_{r=r_0\sqrt{2}}$$

where Vij(r) is the short-range potentials between the ions, which follow

$$V_{ij}(r) = b\beta_{ij}\exp\left(\frac{r_i + r_j - r_j}{\rho}\right) + c_j r_j^{-6} + d_j r_j^{-8}$$

The elastic force constant κ is derived at the equilibrium interionic distance r0 following

$$\kappa = \frac{r_0}{2}\left[\pi^2(C_{11} - C_{12})(C_{11} + C_{12} + 2C_{44})(C_{44})\right]^{\frac{1}{3}}$$

Thus, we have estimated the elastic force constants in terms of the developed EIoIP for a pair such as B-B, Mg-B and Mg-Mg and have the total elastic force constants of the Mg(B1-xCx)2 superconductors. This continuum model thus takes care of the clear physical binding in doped superconductors. We stress that the simple models based on this potential can describe those cohesive properties of such solids that depend on van der Waals interactions. However, the true potential must recognize the correct charge distribution and the relative orientations of the interacting atoms in manganites and which is a complicated task.

The Matsubara gap function, which is, related with upper critical magnetic field yields

$$\frac{1+\lambda}{\lambda-\mu^*} = 2\pi\frac{T}{T_c}\sum_{m=0}^{N_c}\frac{1}{\chi_m^{-1}(\bar{\omega}_m) - (2\tau)^{-1}}$$

Here, is Matsubara frequency, within the standard two-square-well model and is = (1+λ) + $(2\tau)^{-1}$ (sgn), λ is the usual electron-phonon coupling strength with cut off at Nc, and τ is the scattering time. In this approximation Nc follows

$$N_c = \frac{1}{2}\left[\frac{\omega}{\pi T} + 1\right]$$

μ* is the renormalized Coulomb repulsive parameter and the factor χm in Eq. (23) is

$$\chi_m(\bar{\omega}_m) = \frac{2}{\sqrt{\xi^*}}\int_0^{\infty}\exp(-q^2)\tan^{-1}(\phi)dq$$

with

$$\phi = \frac{q\sqrt{\xi^*}}{\left[(2m+1)\pi\frac{T}{T_c}\right] + \left[\frac{1}{2\tau^*}\right]}$$

The upper critical magnetic field is related through

$$\xi^* = \frac{1}{2}eH_{c2}^*v_F^{*2}$$

The physical quantities appearing in equation (23)-(27) involve renormalized values as

$$H_{c2}^* = \frac{H_{c2}}{(1+\lambda)T_c}$$

$$v_F^* = \frac{v_F}{\sqrt{(1+\lambda)T_c}}$$

and impurity scattering time

$$\hat{o}^* = \frac{\hat{o}}{(1+\lambda)T_c}$$

These expressions differ from the BCS limit, as the renormalizations in ξ*, vF*, H^*_{c2} and τ* are introduced. These are valid for any impurity concentration described in equations (23)-(27) by scattering time. In the present analysis Pauli limiting has been neglected as an approximation due to relatively small value of dHc2/dT [1/(1+λ)] in Mg(B(1-x)Cx)2. Physically, the above approach describes quantitatively the renormalization of the physical properties due to electron-phonon interaction and is therefore reduced by 1+ λ.

The zero temperature-limited resistivity within the Drude model is

$$\rho_0 = \frac{4\pi\hat{o}^{*-1}}{\omega_p^2}$$

In Mg(B1-xCx)2, we consider two different channels of electron transport, the resistivity can be written in the limit in which interband scattering is negligible,

$$\frac{1}{\rho_0} = \frac{1}{\rho_0^{\pi}} + \frac{1}{\rho_0^{\sigma}}$$

PARIPEX - INDIAN JOURNAL OF RESEARCH ✠ 164

in accordance with the Matthiessen rule. Here $\rho 0^{\pi}$ ($\rho 0^{\sigma}$) is the residual resistivity of π (σ) bands. Within a two-band picture, the determination of elastic scattering rate essentially needs the Coulomb repulsive parameter, electron phonon coupling strength, Fermi velocity, plasma frequency and upper critical magnetic field. This allows one to estimate the zero temperature limited resistivity where the two π bands and the σ bands are considered as a whole, respectively. we start with the general expression for the temperature dependent part of the resistivity, given by

$$\rho = \frac{3\pi}{\hbar e^2 v_F^2} \int_0^{2k_f} |v(q)|^2 \left\langle |S(q)|^2 \right\rangle \left(\frac{1}{2k_F}\right)^4 q^3 dq \ .$$

v (q) is the Fourier transform of the potential associated with one lattice site, vF being the Fermi velocity and S(q) is the structure factor. Following Debye model it takes the following form

$$|S(q)|^2 \approx \frac{k_B T}{M v_s^2} f(x)$$

$$f(x) = \frac{x}{(e^x - 1)(1 - e^{-x})}$$

f(x) represents the statistical factor with $x = \hbar\omega / k_B T$
Thus the resistivity expression leads to

$$\rho \approx \frac{3 k_B T}{\hbar e^2 v_F^2 M v_s^2} \int_0^{2k_F} |v(q)|^2 \frac{x q^3 dq}{[e^x - 1][1 - e^{-x}]}.$$

v_s being the sound velocity. Equation (36) in terms of acoustic phonon contribution yields the Bloch-Gruneisen function of temperature dependent resistivity, $\rho_{ac}\,\sigma$:

A_{op} is defined analogously to Eq. (38). If the Matthiessen rule is obeyed, the resistivity may be represented as a sum $\rho(T) = \rho_0 + \rho_{e\text{-}ph}$ (T), where ρ_0 is the residual resistivity that does not depend on temperature as electrons also scatter off impurities, defects and disordered regions. Thus, the phonon resistivity can be conveniently modelled by combining both terms arising from acoustic and optical phonons

$$\rho_{e-ph}(T) = \rho_a^{\sigma}(T, \theta_D) + \rho_p^{\sigma}(T, \theta_E)$$

Finally, the total resistivity is now rewritten as

$$\rho(T, \theta_D, \theta_E) = \frac{\rho_0^{\pi} \rho_0^{\sigma}}{\rho_0^{\pi} + \rho_0^{\sigma}} + \rho_{ac}^{\sigma}(T, \theta_D) + \rho_{op}^{\sigma}(T, \theta_E)$$

$$= \frac{\rho_0^{\pi} \rho_0^{\sigma}}{\rho_0^{\pi} + \rho_0^{\sigma}} + 4 A_{ac} (T/\theta_D)^4 T \times \int_0^{\theta_D/T} x^5 \left(e^x - 1\right)^{-1} \left(1 - e^{-x}\right)^{-1} dx$$

$$+ A_{op} \theta_E^2 T^{-1} \left[\exp(\theta_E / T) - 1\right]^{-1} \left[1 - \exp(-\theta_E / T)\right]^{-1}$$

We use the values of various physical parameters in the next section to estimate the temperature-dependent contribution in high-T_c, $Mg(B_{1-x}C_x)_2$ superconductors.

3. Discussion and analysis of results

Any discussion of the $Mg(B_{1-x}C_x)_2$ superconductors necessitates the knowledge of the structural aspects, and this is particularly true of the calculations reviewed here. Also applying the available information's on the developed theory inevitably entails certain complications and one has to find suitable data that varies from technique to technique. Special attention is paid in this approach to address the issue whether long range or short range interactions are at the origin of the substantial properties of the C doped MgB_2

4. Conclusions

Either electron-phonon interaction with low-energy acoustic phonon and high-energy optical phonon or electronic excitations within the framework of two-band mechanism have substantial role to discuss superconducting and normal state resistivity in doped magnesium diborides. The behavior of electrical resistivity and superconductivity in $Mg(B_{(1-x)}C_x)_2$ is investigated with an idea that a pair of electron interacting with a boson field within the boron layer with two differently sized energy gaps associated with π and σ bands leads to a consistent explanation of physical properties.

To conclude, the present model calculations thus lead to both qualitative and quantitative agreement between the calculated and experimental results. Although we have provided a simple explanation of these effects, there is a clear need for good theoretical understanding of the resistivity behaviour in C doped MgB_2 superconductors.

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