January 2009 Volume 5 Issue 1

Trade Science Inc.

Materials Science

An Indian Journal

Full Paper

MSAIJ, 5(1), 2009 [26-28]

Pseudopotential study of the superconducting behaviour of MgB_2 : HFP technique

Jayprakash Yadav*[1], S.M. Rafique[1], Md.Tauhid Alam[1] and Umakant Prasad[2]

[1]University Department of Physics, T M Bhagalpur University, Bhagalpur Bihar -812007

[2]Department of Physics, T.N.B. College, Bhagalpur-812007,(INDIA)

E-mail : dr.jp_yadav@yahoo.co.in

Received: 9th September, 2008 ; Accepted: 9th September, 2008

ABSTRACT

The study of recent literature reveals that the discovery of high T_C (T_C = 39K) superconductivity (SC) in MgB_2 has generated considerable interest in this binary system. The appearance of high T_C SC in such a simple system which does not contain transition metals has led to considerable optimism among workers. The phonon mediated BCS type mechanism has been acknowledged to be a good tool for its theoretical study via McMillan formalism. Recent studies are the milestones in this direction. In this paper, we report the Harrison's First Principle Pseudopotential (HFPP) study of this system so as to bring out the effectiveness of this technique which has not been explored as yet. It has been observed that due to the unique double layered structure of MgB_2 some adjustable parameter is to be introduced in the computation of the form factor so as to predict the SC parameters in reasonable agreement with experiment.

KEYWORDS

Pseudopotential;
Superconducting parameters;
Magnesium diboride (MgB_2).

INTRODUCTION

Superconductivity is a property of many metals, alloys and chemical compounds at temperatures near absolute zero by virtue of which their electrical resistivity vanishes and they become strongly diamagnetic. The discovery of superconductivity (SC) in magnesium diboride (MgB_2) with remarkable high transition temperature (T_C = 39K) has generated considerable interest in this system[1]. MgB_2 adopt a simple primitive hexagonal crystal structure comprising of interleaved two dimensional of magnesium and boron layers. The appearance of high T_C in such a simple system which does not contain transition metal is quite encouraging from theoretical and experimental point of view. It has generated optimism for achieving high value of T_C in binary systems with simple constituents.

It has been noted that the theories developed to explain SC in the layered high T_C curates would not be helpful in understanding MgB_2 and hence Loui and Cohen and their co-workers have used the well established BCS theory to explain the superconducting behaviour of MgB2[2]. The phonon mediated BCS type of mechanism is a good tool for the study of such systems via McMillan formalism[3]. Recently such attempts are being made[4-7] and we have also persued over investigation along these lines using Harrison's first principle pseudopotential (HFPP) technique[8].

Formalism and computation

The HFPP form factor is represented as

$$w(k,q) = \left\{\frac{v_q^{a,b} + v_q^c + v_q^d}{\varepsilon^*(q)}\right\} + \left[\frac{1-G(q)}{\varepsilon^*(q)}\right] v_q^f + W^R \qquad (1)$$

where $v_q^{a,b}$ is the valence charge and core electron potential, v_q^c is the conduction band-core exchange potential, v_q^f is the screening potential, W^R is the repulsive potential, $\varepsilon^*(q)$ is the modified Hartree dielectric screening function and G(q) is the exchange-correlation function. The potentials are computed from first principles on the lines of Harrison[8].

The basic input parameters needed for the computation are the core energy eigenvalue ε_{nl} radial wavefunctions $P_{nl}(r)$, Fermi wave vector k_F, atomic volume Ω_0 and valence Z. The pseudopotential form factor and other parameters of the binary system may be computed through

$$X_{AB} = (1-c)X_A + cX_B \qquad (2)$$

where X_A and X_B are the parameters or the form factor of the constituents and X_{AB} those of the binary system, c is the concentration of the second constituent[9].

The Debye temperature of the binary system is represented by[10]

$$1/(\theta_D)^2_{AB} = (1-c)/(\theta_D)^2_A + c/(\theta_D)^2_B \qquad (3)$$

The SC parameters have been computed through the McMillan formalism[3]. The electron-phonon coupling strength

$$\lambda = \frac{12m^*Z^*}{M<\omega^2>}\int_0^1 \eta^3 \left|w(k,q)\right|^2 d\eta \qquad (4)$$

where m* is the effective mass of the electron, Z* the effective valence, M the atomic mass, $<\omega^2>$ the averaged phonon frequency and $\eta = q / 2k_F$.

The Coulomb pseudopotential is represented by

$$\mu^* = [m_b/(\pi k_F)]I/[1+m_b/(\pi k_F)\ln(E_F/k_B\theta_D)I] \qquad (5)$$

$$\text{With } I = \int_0^1 d\eta/(\eta\varepsilon^*(\eta)) \qquad (6)$$

where m_b is the band mass, E_F the Fermi energy, k_B the Boltzmann's constant, θ_D the Debye temperature and k_F the Fermi wave vector. The superconducting transition temperature is given by

$$T_c = \frac{\theta_D}{1.45}\exp\left[\frac{-1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right] \qquad (7)$$

The computation of the HFPP form factor has been done with Herman-Skillman[11] eigenvalues and eigenfunctions using Xα exchange parameters (α_X) satisfying Virial theorem and exchange-correlation function G(q) suggested by Vashishta-Singwi (V-S)[12] form which satisfies compressibility some rule and provides physically acceptable pair correlation function.

The results which are being presented are only those which reasonably agree with the experimental data of T_C and theoretical data of other authors. It was felt that MgB_2 having special features as regards its structure mentioned earlier needs some adjustable parameter β in the form factor w(k,q) so as to reproduce the reasonable agreement with experimental data T_C. For this Harrison prescription[8] has been adopted. Thus

$$w(k,q) = <k+q|w|k> = (1+\beta)<k+q|w^0|k>/\varepsilon^*(q) \qquad (8)$$

with a suitable choice of β we can obtain a rather good form factor which can predict a reasonable value of T_C. The adjustable parameter β would throw light on the effect of double layered structure of MgB_2.

RESULT AND DISCUSSION

It has been observed that the form factor of MgB_2 is dominated by that of the boron atom. This implies the B-atoms in the boron layers play more.

It is known that at ambient conditions MgB2 crystallises in hexagonal structure where B-atoms form honeycomb lattice consisting of graphite like sheet separated by hexagonal layers of Mg atoms. The pairing mechanism leading to SC is of phononic origin. Thus the domination of B-atoms in shaping the form factor is quite natural. Gaitonde et al.[4] observes that the electronic band structure shows that the bands near the Fermi energy are predominantly due to the boron orbital. The flat bands contribute largely to the density of states near the Fermi level giving high T_C. In our computations also we observe that the most contributing part of the form factor w(k, q) is in the region $1 \le \eta' \le 2$ where $\eta' = q/k_F$. This is because the integrand involves the η^3 and $\Omega' |w(k, q)|^2$ like Ziman integrand for electrical resistivity.

Two experimental values of the Debye temperature θ_D = 750K and 1050K are available[5] and employing these the original form factor w(k, q) yields λ =

0.52, $\mu^* = 0.09$, $T_C = 9.95$K and $\lambda = 0.26$, $\mu^* = 0.26$, $T_C = 0.15$K.

This shows that the ionic interactions are not properly reproduced as they exist in MgB_2 structure and hence and adjustable parameters β has been introduced as

$$w(k, q)_{AB} = (1+\beta)[(1-c)w(k,q)_A + cw(k, q)_B] \quad (9)$$

where c = 0.6666 (stoichiometric composition).

With $\theta_D = 750$K and $\beta = 0.3$ we get $\lambda = 0.88$, $\mu^* = 0.0944$, $T_C = 36.8$K and with $\beta = 0.6$ we obtain $\lambda = 0.83$, $\mu^* = 0.0944$ and $T_C = 37.2$K ($T_C = 39$K expt.). With $\theta_D = 1050$K and $\beta = 0.7$ we obtain $\lambda = 0.77$, $\mu^* = 0.0944$, $T_C = 38.9$K. λ has also been estimated by other techniques[4,5] with similar approximations and $\lambda = 0.69$, $\mu^* = 0.09$ and $T_C = 30.8$K has been obtained heat coefficient Y is given as

$$\lambda = Y_{exp.}/Y_{calc.} - 1 \quad (10)$$

$$\text{where } \lambda_{calc.} = 1/3\pi^2 D(E_F) k_B^2 \quad (11)$$

$D(E_F)$ being the density of states near Fermi level. $Y_{exp.}$ has been reported to lie between 2.6-3 mJ/mol-K^2 which gives $\lambda = 0.53$ and $\lambda = 0.77$ respectively. Taking $\mu^* = 0.1$, $T_C = 9.4$K and 39K have been obtained with $\theta_D = 750$K and 1050K respectively[5]. Thus our results with HFPP technique using $\theta_D = 1050$K agree with[5]. With $\theta_D = 750$K the result of[5] is TC = 9.41K we have been able to improve the form factor by a 30% correction to accommodate the double layer interactions to get $T_C = 36.8$ which is in reasonable agreement with experiment.

CONCLUSION

The HFPP technique has been used to study the superconducting parameter of the high T_C superconductor MgB_2 having double layered structure where boron atoms form honeycomb lattice separated by hexagonal layers of Mg atoms. The study reveals that an adjustable parameter should be introduced in the form factor w(k, q) to take account of this special structure of MgB_2 leading to superconducting behaviour with $T_C = 39$K. It has been observed that the form factor should be at least 30% more negative to consolidate the inter ionic interactions and reproduce the observed transition temperature. This shows that the repulsive component W^R involved in the expression of the form factor is weakened by a substantial amount in the formation of MgB_2 structure. This invites furthers investigation either for the improvement of the formalism or for using other sets of wave functions, exchange-correlation or the orthogonalization hole parameters as previously adopted by various authors in the past decades for pseudopotential calculations.

REFERENCES

[1] J.Nagamats, N.Nakagawa, Y.Zentaani, J.Akimitsu; Nature, 41063 **(2001)**.
[2] Research News, Paul Preurs, **510**, 486-6249 **(2002)**.
[3] W.L.McMillan; Phys.Rev., **167**, 313 **(1968)**.
[4] D.M.Gaitonde, P.Modak, R.S.Rao, B.K.Godwal; Bull.Mat.Sci., **26**, 131 **(2003)**.
[5] P.P.Singh; Bull.Mat.Sci., **26**, 131 **(2003)**.
[6] E.Eaito, Taknenobu, T.Ito, Y.Iwasa, K.Prassides, T.Arima; J.Phys.Condens.Matt., **13**, 1267 **(2001)**.
[7] H.J.Choi, D.Roundy, H.Sun, M.L.Cohen, S.J.Louie; Letters to Nature, **418**, 758 **(2002)**.
[8] W.A.Harrison; Pseudopotential in the Theory of Metals', Benjamin Inc.NY, **(1966)**.
[9] H.Khan, K.S.Sharma; UPAP, **36**, 523 **(1998)**
[10] S.Sharma, H.Khan, K.S.Sharma; UPAP, **41**, 301 **(2003)**.
[11] F.Herman, J.Skillman; 'Atomic Structure Calculation', Prentice Hall Englewood Life, NJ.
[12] P.Vashishta, K.S.Singwi; Phys.Rev.Lett., **86**, 577 **(2001)**.
[13] K.P.Bohen et al.; Phys. Rev., **B6**, 875 **(1972)**.
[14] J.Kourtus et al.; Phys.Rev., **B64**, 20501 **(2001)**.
[15] J.Kourtus et al.; Phys.Rev.Lett., **86**, 1877 **(2001)**.
[16] S.L.Budko et al.; Phys.Rev.Lett., **86**, 1877 **(2001)**.
[17] F.Bouquet et al.; Phys.Rev.Lett., **82**, 47001 **(2001)**.