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A Theoretical Study of Magnetic Impurity Effect on Superconducting Properties of Manganese doped MgB2

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Abstract:- **In the present study we investigated the theoretical calculation of Superconducting state parameter (SSP) by doping of MN on MgB2 superconductor for concentration (x=0.006, 0.007, 0.014, 0.016, 0.020). We use Ashcroft's pseudo potential in conjunction Random phase approximation (RPA) dielectric screening function with methodology based on BCS- Elias berg Mc. Millan framework in which material properties like electron-phonon coupling strength (λ) and Coulomb pseudo potential (μ*) are obtained from the knowledge of electron-ion pseudo potential. The super-conducting state properties like transition temperature (TC), isotope effect exponent (α) and interaction strength (N0V) are then obtained by using the values of λ, μ* and <ω2> relevant to the superconductor .It is also observed that addition of Manganese to superconductor MgB2 causes the parameters λ, μ*, α, N0V, TC decreases with increasing in Manganese concentration. Present calculation also observed that TC for alloys Mg1-xMnxB2 is excellent agreement with the experimental results. It is observed that the increase in doping concentration of MN causes all the superconducting parameters to decrease. This suggests decrease in superconducting behavior of MgB2 due to effect of magnetic impurity MN.**

Index Terms—Electron-phonon coupling strength, Isotope effect, Pseudo potential, Transition temperature

I. INTRODUCTION

There has been a considerable amount of research undertaken in order to understand the influence of dopants to enhance the super conducting properties of the MgB2 [1]. However, it is observed that most of the research work undertaken has been experimental and only few researches have been done theoretically [2],[3].Therefore, we need to study this compound with various substitutions theoretically, which may lead to electron or hole doping, isovalent and magnetic ion substitution. We use the well-established pseudo potential methodology based on BCS-Elias berg- McMillan formulation, in which material properties like electron-phonon coupling strength (λ) and Coulomb pseudo potential (μ*)are obtained from the knowledge of electron-ion pseudo potential, dielectric screening and phonon spectrum which is generally replaced by the use of a most representative phonon 19. % less likely to suffer cataracts frequency or an average phonon frequency $<\omega^2>$. The super-conducting state properties like transition temperature (T_c), isotope effect exponent (α) and interaction strength (N_0V) are then obtained by using the values of λ , μ*, average square phonon frequency $<\omega^2>$ and isotopic mass M relevant to the superconductor. We have employed Ashcroft's empty core model pseudo potential [4] and RPA form of dielectric screening due to Gellman and Bruckner [5] for determination of superconducting parameters of $Mg_{1-x}Mn_xB_2$system which takes care of exchange and correlation effects of the electron gas.

II. THEORY

We follow Mc.Millian [6] in a defining electron-phonon coupling strength by:

$$\lambda = 2\int_0^{\infty}[\alpha^2\ (\omega)F(\omega)/\ \omega\ ] \qquad (1)$$

Where α^2 (ω) F (ω) is the spectral function, which when appropriately evaluated in the plane – wave approximation for scattering on the Fermi surface, yield [7].

$$\lambda = \frac{m^*}{4\pi^2\ k_F\ MN<\omega^2>}\ \int_0^{2k_F} dq\ q^3\ \ |V_s\ (q)|^2 \qquad (2)$$

Where q is change in the electron wave vector k in scattering on the Fermi surface, m* is the effective mass of electron M is the ionic mass, N is the ion number density, k_F is the Fermi radius, and

$$Vs(q) = \frac{<k+q|V|k>}{\varepsilon\ (q)} \qquad (3)$$

Represent the screened atomic form factors, where <**k+q**|V|**k**>is the matrix element for the electron scattering from state |**k**> to state |**k+q**|>on the Fermi surface (or bare ion potential) and ε(q) is the dielectric screening function.

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On using $x= q/2k_F$ and

$$N^{-1} = \Omega_0 = \frac{3\pi^2 z^*}{k_F^3}$$

We obtain electron-phonon coupling strength (λ) [8]:

$$\lambda = \frac{12\, m^* z^*}{M < \omega^2 >} \int_0^1 dx\; x^3 |V_S(x)|^2 \qquad (4)$$

Where Ω_0 is atomic volume and z* is the effective valence of ions, m^* is the component of effective mass of electron.

The repulsive interaction between electron in a superconductor is given by the coulomb pseudopotential (μ*), which on representing band mass by $m_b = m^*$ and Debye temperature by θ_D is given [9] by

$$\mu^* = \frac{\frac{m_b}{\pi k_F}\int_0^1 \frac{dx}{x\,\epsilon(x)}}{[1+\frac{m_b}{\pi k_F}\ln\left(\frac{k_F^{\,2}}{20\,\theta_D}\right)\int_0^1 \frac{dx}{x\,\epsilon(x)}]} \qquad (5)$$

The relevant expression for the transition temperature Tc [10] and isotope effect exponent (α) have been obtained by Mc.Millian [6] from the solution of the Eliashberg equation.

$$T_c = \frac{\theta_D}{1.45}\left\{\exp\left(\frac{-1.04\,(1+\lambda)}{\lambda-\mu^*\,(1+0.62\,\lambda)}\right)\right\} \qquad (6)$$

$$\alpha = \frac{1}{2}[1 - (\mu^* \ln\frac{\theta_D}{1.45 T_c})^2 \frac{1+0.62\lambda}{1.04(1+\lambda)}] \qquad (7)$$

And the relevant expression for effective interaction strength (N_0V) [11] has been obtained in the following form

$$N_0V = \frac{\lambda - \mu^*}{1+(\frac{10}{11})\lambda} \qquad (8)$$

For obtaining screened pseudo potential $V_s(x)$, empty core model pseudo potential $V_b(x)$ due to Ashcroft [4] and ε(x) obtained in Random phase approximation (RPA) [5] screening for $Mg_{1-x}Mn_xB_2$ system used in the present investigation are as given (in a.u.) below :

$$V_S(x) = \frac{V_b(x)}{\varepsilon(x)} \qquad (9)$$

where

$$V_b^{Ash}(x) = \frac{-\pi z^* \cos(2 k_F r_c x)}{\Omega_0 k_F^2 x^2} \qquad (10)$$

$$\varepsilon_{RPA}(x) = 1 + \frac{m^*}{2\pi k_F x^2}\left[1 + \frac{(1-x^2)}{2x}\ln\left|\frac{1+x}{1-x}\right|\right], \qquad (11)$$

Here r_c is the potential parameter, which represents effective atomic core radius .The value of r_c for a superconductor is obtained by fitting it to some experimental property of the superconductor.

III. RESULTS AND DISCUSSIONS

The input parameters relevant to the components of $Mg_{1-x}Mn_xB_2$ system have been assembled in Table I. We have used $m_b = m^*$ for the sake of uniformity.The values of m*, $<\omega^2>$, z*, M for the $Mg_{1-x}Mn_xB_2$ system under investigation are obtained from the relevant values for the component by using Vegard's rule [12], viz.

$$V_s = \tfrac{1}{3}[(1-x)V_s(Mg) + x\,V_s(Mn) + 2\,V_s(B)], \qquad (12)$$

The value of θ_D for the $Mg_{1-x}Mn_xB_2$ system is computed from the relevant values by using Grimvall's formula [13]:

$$\frac{1}{\theta_D^2} = \frac{1}{3}\left[\frac{1-x}{\theta_{DMg}^2} + \frac{x}{\theta_{DMn}^2} + \frac{2}{\theta_{DB}^2}\right], \qquad (13)$$

Table I.Input Parameters.[1],[14]-[18]

Data	Component metals		
	Mg	B	Mn
m*	1.01	1.394	0.84
M(au)×10^4	4.4345	1.8440	10.0820
k_F(au)	0.7242	1.2177	0.90
Ω_0(au)	156.819	51.824	81.9
z^*	2	3	1
$<\omega^2>$×10^{-6}(au)	0.76389	7.4598	0.8026
θ_D(K)	400	1250	410

Table II .Superconducting parameter of $Mg_{1-x}Mn_xB_2$

SSP's	Concentration x				
	0.006	0.007	0.014	0.016	0.020
λ	1.1279	1.0975	0.8841	0.7777	0.5008
μ*	0.1722	0.1721	0.1720	0.1720	0.1720
Tc(K) Cal.	30.93	29.37	18.25	12.67	1.5
Exp(K) [19]	30.9	29.3	18.6	12.6	0.00
α	0.4201	0.4169	0.3867	0.3516	0.1009
N_0V	0.4719	0.4632	0.4016	0.3548	0.2259

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Table II. Shows the computed values of Superconducting parameter of

$Mg_{1-x}Mn_xB_2$ system by using Ashcroft's potential with Random phase approximation screening It is observed there is gradual decrease in all superconducting state properties of MgB_2 as doping of Manganese is increased. We note that the electron-phonon interaction strength (λ) goes on decreasing from the value 1.1279 to 0.5008 as the concentration of Mn is increased from 0.006 to 0.020. The decrease in the value of electron-phonon interaction strength (λ) with increasing concentration of Mn shows decrease in strong coupling behavior to weak coupling behaviour of MgB_2. This may be attributed to Mn that occupies Mg sites thus decreasing the electron-phonon coupling between Mg and B. "Fig.".1 shows the behavior of electron-phonon interaction strength (λ) for different concentrations of Mn .Coulomb pseudo potential (μ*) show almost constant behavior with increase in Mn doping.

The transition temperature (T_c) also show a sharp decline from 30.93K to 1.5K with increase in Mn concentration, which suggests that the superconductivity is suppressed as doping of magnetic impurity in MgB_2 increases. It is observed that T_c decrease up to 1.5K which approximately equals 0K which superconductivity almost vanishes for doping concentration 0.020 of Mn .The T_c values obtained theoretically are in agreement with the experimental results [19]. The variation of T_c with the concentration of Mn in $Mg_{1-x}Mn_xB_2$system has been shown in "Fig.". 2 along with experimental data.

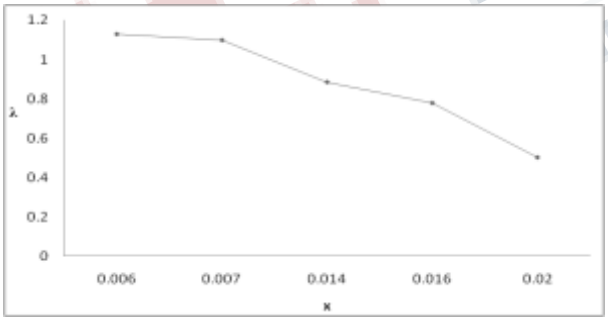

Fig. 1: Variation of λ with Mn- Concentration (at. %) in $Mg_{1-x}Mn_xB_2$ alloys.

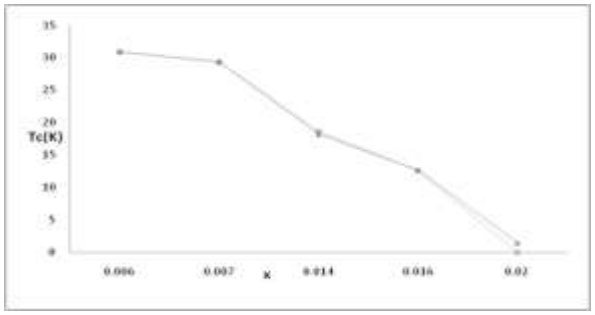

Fig. 2: Variation of T_c with Mn- Concentration (at. %) in $Mg_{1-x}Mn_xB_2$ alloys.

Decrease in values of isotope effect exponent (α) from 0.4201to 0.1009 and effective interaction strength (N_0V) from 0.4719 to 0.2259also indicate change of strong superconducting behavior to weak superconducting behavior with the increase of magnetic doping (Mn).

IV. CONCLUSION

The present investigations show that all the superconducting parameters go on decreasing with the increase in magnetic and isovalent impurity. The magnitude of electron - phonon interaction strength (λ) and transition temperature (T_c) indicates that $Mg1_{-x}Mn_xB_2$ system is strong to weak coupling superconductor. Present computations yield results which are in agreement with the experimental data.

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