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AN EVALUATION OF Al CONCENTRATION DEPENDENCE OF T_c IN TWO GAP NATURE OF $Mg_{1-X}Al_XB_2$ SUPERCONDUCTOR

S. KUMAR[a], D. PRASAD[b] and L. K. MISHRA[*]

Department of Physics, Magadh University, BODH GAYA – 824234 (Bihar) INDIA
[a]Department of Physics, G. L. A. College, DALTANGANGJ (Palamu) (Jharkhand) INDIA
[b]Department of Physics, T. S. College, HISUA (Nawada) (Bihar) INDIA

ABSTRACT

In this paper, we have evaluated the Al concentration of T_c using electron phonon coupling constant and coulomb pseudo potential. Our theoretically evaluated results show that as doping concentration x (Al concentration) increases the zero field T_c decreases. This study shows that the σ bands collapsed gradually with Al doping due to the increase in the number of electrons. It was found that in all doping concentration the σ bands were dirtier than the π bands.

Key words: Two gap superconductor, Clean limit, Dirty limit, Upper critical field, Electron-phonon coupling parameter, Coulomb pseudo potential.

INTRODUCTION

The discovery of the relatively high T_c of 39 K in the very simple-structured magnesium diboride (MgB_2)[1] fascinated the scientific community. Soon after its discovery, MgB_2 was revealed to have a navel two-gap nature, which was found to influence its superconducting properties[2-6]. Among these, the upper critical field (Hc_2) was known to be affected seriously by the two-gap nature[7-11]. In the clean limit, at low temperatures Hc_2 and its anisotropy (γ_H) are determined by the two- dimensional (2D) σ bands, while at high temperatures 3 Dπ bands gradually became important in determining the Hc_2 and γ_H are mostly controlled by the amounts of the impurities[10,11], similar to the conventional one-gap BCS supercanductars[12,13]. In MgB_2 however, there can be different scattering channels; within each band and between different pairs of bands. These are referred to as the intra band and inter band scatterings, respectively. According to the theory[10,11], inter band

[*]Author for correspondence; E-mail: muphysicslkm@gmail.com

scattering allows the different gaps to merge, simultaneously reducing the transition temperature. In the absence of the inter band scatterings, the Hc_2 and γ_H curves essentially depend on the intra band electron diffusivities. Near T_c, the Hc_2 curves are mainly determined by the diffusivities of the cleaner band between σ and π bands. On the other band, the zero-temperature $Hc_2(0)$ is controlled by the dirtier band. This feature of two-gap superconductivity in the dirty limit causes the upward curvature near T_c and the significant enhancement of $Hc_2(0)$ beyond the prediction of the one-gap BCS theory[10,14].

To address the above mentioned effects of the impurities, it should be noted that substituting Mg or B with other elements can differently affect the σ and π bands. It is expected that the B-site substitutions enhance the scattering within the σ bands, whereas Mg-site substitutions do the same thing in the π bands of course, these can accompany the alterations of the electronic structure. However, detailed information on the modified electronic structure can be obtained in first principles calculation[I5,16]. For instance, the main effect of Al doping in the Mg site was found to reduce the density of states at the Fermi level by increasing the number of electrons and to produced a band broadening by reducing the cell volume[15]. However, even though several studies on AI-doped MgB_2 exist[I7-20] the evolution of the impurity scattering with Al doping was not addressed until now.

In this work, we .investigated the effect of Al doping on $HC_2(T)$ for $Mg_{1-x}Al_xB_2$ (x = 0, 0.1, 09.2, 0.3). The $HC_2(T)$ values, determined by the resistivity measurements, were analysed by using the two-gap dirty-limit theory, along with the electron-phonon coupling constants and Coulomb pseudo potentials that were calculated in the first principles calculation.

The samples were synthesis in high-pressure and high temperature conditions. A stoichiometric mixture of Mg, B and Al powders was ground in a glove bag filled with inert Ar gas. The resulting precursor was pelletized, wrapped in Ta foil and put into a high pressure cubic cell. It was pressed up to 3.5 GPa and heat treated at 950^{o}C for 2 h. It was then quenched to room temperature.

The structure of the samples was examined by x-ray diffraction measurements. The surface of morphology and the local compositions were investigated by using a field emission scanning electron microscope and energy dispersive spectroscopy, respectively.

Mathematical formulae used in the analysis

We used the theoretical formalism of A. Golubovand A. E. Koshelev[10,11] of two-gap dirty limit theory of $Hc_2(T)$ which takes the form in the absence of inter band scattering

$$a_o[\ln t + U(h)][\ln t + U(\eta h)] + a_2[\ln t + U(\eta h)] + a_1[\ln t + U(\eta h) + U(h)] = 0 \quad \ldots(1)$$

Here

$$h = \frac{H_{C2} D_\sigma^{eff}}{2\Phi_0 T}$$

$$\eta = \frac{D_\pi^{eff}}{D_\sigma^{eff}}$$

$$U(x) = \psi\left(\frac{1}{2} + x\right) - \psi(x) \quad \ldots(2)$$

Ψ (x) is the digamma function a_0, a_1, a_2 are the constants derived from the electron-phonon coupling constant (λ^{ep}_{mn}) and coulomb pseudo potential μ_{mn}

$$\lambda_{mn} = \lambda_{mn}^{ep} - \mu_{mn}$$

Φ_0 = flux quanta …(3)

For the isotropic case, the electron diffusivity is given by D = $lv_F^2/3$ is the Fermi velocity and *l* is the electron mean free path. The numerical values of the data are given in Table T_3.

If the system is sufficiently impure than the electronic mean free path l is much smaller than the coherence length ξ_0 of the pure material.

For dirty limit $\Delta << (1/\tau) << E_F$

For clean limit $l >> \xi_0$ …(4)

The electron diffusivities are actually related to the value of the resistivity. The resistivity can be expressed in terms of the electron diffusivities [10] by -

$$\frac{1}{\rho} = e^2 (N_\sigma D_\sigma^{\ eff} + N_\pi D_\pi^{\ eff}) \quad \ldots(5)$$

Where N_π and N_σ are the partial densities of states in the π and σ band respectively.

RESULTS AND DISCUSSION

In this paper, we have evaluated the Al concentration dependence of T_c in two gap nature of $Mg_{1-x}AL_xB_2$ superconductor. In table 1 we have shown the Al concentration of T_c. The theoretical results were compared with the experimental data[15]. Our theoretically evaluated results show that as x (Al-concentration) increases zero-field T_c decreases. This shows that σ bands collapse gradually with Al doping due to the increase in the number of electrons. At x = 0.3 an abrupt topological change of the σ bands in the open section of the Fermi surface was found. Al x = 0.6 the σ bands vanishes completely. In table 2, we have presented the temperature dependence of the Hc_2 at different doping concentration. From our theoretical results it appears that Hc_2 is highest at x=0.0 and lower for x = 0.3. For all doping Hc_2 (T) decrease with T and at $T \rightarrow T_c$ its value tends to zero. In one gap BCS theory, Hc_2 (T) enhances as the impurity scattering increase. In one gap BCS theory Hc_2 (T) is linear near T_c. On the other hand in two gap nature of $Mg_{l-x}Al_xB_2$ superconductor as the Al contents increase both T_c and Hc_2 (0) decrease. It shows that the three dimensional π bands become much dirtier when Al was doped. In contrast the inter band scattering of the two dimensional σ bands are relatively unaffected by the Al doping[25-30].

Table 1: An Evaluated results of Al concentration dependence of T_c for $Mg_{1-x}Al_xB_2$. The results were compared with experimental data[15]

Doping (x)	T_c(K)	
	Theory	Expt.
0.00	40.2	39.0
0.05	39.6	
0.10	38.4	36.5
0.15	34.2	
0.20	30.8	32.8
0.25	28.7	
0.30	26.5	28.4
0.35	24.8	
0.40	21.9	
0.45	19.8	
0.50	17.5	
0.55	11.2	
0.60	10.6	

Table 2: An evaluated results for temperature dependence of Hc_2 (T) at different doping concentration

T (K)	Hc_2 (T)			
	X = 0.0	**X = 0.1**	**X = 0.2**	**X = 0.3**
5	13.26	10.58	8.39	5.11
10	11.85	9.45	7.18	4.28
12	10.97	8.27	6.98	3.46
15	9.45	7.42	4.36	3.21
17	8.27	6.38	3.10	2.95
20	7.66	5.95	2.89	2.27
22	6.85	5.22	2.26	1.88
25	5.39	4.85	1.88	1.18
30	4.12	3.86	1.73	0.92
32	3.98	3.10	1.44	0.76
35	3.30	2.75	1.26	0.52
37	2.17	2.08	1.06	0.39
40	1.86	1.78	0.95	0.22

Table 3: Parameter used in the calculation

X	$\lambda_{\sigma\sigma}$	$\lambda_{\sigma\pi}$	$\lambda_{\pi\sigma}$	$\lambda_{\pi\pi}$	D_π^{eff} m^2S^{-1}	D_σ^{eff} m^2S^{-1}
0.0	0.810	0.119	0.090	0.285	7.0×10^{-3}	2.0×10^{-3}
0.1	0.670	0.170	0.115	0.366	6.0×10^{-3}	2.3×10^{-3}
0.2	0.511	0.185	0.121	0.395	1.7×10^{-3}	2.0×10^{-3}
0.3	0.407	0.166	0.145	0.376	1.1×10^{-3}	2.5×10^{-3}

X = Doping concentration

$\lambda_{\sigma\sigma}$ = Coupling constant for $\sigma\sigma$ band; $\lambda_{\sigma\pi}$ = Coupling constant for $\sigma\pi$ band

$\lambda_{\pi\sigma}$ = Coupling constant for $\pi\sigma$ band; $\lambda_{\pi\pi}$ = Coupling constant for $\pi\pi$ band

D_π^{eff} = Effective diffusivities for π band; D_σ^{eff} = Effective diffusivities for σ band

The Hc_2 (T) of $Mg_{1-x}Al_xB_2$ (x = 0, 0.1, 0.2 and 0.3) was studied based on the two-gap dirty-limit. The following facts were found:

1. The reduction of Hc_2 (0) with x is related to the modifications of the electronic structure.
2. The 3D π band became much dirtier when the Al was doped, whereas the 2D σ bands were unaffected by such doping, which indicates that Al doping is band sensitive when it acts as an impurity.
3. On examining over different doping concentrations, we have found that the σ bands were dirtier than the π bands.

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