

Density of States and Debye Temperature for Superconductors

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Abstract: *The Debye continuum model is most relevant at low temperatures where only low frequencies can be excited and therefore, waves of only long wavelength will be present. The mole fraction or atom-volume ratio fraction methods are effective methods for high temperature super conductor to calculate the electronic density of state.*

Keywords: Density of states, Debye temperature

1. Introduction

Due to limitation of low temperature superconductor, working with devices that have to be cooled to temperature in the range of liquid helium temperature (4.2 K) is obviously not viable on any count. This has kept the scientists world over relentlessly trying to discover superconductivity near room temperature. A decisive boost to this optimism came in 1986, when Bednorz and Muller synthesized metallic oxygen-deficient copper oxide compound of La-Ba- (Sr)-Cu-O system with the transition temperature of about 30K. A vigorous activity towards the search for materials with higher critical temperature ensued following this Nobel Prize winning announcement. It has resulted in the development of a variety of materials with the highest critical temperature to in the vicinity of 135 K. The T_c values being so high compared to those of conventional superconductors. These materials are called high temp superconductors or high T_c Superconductors [1] [2] [3].

V_3Si , Nb_3Sn , Nb_3Ge , Nb_3Al , Say these are in general A_3B superconductors, having six transition metal atoms A on the faces of background of BCC lattice of B atom. Here three sets of perpendicular chains of transition atoms A along the unite cell edges and the nearest neighbours distance $a/2$, where a = lattice parameter. The highest superconductor transition temp for Nb_3Ge structure was $T_c = 24K$ but know for intermetallic MgB_2 , $T_c = 40k$ is the high temperature for intermetallic superconductor [4][5]. We know that V_3Si and Nb_3Sn have two gaps [6][7]. The density of state is very important in all superconductor compounds.

$$\left. \begin{aligned} Kx &= \frac{\pi}{L} nx \\ Ky &= \frac{\pi}{L} ny \\ Kz &= \frac{\pi}{L} nz \end{aligned} \right\}$$

Above all equations provides the clue to the determination of density of electron states. We have excluded the zero value of n_x , n_y and n_z since the respective solutions cannot

be normalized over the potential box. Further, no new linearly independent solutions are found for the negative values of these integers and as such these values are not considered. Thus for the fixed boundary condition as given below,

$$\begin{aligned} \Psi &= 0 \text{ for } x = 0 \text{ and } L, \text{ and } 0 < y, z < L \\ y &= 0 \text{ and } L, \text{ and } 0 < z, x < L \\ z &= 0 \text{ and } L, \text{ and } 0 < x, y < L \end{aligned}$$

The useful possible values of K totally lie in the positive octant of the K space. The density of state for Nb_3Ge , Nb_3Al are 7.6 and 7.8 (State / eV.spin.cell) respectively [8], [9]. The highest value of density of state was for Nb_3Sn , 21.34 states /eV. Cell. MgB_2 is high temp superconductor. The density of state for this is 0.21 state/eV. Spin atom [10]. The Debye temperature value is important to calculate the transition temperature of compound. The characteristic of low temperature is high density of state near Fermi level but it is small at high temperature superconductor MgB_2 or cuprate $YBa_2Cu_3O_7$.

The main aspect of this study is trying to present the relation between the electron density of state for compound $AnBm$ and the electron density of state at Fermi level for the elements A, B by Debye temperature and free electron approximation of compounds $AnBm$ either this compound are low or high temperature superconductivities.

We consider Nb_3Sn and Nb_3Al is low temperature superconductor and MgB_2 and $YBa_2Cu_3O_7$ is high temperature superconductor.

The free energy in three dimensions,

$$E = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}$$

and we know there is one electron state in volume $(\pi/L)^3$ of the K -space

$$\frac{D(\varepsilon)}{V} = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \varepsilon^{1/2}$$

The density of states as a function of energy is graphically represented as

$$\frac{dN}{dE} = \left(\frac{V}{2\pi^2}\right) \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}} \dots\dots\dots (1)$$

Methods of calculation the electron density of states (EDOS) of compound AnBm are

$$D(E)_{AB} = \left(\frac{1}{r_A}\right)^{\frac{1}{3}} D(E)_A + \left(\frac{1}{r_B}\right)^{\frac{2}{3}} D(E)_B \dots\dots\dots (2) \text{ (Free electron approximation)}$$

$$D(E)_{AB} = \left(\frac{n}{n+m}\right) D(E)_A + \left(\frac{m}{n+m}\right) D(E)_B \dots\dots\dots (3) \text{ (Mole Function)}$$

$$D(E)_{AB} = \left(\frac{r_B}{r_A+r_B}\right) D(E)_A + \left(\frac{r_A}{r_A+r_B}\right) D(E)_B \dots\dots\dots (4) \text{ (Atom-volume ratio fraction)}$$

r_A and r_B are defined as

$$r_A = \left(\frac{(N_A)_{AB}}{N_A}\right) \left(\frac{V_A}{V_{AB}}\right) \dots\dots\dots (5)$$

$$r_B = \left(\frac{(N_B)_{AB}}{N_B}\right) \left(\frac{V_B}{V_{AB}}\right) \dots\dots\dots (6)$$

Where $(N_A)_{AB}$, $(N_B)_{AB}$ = the atomic No. in unit cell (in a compound AnBm) of elements A and B

N_A , N_B = the atomic No in unit cell of elements A and B, respectively

V_{AB} = the lattice's volume of AnBm

V_A , V_B = the lattice's volumes of elements A and B.

The Debye continuum model is most relevant at low temperatures where only low frequencies can be excited and therefore, waves of only long wavelength will be present. Thus a Debye characteristic temp θ_D is defined below for which the model is valid. It is given by

$$\theta_D = \frac{\hbar\omega_D}{K_B} \dots\dots\dots (7)$$

Using above equation and

$$C_V = 9NK_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx \dots\dots\dots (8)$$

So, initial Debye temperature for compound AnBm can be obtained by an equation (8).

2. Results

There are many theoretically methods used to obtain the EDOS at Fermi level at 0K but here the effort is by using the free electron model with ratios of the atoms number in unit cell from the lattice of compound and lattices of elements also the volumes. The initial Debye temperature of Nb₃Sn, Nb₃Al, MgB₂ Calculated from equation (8) leads to values close to experiments values.

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