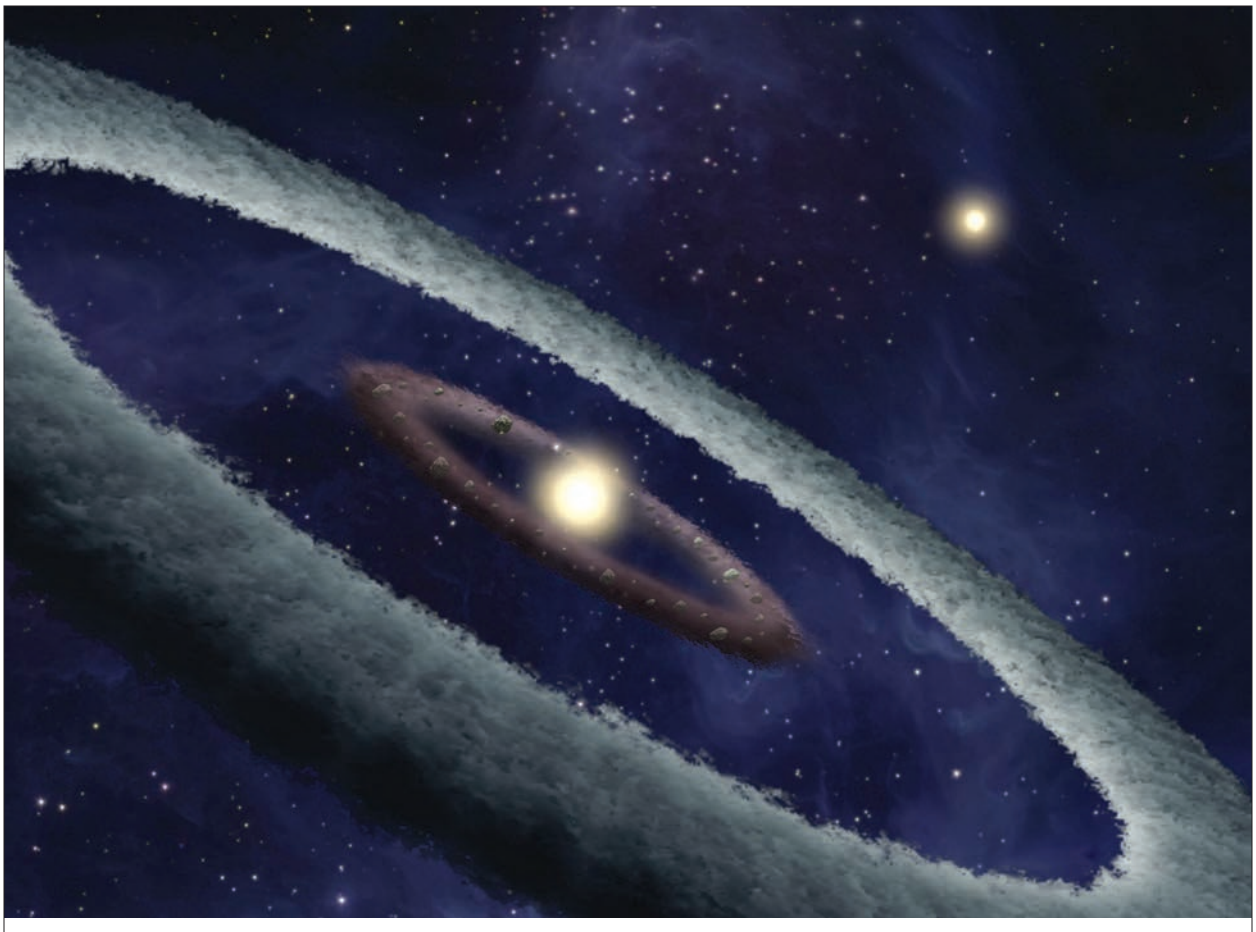

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Electronic Density of State and Debye Temperature for Low (Nb_3Sn, Nb_3Al) and High (MgB_2, $YBa_2Cu_3O_7$) Temperature Superconductors

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Abstract: The free electron approximation model can be used to calculate the electronic density of state of low temperature superconductivities Nb_3Sn and Nb_3Al but the mole fraction or atom-volume ratio fraction methods are effective methods for high temperature MgB_2 and $YBa_2Cu_3O_7$ superconductivities. The smallest value of the Debye temperature of many compounds depends ouly on the atom-volume ratios. However, the initial Debye temperature can evaluated from the smallest value and a constant related to the interaction coupling between electron-phonon for the components of compound, this result is a reasonable and approximately value close to experimental value of initial Debye temperature.

Key words: Free electron approximation, mole fraction, atom-volume fraction, electronic specific heat constant

INTRODUCTION

The unit cell of A_3B superconductors having six transition metal atoms A on the faces of background of bcc lattice of B atom. The most significant feature of the crystal structure is that three sets of orthogonal chains of transition atoms A along the unite cell edges and the nearest neighbors distance a/2, a is the lattice parameter the highest superconductor transition temperatures for A-15, Nb_3Ge (Gavaler, 1973) structure was T_c = 23K but know for intermetallic MgB_2, T_C = 39 (Nagamatsu *et al*., 2001) is the high temperature for intermetallic superconductor. Some of this structure has two gaps as V_3Si (Nefyodov *et al*., 2005), Nb_3Sn (Guritanu *et al*., 2004). The density of state is very important in all superconductor compounds where many physical quantities depend on it's magnitude. Several studies calculated the density of state for this compounds; Nb_3Ge, Nb_3Al (Pickett *et al*., 1979) the density of state for them respectively was $D(E_F)$ = 7.6, 7.8 (state/ev.spin.cell) also the study of compounds Nb_3B, B = Al, Ga, Ge and in (Paduani, 2007), the highest value of density of state was for Nb_3Sn, $D(E_F)$ = 21.34 staes/ev.cell. High temperature superconductor MgB_2 the density of state was D (E_F) = 0.21 state/ev.spin.atom (Kortus *et al*., 2001). The Debye temperature value is important to calculate or estimate the critical temperature of compound. The experiment results for two samples was 800 and 930K (Wang *et al*., 2001). 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 $YBa_2Cu_3O_7$.

Here, the main goal of this study is trying to present the relation between the electron density of state at Fermi level for the elements A, B and the electron density of state for compound A_nB_m by using free electron approximation and new method to calculate the Debye temperature of compounds A_nB_m either this compounds are low or high temperature super-conductivities.

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MATERIALS AND METHODS

Present Compounds

The present compounds are low temperature superconductor compounds Nb_3Sn and Nb_3Al belong to the structure A15, intermetallic high temperature superconductivity as magnesium diboride MgB_2 and cuprate high temperature superconductivity $YBa_2Cu_3O_7$.

Methods

The Fermi energy in three dimensions:

$$E = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3} \tag{1}$$

Electronic Densities Of State (EDOS) contain spin:

$$D(E) = \frac{dN}{dE} = (V/2\pi^2)(2m/\hbar^2)^{3/2}E^{1/2} \tag{2}$$

Methods of calculation the EDOS of compound A_nB_m are:

$$D(E)_{AB} = (1/r_A)^{2/3}D(E)_A + (1/r_B)^{2/3}D(E)_B \quad \text{(Free electron appro.)} \tag{3}$$

$$D(E)_{AB} = (n/(n+m))D(E)_A + (m/(n+m))D(E)_B \quad \text{(Mole fraction)} \tag{4}$$

$$D(E) = \left(\frac{r_B}{r_A + r_B}\right)D(E)_A + \left(\frac{r_A}{r_A + r_B}\right)D(E)_B \quad \text{(Atom-volume ratio fraction)} \tag{5}$$

r_A and r_B are defined as:

$$r_A = \left(\frac{(N_A)_{AB}}{N_A}\right)\left(\frac{V_A}{V_{AB}}\right), \qquad r_B = \left(\frac{(N_B)_{AB}}{N_B}\right)\left(\frac{V_B}{V_{AB}}\right) \tag{6}$$

Where:

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

N_A, N_B = The atomic No. in unit cell (in their original lattice) of elements A and B, respectively

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

V_{AB} = The lattice's volume of A_nB_m

An initial Debye temperature for compound A_nB_m can be obtained by the following:

$$\Theta_D = \delta(\Theta_D)_S$$
$$(\Theta_D)_S = \frac{(\Theta_D)_A(\Theta_D)_B}{(r_B(\Theta_D)_A + r_A(\Theta_D)_B)} \tag{7}$$
$$\delta = \left(\frac{Z_A(\Theta_D)_A r_A(1+\lambda_A) + Z_B(\Theta_D)_B r_B(1+\lambda_B)}{Z_A(\Theta_D)_A(V_{AB}/V_A) + Z_B(\Theta_D)_B(V_{AB}/V_B)}\right)^{1/3}$$

where, $(\Theta_D)_A$ and $(\Theta_D)_B$ are Debye temperatures of an element A and B, respectively and $(\Theta_D)_S$ is the smallest value of Debye temperature and z is the number of valence electrons.

RESULTS AND DISCUSSION

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. This effort led to approximative value or close to that obtained by other methods as self-consistent-pseudoptiential method. The density of state which obtained by Eq. 3 is a reasonable value for some compound superconductors A_nB_m as structure A_3B (A15). The compounds Nb_3B, B = Sn, Al are low temperature superconductors, the average of interaction coupling for Nb and Sn is a strong ($\lambda \geq 0.82$) but the average is intermediate coupling for Nb, Al elements ($\lambda \leq 0.6$), they also have high EDOS. However, the EDOF of Nb_3Sn and Nb_3Al calculated by Eq. 3. The high temperature intermetallic MgB_2, T_C = 39 (Nagamatsu *et al*., 2001) and high temperature cuprate $Yba_2Cu_3O_7$, T_C = 93K (Wu *et al*., 1987); the average of interaction coupling between electron-phonon either for MgB_2 component or $YBa_2Cu_3O_7$ is small. As a result of that, the EDOS obtained from mole fraction method (Eq. 4). This results are shown in Table 1 column a of electronic density of state.

The smallest value of Debye temperature; perhaps there is no experimental values smaller than it. The initial Debye temperature of Nb_3Sn, Nb_3Al, MgB_2 calculated from $(\Theta_D)_S$ multiplied by a constant value δ leads to values close to experiments values.

The initial Debye temperature of cuprate $YBa_2Cu_3O_7$ can also be obtained by mole fraction which takes the form:

$$(1/\Theta_D) = (1/13)(1/\Theta_D)_Y + (2/13)(1/\Theta_D)_{Ba} + (3/13)(1/\Theta_D)_{Cu} + (7/13)(1/\Theta_D)_O$$

or by fraction of atom-volume ratios method that gives the same results. Electronic specific heat constant (γ) for all compounds is determined from: D (E) $(1+\gamma) = 0.212\ \gamma$, under the condition that the density of state in unite (states/atom.ev.spin).

All results are shown in Table 1., compare with experiment results taken from references (Junod *et al*., 1983; Wang *et al*., 2001), where, the columns (a) represents the results of these methods and (b) columns are the experiment results Debye temperature (Θ_D) and electronic specific heat constant (γ).

CONCLUSIONS

The free electron approximation can be used to calculate the EDOS of superconducting compounds that are strong or intermediate interaction coupling between electron-phonon (λ) or the average λ of it's components are strong or intermediate and the components have high EDOS, but the mole fraction is an effective method to obtain. The EDOS for weak λ superconducting compounds or

Table 1: Calculation (a columns) compare with experiment results for Θ_D and γ (b columns) from tables of Junod *et al.* (1983) and Wang *et al.* (2001)

	D (E) (States/Atom.eV.spin)		γ (mJ/gat.k^2)		Θ_D (K)			
Compounds	a	b	a	b	a	b	λ	T_C (K)
Nb_3Sn	0.873	0.99	11.52	14.3	228.7	230	1.78	18.00
Nb_3Al	0.788	0.84	9.62	8.72	320.0	292	1.59	18.07
MgB_2	0.138	0.12	1.04	0.89	927.0	930	0.58	36.70
$YBa_2Cu_3O_7$	0.128	0.13	1.51	≈1.5	436.0	420	≈1.5	90.00

the average λ of it's components and EDOS are small. The Debye temperatures which derived from the Eq. 7 are reasonable and closed to experiments result for many compounds. The atom-volume ratios has two properties. First, it is a direction relation to calculate the mass density for any compound. Second, the total ratios of high temperature compounds are larger than of low temperature compounds.

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