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SUPERCONDUCTING STATE PARAMETERS OF Pb-Tl-Bi ALLOYS

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The theoretical study of the superconducting state parameters (SSP) viz. electron-phonon coupling strength λ, Coulomb pseudopotential μ^*, transition temperature T_C, isotope effect exponent α and effective interaction strength $N_O V$ of Pb-Tl-Bi alloys viz. $Tl_{0.90}Bi_{0.10}$, $Pb_{0.40}Tl_{0.60}$, $Pb_{0.60}Tl_{0.40}$, $Pb_{0.80}Tl_{0.20}$, $Pb_{0.60}Tl_{0.20}Bi_{0.20}$, $Pb_{0.90}Bi_{0.10}$, $Pb_{0.80}Bi_{0.20}$, $Pb_{0.70}Bi_{0.30}$, $Pb_{0.65}Bi_{0.35}$ and $Pb_{0.45}Bi_{0.55}$ have been made extensively in the present work using a model potential formalism for the first time. A considerable influence of various exchange and correlation functions on λ and μ^* is found from the present study. The present results of the SSP are found in qualitative agreement with the available experimental data wherever exist.

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1. Introduction

During last several years, the superconductivity remains a dynamic area of research in condensed matter physics with continual discoveries of novel materials and with an increasing demand for novel devices for sophisticated technological applications. A large number of metals and amorphous alloys are superconductors, with critical temperature T_C ranging from 1-18K. Even some heavily doped semiconductors have also been found to be superconductors. Basically, all the metal superconductors are type-I superconductors at room temperature [1-13]. The pseudopotential theory has been used successfully in explaining the superconducting state parameters (SSP) for metallic complexes by many workers [1-13]. Many of them have used well known model pseudopotential in the calculation of the SSP for the metallic complexes. Recently, Vora *et al.* [3-11] have studied the SSP of some metals, In-based binary alloys, alkali-alkali binary alloys and large number of metallic glasses using single parametric model potential formalism. The study of the SSP of the binary alloy based superconductors may be of great help in deciding their applications; the study of the dependence of the transition temperature T_C on the composition of metallic elements is helpful in finding new superconductors with high T_C. The application of pseudopotential to binary alloys involves the assumption of pseudoions with average properties, which are assumed to replace three types of ions in the binary systems, and a gas of free electrons is assumed to permeate through them. The electron-pseudoion is accounted for by the pseudopotential and the electron-electron interaction is involved through a dielectric screening function. For successful prediction of the superconducting properties of the alloying systems, the proper selection of the pseudopotential and screening function is very essential [3-11].

A well known empty core (EMC) model potential of Ashcroft [14] is applied here in the study of the SSP viz. electron-phonon coupling strength λ, Coulomb pseudopotential μ^*, transition temperature T_C, isotope effect exponent α and effective interaction strength $N_O V$ of Pb-Tl-Bi alloys viz. $Tl_{0.90}Bi_{0.10}$, $Pb_{0.40}Tl_{0.60}$, $Pb_{0.60}Tl_{0.40}$, $Pb_{0.80}Tl_{0.20}$, $Pb_{0.60}Tl_{0.20}Bi_{0.20}$, $Pb_{0.90}Bi_{0.10}$, $Pb_{0.80}Bi_{0.20}$, $Pb_{0.70}Bi_{0.30}$, $Pb_{0.65}Bi_{0.35}$ and $Pb_{0.45}Bi_{0.55}$. To see the impact of various exchange and correlation functions on the aforesaid properties, we

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have used five different types of local field correction functions proposed by Hartree (H) [15], Taylor (T) [16], Ichimaru-Utsumi (IU) [17], Farid *et al.* (F) [18] and Sarkar *et al.* (S) [19]. We have incorporated for the first time the more advanced and newly developed local field correction functions i.e. IU [17], F [18] and S [19] in the investigation of the SSP of Pb-Tl-Bi alloys.

To describe electron-ion interactions in the binary systems, the Ashcroft's empty core (EMC) single parametric local model potential [14] is employed in the present investigation. The form factor $W(q)$ of the EMC model potential in wave number space is (in au) [14]

$$W(q) = \frac{-8\pi Z}{\Omega_O q^2 \varepsilon(q)} \cos(q r_C). \tag{1}$$

here, Z, Ω_O $\varepsilon(q)$ and r_C are the valence, atomic volume, Hartree dielectric function and parameter of the model potential of Pb-Tl-Bi alloys, respectively.

2. Method of computation

In the present investigation for binary mixtures, the electron-phonon coupling strength λ is computed using the relation [3-11]

$$\lambda = \frac{m_b \Omega_0}{4\pi^2 k_F M \langle \omega^2 \rangle} \int_0^{2k_F} q^3 \left| W(q) \right|^2 dq. \tag{2}$$

Here m_b is the band mass, M the ionic mass, Ω_O the atomic volume, k_F the Fermi wave vector and $W(q)$ the screened pseudopotential. The effective averaged square phonon frequency $\langle \omega^2 \rangle$ is calculated using the relation given by Butler [20], $\langle \omega^2 \rangle^{1/2} = 0.69\theta_D$, where θ_D is the Debye temperature of the Pb-Tl-Bi alloys.

Using $X = q/2k_F$ and $\Omega_O = 3\pi^2 Z/(k_F)^3$, we get Eq. (2) in the following form,

$$\lambda = \frac{12\, m_b Z}{M \langle \omega^2 \rangle} \int_0^1 X^3 \left| W(X) \right|^2 dX, \tag{3}$$

where Z and $W(X)$ are the valence and the screened EMC pseudopotential [13] of the Pb-Tl-Bi alloys, respectively.

The Coulomb pseudopotential μ^* is given by [3-11]

$$\mu^* = \frac{\dfrac{m_b}{\pi k_F} \displaystyle\int_0^1 \frac{dX}{\varepsilon(X)}}{1 + \dfrac{m_b}{\pi k_F} \ln\left(\dfrac{E_F}{10\,\theta_D}\right) \displaystyle\int_0^1 \frac{dX}{\varepsilon(X)}}. \tag{4}$$

Where E_F is the Fermi energy, m_b the band mass of the electron and $\varepsilon(X)$ the modified Hartree dielectric function, which is written as [15]

$$\varepsilon(X) = 1 + (\varepsilon_H(X) - 1)(1 - f(X)). \tag{5}$$

$\varepsilon_H(X)$ is the static Hartree dielectric function [15] and $f(X)$ the local field correction function. In the present investigation, the local field correction functions due to H [15], T [16], IU [17], F [18] and S [19] are incorporated to see the impact of exchange and correlation effects.

After evaluating λ and μ^*, the transition temperature T_C and isotope effect exponent α are investigated from the McMillan's formula [3-11]

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

$$\alpha = \frac{1}{2}\left[1 - \left(\mu^* \ln\frac{\theta_D}{1.45T_C}\right)^2 \frac{1+0.62\lambda}{1.04(1+\lambda)}\right]. \tag{7}$$

The expression for the effective interaction strength $N_O V$ is studied using [3-11]

$$N_O V = \frac{\lambda - \mu^*}{1 + \frac{10}{11}\lambda}. \tag{8}$$

3. Results and discussion

The input parameters and constants used in the present calculations are given in Table 1. Table 2 shows the presently calculated values of the SSP viz. electron-phonon coupling strength λ, Coulomb pseudopotential μ^*, transition temperature T_C, isotope effect exponent α and effective interaction strength $N_O V$ at various concentrations for Pb-Tl-Bi alloys with available experimental findings [21].

Table 1. Input parameters and other constants.

Alloys	Z	r_C (au)	Ω_O (au)^3	k_F (au)	M (amu)	θ_D (K)	$\langle\omega^2\rangle^2$ (au)^2 x 10^{-6}
$Tl_{0.90}Bi_{0.10}$	3.20	0.9910	196.47	0.7842	204.83	90.20	0.15644
$Pb_{0.40}Tl_{0.60}$	3.40	0.8935	196.38	0.8003	205.5	90.72	0.15825
$Pb_{0.60}Tl_{0.40}$	3.60	0.8482	198.72	0.8125	206.06	92.58	0.16481
$Pb_{0.80}Tl_{0.20}$	3.80	0.8237	201.06	0.8241	206.63	94.44	0.17150
$Pb_{0.60}Tl_{0.20}Bi_{0.20}$	4.00	0.2349	208.26	0.8285	206.98	190.00	0.69415
$Pb_{0.90}Bi_{0.10}$	4.10	0.8004	207.00	0.8370	207.37	98.57	0.18682
$Pb_{0.80}Bi_{0.20}$	4.20	0.7874	210.60	0.8390	207.55	100.84	0.19553
$Pb_{0.70}Bi_{0.30}$	4.30	0.7662	214.20	0.8408	207.73	103.11	0.20443
$Pb_{0.65}Bi_{0.35}$	4.35	0.7452	216.00	0.8417	207.82	104.25	0.20898
$Pb_{0.45}Bi_{0.55}$	4.55	0.8157	223.20	0.8451	208.17	108.79	0.22757

The calculated values of the electron-phonon coupling strength λ for Pb-Tl-Bi alloys, using five different types of the local field correction functions with EMC model potential, are shown in Table 2 with the experimental data [21]. It is noticed from the present study that, the percentile influence of the various local field correction functions with respect to the static H-screening function on the electron-phonon coupling strength λ is 26.52%-49.52%, 26.42%-51.81%, 26.08%-52.21%, 25.67%-51.91%, 25.72%-60.06%, 25.20%-51.46%, 25.14%-51.69%, 25.11%-52.15%, 25.11%-52.67% and 25.28%-51.24% for $Tl_{0.90}Bi_{0.10}$, $Pb_{0.40}Tl_{0.60}$, $Pb_{0.60}Tl_{0.40}$, $Pb_{0.80}Tl_{0.20}$, $Pb_{0.60}Tl_{0.20}Bi_{0.20}$, $Pb_{0.90}Bi_{0.10}$, $Pb_{0.80}Bi_{0.20}$, $Pb_{0.70}Bi_{0.30}$, $Pb_{0.65}Bi_{0.35}$ and $Pb_{0.45}Bi_{0.55}$ alloys,

respectively. Also, the H-screening yields lowest values of λ, whereas the values obtained from the F-function are the highest. It is also observed from the Table 2 that, λ goes on increasing from the values of 0.9788→1.8834 as the concentration 'x' of 'Tl' is decreased from 0.60→0.20, while for concentration 'x' of 'Bi' increases except $\alpha Pb_{0.45}Bi_{0.55}$ alloys, λ goes on increasing. The increase or decrease in λ with concentration 'x' of 'Tl' and 'Bi' shows a gradual transition from weak coupling behaviour to intermediate coupling behaviour of electrons and phonons, which may be attributed to an increase of the hybridization of sp-d electrons of 'Tl' and 'Bi' with increasing or decreasing concentration (x). This may also be attributed to the increase role of ionic vibrations in the Tl or Bi-rich region. The present results are found in qualitative agreement with the available experimental data [21]. The calculated results of the electron-phonon coupling strength λ for $Tl_{0.90}Bi_{0.10}$, $Pb_{0.40}Tl_{0.60}$, $Pb_{0.60}Tl_{0.40}$, $Pb_{0.80}Tl_{0.20}$, $Pb_{0.60}Tl_{0.20}Bi_{0.20}$, $Pb_{0.90}Bi_{0.10}$, $Pb_{0.80}Bi_{0.20}$, $Pb_{0.70}Bi_{0.30}$, $Pb_{0.65}Bi_{0.35}$ and $Pb_{0.45}Bi_{0.55}$ deviate in the range of 8.68%-36.54%, 7.60%-29.21%, 3.40%-24.83%, 1.84%-23.10%, 23.27%-52.06%, 0.81%-20.78%, 1.36%-29.07%, 1.58%-31.30%, 2.70%-32.31% and 33.28%-55.88% alloys from the available experimental findings [21], respectively.

The computed values of the Coulomb pseudopotential μ^*, which accounts for the Coulomb interaction between the conduction electrons, obtained from the various forms of the local field correction functions are tabulated in Table 2. It is observed from the Table 2 that for all binary alloys, the μ^* lies between 0.11 and 0.14, which is in accordance with McMillan [22], who suggested $\mu^* \approx 0.13$ for simple and non-simple metals. The weak screening influence shows on the computed values of the μ^*. The percentile influence of the various local field correction functions with respect to the static H-screening function on μ^* for the Pb-Tl-Bi alloys is observed in the range of 4.77%-9.04%, 4.73%-8.86%, 4.66%-8.82%, 4.60%-8.77%, 5.02%-9.56%, 4.52%-8.70%, 4.60%-8.69%, 4.59%-8.76%, 4.59%-8.75% and 4.63%-8.84% for $Tl_{0.90}Bi_{0.10}$, $Pb_{0.40}Tl_{0.60}$, $Pb_{0.60}Tl_{0.40}$, $Pb_{0.80}Tl_{0.20}$, $Pb_{0.60}Tl_{0.20}Bi_{0.20}$, $Pb_{0.90}Bi_{0.10}$, $Pb_{0.80}Bi_{0.20}$, $Pb_{0.70}Bi_{0.30}$, $Pb_{0.65}Bi_{0.35}$ and $Pb_{0.45}Bi_{0.55}$ alloys, respectively. Again the H-screening function yields lowest values of the μ^*, while the values obtained from the F-function are the highest. The theoretical or experimental data of the μ^* is not available for the further comparisons.

Table 2. Superconducting state parameters of the Pb-Tl-Bi alloys.

Alloys	SSP	Present results					Expt. [30]
		H	T	IU	F	S	
$Tl_{0.90}Bi_{0.10}$	λ	0.7123	1.0067	1.0621	1.0650	0.9012	0.78
	μ^*	0.1195	0.1288	0.1300	0.1303	0.1252	–
	T_C (K)	2.3011	4.5437	4.9372	4.9540	3.7799	2.30
	α	0.4372	0.4558	0.4580	0.4580	0.4515	–
	N_0V	0.3598	0.4584	0.4742	0.4749	0.4265	–
$Pb_{0.40}Tl_{0.60}$	λ	0.9788	1.3999	1.4795	1.4859	1.2374	1.15
	μ^*	0.1185	0.1276	0.1288	0.1290	0.1241	–
	T_C (K)	4.6004	7.2982	7.7222	7.7522	6.3648	4.60
	α	0.4627	0.4719	0.4730	0.4730	0.4695	–
	N_0V	0.4553	0.5599	0.5760	0.5772	0.5239	–
$Pb_{0.60}Tl_{0.40}$	λ	1.1317	1.6220	1.7141	1.7226	1.4269	1.38
	μ^*	0.1179	0.1269	0.1281	0.1283	0.1234	–
	T_C (K)	5.9021	8.6916	9.1119	9.1465	7.7143	5.90
	α	0.4697	0.4764	0.4773	0.4773	0.4746	–
	N_0V	0.4997	0.6042	0.6199	0.6213	0.5674	–
$Pb_{0.80}Tl_{0.20}$	λ	1.2398	1.7739	1.8738	1.8834	1.5581	1.53
	μ^*	0.1174	0.1263	0.1275	0.1277	0.1228	–
	T_C (K)	6.8014	9.6015	10.0139	10.0497	8.6140	6.80
	α	0.4733	0.4788	0.4794	0.4795	0.4772	–

	N_0V	0.5277	0.6306	0.6460	0.6473	0.5940	–
$Pb_{0.60}Tl_{0.20}Bi_{0.20}$	λ	0.8677	1.2976	1.3726	1.3888	1.0909	1.81
	μ^*	0.1276	0.1382	0.1396	0.1398	0.1340	–
	T_C (K)	7.2606	13.4096	14.3079	14.4995	10.6459	7.26
	α	0.4460	0.4625	0.4641	0.4645	0.4564	–
	N_0V	0.4137	0.5319	0.5485	0.5520	0.4804	–
$Pb_{0.90}Bi_{0.10}$	λ	1.3151	1.8770	1.9815	1.9919	1.6465	1.66
	μ^*	0.1172	0.1260	0.1272	0.1274	0.1225	–
	T_C (K)	7.6521	10.5294	10.9469	10.9849	9.5032	7.65
	α	0.4753	0.4800	0.4806	0.4806	0.4787	–
	N_0V	0.5456	0.6470	0.6619	0.6633	0.6104	–
$Pb_{0.80}Bi_{0.20}$	λ	1.3335	1.9055	2.0117	2.0228	1.6688	1.88
	μ^*	0.1174	0.1262	0.1274	0.1276	0.1228	–
	T_C (K)	7.9501	10.8947	11.3199	11.3602	9.8361	7.95
	α	0.4756	0.4802	0.4808	0.4808	0.4789	–
	N_0V	0.5497	0.6512	0.6661	0.6676	0.6142	–
$Pb_{0.70}Bi_{0.30}$	λ	1.3809	1.9782	2.0888	2.1011	1.7277	2.01
	μ^*	0.1176	0.1265	0.1277	0.1279	0.1230	–
	T_C (K)	8.4518	11.4578	11.8872	11.9309	10.3650	8.45
	α	0.4765	0.4808	0.4814	0.4814	0.4795	–
	N_0V	0.5601	0.6617	0.6765	0.6781	0.6243	–
$Pb_{0.65}Bi_{0.35}$	λ	1.4418	2.0711	2.1875	2.2012	1.8039	2.13
	μ^*	0.1177	0.1266	0.1278	0.1280	0.1231	–
	T_C (K)	8.9511	11.9763	12.4032	12.4496	10.8663	8.95
	α	0.4776	0.4816	0.4821	0.4821	0.4804	–
	N_0V	0.5730	0.6745	0.6892	0.6908	0.6367	–
α $Pb_{0.45}Bi_{0.55}$	λ	1.1426	1.6289	1.7195	1.7281	1.4315	2.59
	μ^*	0.1188	0.1278	0.1291	0.1293	0.1243	–
	T_C (K)	7.0042	10.2267	10.7090	10.7508	9.0714	7.0
	α	0.4696	0.4761	0.4769	0.4770	0.4743	–
	N_0V	0.5022	0.6051	0.6205	0.6219	0.5680	–

Table 2 contains calculated values of the transition temperature T_C for Pb-Tl-Bi alloys computed from the various forms of the local field correction functions along with the experimental findings [21]. From the Table 2 it can be noted that, the static H-screening function yields lowest T_C whereas the F-function yields highest values of the T_C. The present results obtained from the H-local field correction functions are found in good agreement with available experimental data [21]. The calculated results of the transition temperature T_C for Pb-Tl-Bi alloys viz. $Tl_{0.90}Bi_{0.10}$, $Pb_{0.40}Tl_{0.60}$, $Pb_{0.60}Tl_{0.40}$, $Pb_{0.80}Tl_{0.20}$, $Pb_{0.60}Tl_{0.20}Bi_{0.20}$, $Pb_{0.90}Bi_{0.10}$, $Pb_{0.80}Bi_{0.20}$, $Pb_{0.70}Bi_{0.30}$, $Pb_{0.65}Bi_{0.35}$ and $Pb_{0.45}Bi_{0.55}$ deviate in the range of 0.05%-115.39%, 0.01%-68.53%, 0.04%-55.03%, 0.02%-47.79%, 0.01%-99.72%, 0.03%-43.59%, 0.00%-42.90%, 0.02%-41.19%, 0.01%-41.10% and 0.06%-53.58% from the experimental findings [21], respectively.

The values of the isotope effect exponent α for Pb-Tl-Bi alloys are tabulated in Table 2. The computed values of the α show a weak dependence on the dielectric screening, its value is being lowest for the H- screening function and highest for the F-function. Since the experimental value of α has not been reported in the literature so far, the present data of α may be used for the study of ionic vibrations in the

superconductivity of alloying substances. Since H-local field correction function yields the best results for λ and T_C, it may be observed that α values obtained from this screening provide the best account for the role of the ionic vibrations in superconducting behaviour of this system. The theoretical or experimental data of the α is not available for the further comparisons.

The values of the effective interaction strength $N_O V$ are listed in Table 2 for different local field correction functions. It is observed that the magnitude of $N_O V$ shows that the Pb-Tl-Bi alloys under investigation lie in the range of weak coupling superconductors. The values of the $N_O V$ also show a feeble dependence on dielectric screening, its value being lowest for the H-screening function and highest for the F-screening function. The variation of present values of the $N_O V$ show that, the Pb-Tl-Bi alloys under consideration falls in the range of weak coupling superconductors. The theoretical or experimental data of the $N_O V$ is not available for the further comparisons.

From the study of the Table 2, one can see that among the five screening functions the screening function due to H (only static–without exchange and correlation) gives the minimum value of the SSP while the screening function due to F gives the maximum value. The present findings due to T, IU and S-local field correction functions are lying between these two screening functions. The local field correction functions due to IU, F and S are able to generate consistent results regarding the SSP of Pb-Tl-Bi alloys as those obtained for more commonly employed H and T functions. The effect of local field correction functions plays an important role in the computation of λ and μ^*, which makes drastic variation on T_C, α and $N_O V$. Thus, the use of these more promising local field correction functions is established successfully. The computed results of α and $N_O V$ are not showing any abnormal values for Pb-Tl-Bi alloys.

The values of the electron-phonon coupling strength λ and the transition temperature T_C show an appreciable dependence on the local field correction function, whereas for the Coulomb pseudopotential μ^*, isotope effect exponent α and effective interaction strength $N_O V$ a weak dependence is observed. The magnitude of the λ, α and $N_O V$ values shows that Pb-Tl-Bi alloys are weak to intermediate superconductors. In the absence of experimental data for α and $N_O V$, the presently computed values of these parameters may be considered to form reliable data for Pb-Tl-Bi alloys, as they lie within the theoretical limits of the Eliashberg-McMillan formulation.

Lastly, we would like to emphasize the importance of involving a precise form for the pseudopotential. It must be confessed that although the effect of pseudopotential in strong coupling superconductor is large, yet it plays a decisive role in weak coupling superconductors i.e. those substances which are at the boundary dividing the superconducting and nonsuperconducting region. In other words, a small variation in the value of electron-ion interaction may lead to an abrupt change in the superconducting properties of the material under consideration. In this connection we may realize the importance of an accurate form for the pseudopotential.

4. Conclusions

The comparison of presently computed results with available experimental findings is highly encouraging in the case of Pb-Tl-Bi alloys, which confirms the applicability of the model potential. The theoretically observed values of SSP are not available for most of the Pb-Tl-Bi alloys therefore it is difficult to draw any special remarks. However, the comparison with other such theoretical data supports the present computations of the SSP. Such study on SSP of other binary and multi component alloys as well as metallic glasses is in progress.

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