TÜBİTAK

Turk J Phys
33 (2009) , 57 – 62.

doi:10.3906/fiz-0807-17

Superconducting State Parameters of Al-Li Binary Alloys

Aditya M. VORA
Humanities and Social Science Department, S. T. B. S. College of Diploma Engineering
Opp. Spinning Mill, Varachha Road, Surat 395 006, Gujarat, INDIA
e-mail: voraam@rediffmail.com

Received 29.07.2008

Abstract

Theoretical computation of 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 $N_\circ V$ of face centered cubic $Al_{1-C}Li_C$ binary alloys 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.

Key Words: Pseudopotential, Superconducting state parameters, Binary alloys.
PACS: 61.43.Dq; 71.15.Dx; 74.20.-z; 74.70.Ad

1. Introduction

Extensive research on cuprate superconductors has revealed their many unique characteristics, but detailed mechanism leading to observed critical phenomenon remains elusive. For traditional superconductors, the BCS theory [1] provides an elegant description of the superconducting electron pair formation induced by attractive electron–phonon interaction. Al-Li based alloys can be distinguished from other aluminium alloys due to their higher strength at a lower density and they are, therefore, promising structural materials for aviation and space engineering. Recently, their plastic and elastic properties have been the subject of numerous papers. The studies were usually performed at cryogenic temperatures, mainly covering the range down to 77.3 K. Only some of them were done at 4.2 K and therefore not all the studies were concerned with the possible superconductivity of the Al-Li alloys and the specific plastic effects which show up during the superconducting transition [2, 3]. Very recently, Ou et al. [2] have reported superconducting transition parameters using fitting of the density of states as well as Coulomb psudopotential. Experimental study is also narrated in the respective paper.

There are very few scattered attempts to study superconducting state parameters (SSP) of metallic superconductors based on model potential [4–6]. Here, we have avoided any fitting procedure to compute the superconducting state parameters (SSP) of binary alloys. Hence, we thought it worthwhile to under take an investigation of the superconducting state parameters (SSP) of $Al_{1-C}Li_C$ binary alloys on the basis of well-known empty core (EMC) model potential of Ashcroft [7]. We have employed five different types of local field correction functions proposed by Hartree (H) [8], Taylor (T) [9], Ichimaru-Utsumi (IU) [10], Farid et al. (F) [11] and Sarkar et al. (S) [12] to show the effect of the exchange and correlation on the aforesaid properties. For the investigations of electron-phonon coupling strength λ, Coulomb pseudopotential μ^*, transition temperature T_C, isotope effect exponent α and effective interaction strength N_OV for the $Al_{1-C}Li_C$ binary alloys, we have extended the way followed by McMillan for metals [4–6, 13].

2. Computational Methodology

The mathematical expressions used for the present investigation of λ, μ^*, T_C, α and N_OV are [4–6, 13]

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

$$\mu^* = \frac{\frac{m_b}{\pi k_F}\int_0^1 \frac{dx}{X\varepsilon(X)}}{1+\frac{m_b}{\pi k_F}\ln\left(\frac{E_F}{10\theta_D}\right)\int_0^1 \frac{dx}{X\varepsilon(X)}}, \tag{2}$$

$$T_C = \frac{\theta_D}{1.45}\exp\left[\frac{-1.04\left(1+\lambda\right)}{\lambda-\mu^*\left(1+0.62\lambda\right)}\right], \tag{3}$$

$$\alpha = \frac{1}{2}\left[1-\left(\mu^*\ln\left(\frac{\theta_D}{1.45T_C}\right)\right)^2\frac{1+0.62\lambda}{1.04\left(1+\lambda\right)}\right], \tag{4}$$

$$N_oV = \frac{\lambda-\mu^*}{1+\frac{10}{11}\lambda}. \tag{5}$$

Here, m_b is the band mass, M is the ionic mass, Ω_O is the atomic volume, k_F is the Fermi wave vector and $\langle\omega^2\rangle$ is the averaged square phonon frequency. $\langle\omega^2\rangle$ is calculated using the relation given by Butler [14], $\langle\omega^2\rangle^{1/2} = 0.69\theta_D$, where θ_D is the Debye temperature of $Al_{1-C}Li_C$ alloys, respectively. The Debye temperature of the pure metallic components is taken from the standard literature [15].

The well known screened Ashcroft's empty core (EMC) model potential [7] used in the present computations of the SSP of $Al_{1-C}Li_C$ alloys is of the form

$$W\left(X\right) = \frac{-\pi Z^*}{\Omega_O X^2 k_F^2 \varepsilon\left(X\right)}\cos\left(2k_F X r_C\right). \tag{6}$$

Here, r_C is the parameter of the model potential of $Al_{1-C}Li_C$ alloys. The Ashcroft's empty core (EMC) model potential is a simple one-parameter model potential [7], which has been successfully found for various metallic

complexes [4–6]. When used with a suitable form of dialectic screening function, this potential has been found to yield good results in computing the SSP of $Al_{1-C}Li_C$ alloys [4–6]. As such we decided to employ this EMC form in the present work. The parameter r_C is adjusted such that the calculated values of T_C agree well with the experimental value of T_C [2, 3] as close as possible.

While $\varepsilon(X)$ the modified Hartree dielectric function, which is written as [8]

$$\varepsilon(X) = 1 + (\varepsilon_H(X) - 1)(1 - f(X)). \tag{7}$$

$\varepsilon_H(X)$ is the static Hartree dielectric function [8] and $f(X)$ is the local field correction function. In the present investigation, the local field correction functions due to Hartree (H) [8], Taylor (T) [9], Ichimaru-Utsumi (IU) [10], Farid et al. (F) [11] and Sarkar et al. (S) [12] are incorporated to see the impact of exchange and correlation effects.

3. Results and Discussion

The input parameters and constants used in the present investigation for pure metallic elements are taken from the literature [15, 16]. Superconducting state parameters of $Al_{1-C}Li_C$ binary alloys are displayed in Table 1 along with other such experimental findings [9]. The present results of superconductivity are found to be in qualitative agreement with available experimental data [2, 3].

Table 1. Input parameters and other constants.

Metallic glass	Z	Ω_O (au)^3	M (amu)	θ_D (K)	r_C (au)
Li	1.00	144.90	6.94	344.00	1.1514
$Al_{0.01}Li_{0.99}$	1.02	144.56	7.14	344.84	1.1548
$Al_{0.03}Li_{0.97}$	1.06	143.89	7.54	346.52	1.1502
$Al_{0.038}Li_{0.962}$	1.08	143.62	7.70	347.19	1.1488
$Al_{0.05}Li_{0.95}$	1.10	143.22	7.94	348.20	1.1417
$Al_{0.10}Li_{0.90}$	1.20	141.54	8.94	352.40	1.1225
$Al_{0.104}Li_{0.896}$	1.21	141.41	9.03	352.74	1.1250

It is seen from Table 2 that, among all five screening functions, the screening function due to Hartree (H) (static only, without exchange and correlation) [8] gives the minimum value of the superconducting state parameters; while the screening function due to Farid et al. (F) [11] gives the maximum value. Findings due to Taylor (T) [9], Ichimaru-Utsumi (IU) [10] and Sarkar et al. (S) [12] local field correction functions lie between these two screening functions. These local field correction functions are able to generate consistent results regarding the SSP of $Al_{1-C}Li_C$ alloys. The numerical values of the aforesaid properties are found to be quite sensitive to the selection of the local field correction function and showing a significant variation with the change in the function. Note the increase in λ from $0.5066 \rightarrow 0.8733$ as the concentration of Li increased from $0.01 \rightarrow 0.104$. The increase in λ shows a gradual transition from weak coupling behavior to intermediate coupling behavior of electrons and phonons, which may be attributed to an increase of the hybridization of sp-d electrons. Generally, Li exhibits non-superconducting nature in normal laboratory condition. But, in the present case it exhibits superconducting nature. The computed results of the electron-phonon coupling strength λ for $Al_{1-C}Li_C$ alloys deviate in the range of 32.96%–133.48% from the experimental findings [2]. With respect

to the static Hartree (H) dielectric function [8] the influence of various local field correction functions on λ is 33.98%–72.82%. Such influence on μ^* is observed in the range of 7.40%–14.24%. These changes in λ and μ^* in turn lead to large changes in T_C, α and $N_O V$. μ^* accounts for the Coulomb interaction between the conduction electrons and has values that lie between 0.16 and 0.19, which is in accordance with McMillan [13].

Table 2. Superconducting state parameters of the $Al_{1-C}Li_C$ binary alloys.

Glass	SSP	Present results					Expt. [2, 3]
		H	T	IU	F	S	
Li	λ	0.5161	0.8227	0.8859	0.8919	0.7066	0.382
	μ^*	0.1664	0.1868	0.1896	0.1901	0.1796	0.10
	T_c (K)	1.1610	7.1197	8.6427	8.7714	4.5256	1.16
	α	0.1718	0.3292	0.3442	0.3449	0.2950	–
	N_0V	0.2380	0.3638	0.3857	0.3876	0.3209	–
$Al_{0.01}Li_{0.99}$	λ	0.5084	0.8064	0.8678	0.8733	0.6943	0.377
	μ^*	0.1658	0.1859	0.1888	0.1892	0.1789	0.10
	T_c (K)	1.0710	6.7526	8.2289	8.3485	4.2734	1.07
	α	0.1636	0.3249	0.3404	0.3411	0.2902	–
	N_0V	0.2343	0.3580	0.3796	0.3814	0.3160	–
$Al_{0.03}Li_{0.97}$	λ	0.5048	0.7956	0.8554	0.8606	0.6867	0.375
	μ^*	0.1648	0.1846	0.1874	0.1878	0.1777	0.10
	T_c (K)	1.0506	6.5829	8.0270	8.1399	4.1753	1.05
	α	0.1644	0.3242	0.3396	0.3403	0.2899	–
	N_0V	0.2330	0.3545	0.3758	0.3775	0.3134	–
$Al_{0.038}Li_{0.962}$	λ	0.5066	0.7945	0.8536	0.8586	0.6873	–
	μ^*	0.1640	0.1836	0.1863	0.1867	0.1767	–
	T_c (K)	1.1005	6.6380	8.0730	8.1811	4.2516	1.10
	α	0.1732	0.3268	0.3418	0.3424	0.2939	–
	N_0V	0.2346	0.3547	0.3757	0.3773	0.3143	–
$Al_{0.05}Li_{0.95}$	λ	0.5075	0.7936	0.8523	0.8572	0.6871	0.378
	μ^*	0.1634	0.1828	0.1855	0.1859	0.1760	0.10
	T_c (K)	1.1309	6.6855	8.1176	8.2249	4.2991	1.13
	α	0.1784	0.3286	0.3434	0.3440	0.2964	–
	N_0V	0.2354	0.3548	0.3757	0.3773	0.3146	–
$Al_{0.10}Li_{0.90}$	λ	0.5119	0.7886	0.8449	0.8494	0.6866	0.385
	μ^*	0.1608	0.1792	0.1818	0.1823	0.1727	0.10
	T_c (K)	1.2900	6.8745	8.2813	8.3786	4.5289	1.29
	α	0.2029	0.3365	0.3500	0.3505	0.3078	–
	N_0V	0.2397	0.3549	0.3750	0.3765	0.3164	–
$Al_{0.104}Li_{0.896}$	λ	0.5082	0.7811	0.8366	0.8409	0.6809	–
	μ^*	0.1605	0.1789	0.1815	0.1819	0.1724	–
	T_c (K)	1.2407	6.6936	8.0772	8.1702	4.4025	1.24
	α	0.1991	0.3344	0.3481	0.3486	0.3054	–
	N_0V	0.2378	0.3521	0.3721	0.3735	0.3141	–

Ou et al. [2] have fitted the values of μ^* in the range of 0.09 to 0.11 for obtaining better λ from the experimental data of T_C. But, we have avoided such fits in the computation. The higher values of μ^* in comparison of those of Ou et al. [2] may be due to the screening effects. The calculated results of the transition temperature T_C for $Al_{1-C}Li_C$ alloys deviate in the range of 0.05%–680.23% from the experimental findings [2, 3].

The computed values of α shows a weak dependence on dielectric screening. Since no experimental value of α has yet been reported in the literature, the present data of α may be used for the study of ionic vibrations in the superconductivity of alloying substances. Since Hartree (H) dielectric function [8] 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 behavior of this system. It is also observed that the magnitude of N_OV lie in the range of weak coupling superconductors and also show a feeble dependence on dielectric screening. The effective interaction strength N_OV represents combined effect of the electronic density of states at the Fermi surface, which is related to the Coulomb pseudopotential μ^*, and the pairing potential arising from the electron-phonon interaction related to the electron-phonon coupling strength λ, respectively. Hence, the physical nature of the effective interaction strength N_OV is same as those of the electron-phonon coupling strength λ. In the absence of experimental data for the SSP, the presently computed values of these parameters may be considered to form reliable data for aforesaid alloys, as they lie within the theoretical limits of the Eliashberg-McMillan formulation [13].

Local field correction functions play an important role in the SSP of $Al_{1-C}Li_C$ binary alloys. The Hartree (H) dielectric function [8] is purely static and it does not include exchange and correlation effects. Taylor (T) [9] has introduced an analytical expression for the local field correction function which satisfies the compressibility sum rule, exactly. The Ichimaru-Utsumi (IU) local field correction function [10] is a fitting formula for the dielectric screening function of the degenerate electron liquids at metallic and lower densities, which accurately reproduces Monte-Carlo results and satisfies the self consistency condition in the compressibility sum rule and short range correlations. Therefore, Hartree (H) dielectric function [8] gives qualitative agreement with experimental data [2, 3] with EMC model potential and is found suitable in the present case.

On the basis of Ichimaru-Utsumi (IU) local field correction function [10], Farid et al. (F) [11] and Sarkar et al. [12] have given a local field correction function. Hence, Farid et al. (F) [11] function represents same characteristic nature like Ichimaru-Utsumi (IU) local field correction function [10]. The SSP computed from Sarkar et al. [12] local field correction are found in qualitative agreement with available experimental data [2, 3].

According to Matthias' rules [17, 18], $Al_{1-C}Li_C$ binary alloys having $Z < 2$ do not exhibit superconducting nature. Hence, the presently studied alloys are non-superconductors. In the present case, however, they exhibit superconducting nature correctly. When we go from $Z = 1.00$ to $Z = 1.21$, the electron-phonon coupling strength λ changes with lattice spacing a. Similar trends are also observed in the values of T_C for most of the $Al_{1-C}Li_C$ binary alloys. Hence, a strong dependency of the SSP of the $Al_{1-C}Li_C$ binary alloys on the valence Z is found.

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, it plays a decisive role in weak coupling superconductors, i.e. those substances which are at the boundary dividing the superconducting and non-superconducting 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 $Al_{1-C}Li_C$ binary alloys, which confirms the applicability of the model potential. The theoretically observed values of SSP are not available for most of the $Al_{1-C}Li_C$ binary 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.

References

[1] J. Bardeen, L. N. Cooper, J. R. Schrieffer, *Phys. Rev.*, **108**, (1957), 1175.

[2] M. N. Ou, T. J. Yang, B. J. Chen, Y. Y. Chen, J. C. Ho, *Solid State Commun.*, **142**, (2007), 421.

[3] V. V. Pustovalov, N. V. Isaev, V. S. Fomenko, S. E. Shumilin, N. I. Kolobnev, I. N. Fridlyander, *Cryogenics*, **32**, (1992), 707.

[4] Aditya M. Vora, *Physica* C, **468,** (2008), 937; *Turkish J. Phys.*, **32**, (2008), 199; *Turkish J. Phys.*, **32**, (2008), 219.

[5] Aditya M. Vora, *J. Phys. Chem. Sol.*, **69**, (2008), 1841.

[6] Aditya M. Vora, *Comp. Mater. Sci.*, **40**, (2007), 492.

[7] N. W. Ashcroft, *Phys. Lett.*, **23**, (1966), 48.

[8] W. A. Harrison, *Pseudopotentials in the Theory of Metals*, W. A. Benjamin, Inc., New York (1966).

[9] R. Taylor, *J. Phys. F: Met. Phys.*, **8**, (1978), 1699.

[10] S. Ichimaru and K. Utsumi, *Phys. Rev. B*, **24**, (1981), 3220.

[11] B. Farid, V. Heine, G. E. Engel and I. J. Robertson, *Phys. Rev. B*, **48**, (1993), 11602.

[12] A. Sarkar, D. S. Sen, S. Haldar and D. Roy, *Mod. Phys. Lett.*, **B12**, (1998), 639.

[13] W. L. McMillan, *Phys. Rev.*, **167**, (1968), 331.

[14] W. H. Butler, *Phys. Rev. B*, **15**, (1977), 5267.

[15] C. Kittel, *Introduction to Solid State Physics*, 7^{th} Ed., John Wiley & Sons, Inc., Singapore (1996).

[16] Aditya M. Vora, *Physica C*, **458**, (2007), 21.

[17] B. T. Matthias, *Progress in Low Temperature Physics*, Ed. C. J. Gorter, Vol. 2. (North Holland, Amsterdam, 1957).

[18] B. T. Matthias, *Physica*, **69** (1973), 54.