

Theoretical study of pressure dependence of superconducting state parameters of alkali metals lithium and sodium using pseudopotential

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Abstract

Theoretical calculation of superconducting state parameters (SSPs) like electron-phonon coupling strength (λ), Coulomb pseudopotential (μ^*), transition temperature (T_C), effective interaction strength (N_0V) and isotopic effect parameter (α_I) of alkali metals Li and Na have been carried out in the framework of pseudopotential theory. Presently computed SSPs are found to be in good agreement with other reported results. Further, the dependence of SSPs on pressure and hence compressed volume has also been investigated by including the volume dependence of Fermi momentum (k_F), Debye temperature (θ_D) and phonon frequency. It is found that μ^* very feebly depends on compression in volume. The compressed volume at which Coulomb repulsion and attractive electron-phonon interaction are equal is known as critical volume and the corresponding pressure is known as critical pressure. At critical volume, transition temperature and effective interaction strength become zero. It is observed that the results of critical volume predicted by different approaches are in good agreement.

Keywords: transition temperature, superconductor, pseudopotential, alkali metals, critical volume

1. INTRODUCTION

The monovalent alkali metals are free electron systems in which s and p conduction electrons are far away from d and f levels [1, 2]. The Fermi surfaces of alkali metals are spherical and very close to the free electron sphere [2]. In these metals, electron-ion scattering can be described by pseudopotential as there is a very weak electron-ion scattering [1, 2]. Moreover, the electron density at the Fermi surface is low in these metals. Thus, alkali metals are non-superconductors at ambient pressure excluding Li and Cs which are found to be superconducting under pressure [2]. Various theoretical studies predicted that Li exhibits superconductivity at very low temperature which is in the range of 1 K to a few mK [1, 3-7]. A recent experimental study did not find any evidence of superconductivity in Li above 100 μ K at ambient pressure [8]. It is also observed during the literature survey that Li and Cs have exceptional behaviour among alkali metals as their superconductivity does not destroy with increasing pressure [2, 9]. Such complicated behavior of alkali metals motivated us to investigate the superconducting behaviour of both Li and Na which behave differently under pressure.

During literature survey, it is observed that pseudopotential theory is found to be successful in the study of superconducting behaviour of materials [10-19].

It is also found during literature survey that only few attempts have been made to study effect of pressure on superconducting behaviour of materials using pseudopotential framework [10-13]. It is well established fact that theoretical study based on density functional theory (DFT) is more accurate as compared to pseudopotential theory. But, DFT based calculation, especially computation of μ^* and hence other SSPs are computationally expensive and complicated to implement as suggested by Szczesniak and Duraski [20]. Such fact encouraged us to use an alternative simple method based on pseudopotential theory that involves valence electrons only.

In the present study, the pseudopotential due to Fiolhais et al. [21, 22] that is an improved version of stabilized jellium or structureless pseudopotential has been used to study the SSPs and their pressure dependence of Li and Na. Formulation of the pseudopotential is based on the fact that the electrostatic potential due to the positive background of the jellium model represents long range potential and short-range part of the potential is represented by a constant that is used to achieve equilibrium at observed bulk valence-electron density [21, 22]. These interactions are incorporated by stabilized jellium or structureless pseudopotential. The pseudopotential has two adjustable input density parameters namely: the radius of the sphere containing one electron- R_S which describes equilibrium average valence electron and valence-Z [21, 22]. This

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pseudopotential is found to be successful in the study of void and cluster properties of simple metals. On the other hand, it is also observed that bulk modulus and its pressure derivative for the polyvalent metals studied by this pseudopotential are not good where crystal structure plays an important role [21, 22].

Looking to such shortcoming, Fiolhais et al. [21, 22] as a refinement, proposed a structured electron ion pseudopotential having an additional third input parameter N_{int} that is related with bulk modulus along with R_S and Z [21, 22]. N_{int} is the equilibrium number of valence electrons in the interstitial region that describes density on the surface of the Wigner–Seitz cell. The pseudopotential has successfully been used to study binding energy, bulk moduli and pressure derivatives of bulk moduli by using second order perturbation theory. The results of bulk moduli computed by using this pseudopotential are found to be better than results obtained by using first principal nonlocal norm conserving pseudopotentials. Therefore, this pseudopotential can be used as an alternative method of first principal nonlocal norm conserving pseudopotentials to study SSPs.

The pseudopotential used in the present study has two adjustable parameters: the core decay length R and a positive parameter α . Two set of parameters namely universal and individual are determined by the authors using different approaches. During determination of the universal set of parameters, authors have minimized binding energy at observed value of density parameter R_S and valence Z so that N_{int} is equal to its uniform electron gas value [21, 22]. On the other hand, the individual set of parameters are determined by using actual value of N_{int} , R_S and Z [21, 22]. Authors have computed the first zero of the pseudopotential form factor using individual and universal set of parameters and it is observed that individual set of parameters gives results that are closer to the conventional values. Pollack et al. [23] suggested that the pseudopotential may be termed as density based because it describes the density of electrons outside the core. They have studied lattice dynamics, elastic moduli and liquid metal resistivity of simple metals using this pseudopotential with good degree of success. The pseudopotential is also found to be successful for the study of liquid state properties of alkali and alkaline earth metals [24-26]. Further, the pseudopotential has been used to study thermodynamic properties of metals by Bhatt et al. [27-29] at extreme environment (high temperature and high pressure). They also pointed out that individual set of parameters are better and transferable at extreme environment. Recently, the pseudopotential, with its individual set of parameters is further extended to study pressure dependence of SSPs of some polyvalent metals and alloys successfully [10-12].

Though, DFT based ab-initio methods are reliable and accurate, use of local pseudopotential is also worthwhile due to its computational simplicity, physical transparency, ability to reproduce physical properties of materials with good degree of success and suitability for the use of density functional approximations [21-23].

Encouraged by such facts, we have carried out study of Superconducting state parameters (SSPs) such as electron-

phonon coupling strength (λ), Coulomb pseudopotential (μ^*), transition temperature (T_C), effective interaction strength (N_0V) and isotopic effect parameter (α_l) of Li and Na as a function of compressed volume by using the well-established local form of the pseudopotential due to Fiolhais et al [21, 22].

2. THEORY

Following equation has been used to compute electron-phonon coupling strength- λ [10, 11].

$$\lambda = \frac{12m^*Z}{16M(\omega^2)} \int_0^2 x^3 |V(x)|^2 dx \quad (1)$$

In equation (1), m^* , M and $\langle\omega^2\rangle$ represent specific heat mass, ionic mass and square of average phonon frequency respectively. $V(x)$ is screened pseudopotential with $x = q/k_F$. Here, k_F is the Fermi wave vector and q is the change in electron wave vector on the Fermi Surface. The form of the pseudopotential used in the present study has two adjustable parameters- α and R that can be found in ref [21]. Authors have suggested two set of parameters, namely universal and individual. We have used individual set of parameters [22] (shown in Table 1) because it is found to be good working for the study of the physical properties of metals and alloys [10-12, 27-29]. The exchange and correlation function due to Hubbard and Sham [30, 31] has been used to screen the pseudopotential.

Theoretically calculated longitudinal and transverse phonon frequencies (ω_L and ω_T) of Li and Na [23] using the same pseudopotential have been used to find $\langle\omega^2\rangle$ [1].

$$\langle\omega^2\rangle = \left(\frac{\omega_L + \omega_T}{2}\right)^2 \quad (2)$$

Following equation has been used to compute Coulomb pseudopotential μ^* [1, 10, 11].

$$\mu^* = \frac{\mu}{1 + \mu \ln\left(\frac{E_F}{k_B \theta_D}\right)} \quad (3)$$

Here E_F is Fermi energy while θ_D is Debye temperature. μ is given by Following equation.

$$\mu = \frac{m_b}{\pi k_F} \int_0^2 \frac{dx}{x \varepsilon(x)} \quad (4)$$

The Debye temperature- θ_D has been obtained by $\hbar\omega = k_B \theta_D$. The band structure density of mass- m_b at Fermi surface has been computed by using following equation [1].

$$m_b = m^*/(1 + \lambda) \quad (5)$$

Superconducting transition temperature- T_C , effective interaction strength- N_0V and isotopic effect parameter- α_l have been calculated by following equations [1, 10, 11].

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

$$N_0V = \frac{\lambda - \mu^*}{1 + \frac{10}{11}\lambda} \quad (7)$$

$$\alpha_l = \frac{1}{2} \left[1 - \left(\mu^* \ln \frac{\theta_D}{1.45 T_C}\right)^2 \frac{1+0.62\lambda}{1.04(1+\lambda)}\right] \quad (8)$$

Further, SSPs as a function of compressed volume (and hence pressure) have been studied by including volume dependence of physical quantities ω , θ_D , E_F , k_F and $V(q)$. Volume dependence of phonon frequency and Debye temperature are incorporated by relations $\omega = \omega_0 \left(\frac{\Omega}{\Omega_0}\right)^{-\gamma_G}$ and $\theta_D = \theta_{D0} \left(\frac{\Omega}{\Omega_0}\right)^{-\gamma_G}$ respectively [10-13]. Here

subscript 0 represents variables at ambient condition.

The variation of Fermi-momentum- k_F is considered by following equation [10-13]

$$k_F = \frac{k_{F0}}{3} \left(4 - \frac{\Omega}{\Omega_0} \right) \quad (9)$$

Coulomb pseudopotential μ^* as a function of compressed volume has been computed using volume dependence of Fermi-momentum- k_F , phonon frequency - ω and Debye temperature- θ_D . Volume dependent results of λ and μ^* are used to compute volume dependence of other SSPs such as T_C , N_0V and α_I .

The Gruneisen parameter- γ_G has been considered as independent of volume as suggested in literature [13].

3. RESULTS AND DISCUSSION

Table 1 lists the input data and pseudopotential parameters of alkali metals Li and Na used in the present study.

Presently computed results of SSPs are tabulated in Table 2 along with available experimental and other theoretical results. The results of SSPs obtained in the present study are found to be in the range of other reported results except α_I of Na. In conventional low T_C superconductors, α_I decreases with a decrease in T_C [35, 36]. Even the negative value of α_I i.e inverse isotopic coefficient may be obtained for superconductor having T_C less than 1K [36]. Thus, the negative value of α_I for both the metals is expected as T_C of both the metals is very small. But the computed result of α_I of Na is very small (see Table 2). It may be due to negligibly small T_C (0K [14]) of Na.

It is well known that superconductivity in metals arises due to interaction between electrons and lattice vibrations (phonons). Phonon - induced attractive electron-electron interaction- λ should dominate over electron-electron Coulomb repulsion- μ^* for metallic superconductors [1, 18, 19].

It is also well-established fact that there is broadening of energy bands and reduction in energy gaps when atoms come closer to each other [2].

TABLE 1
INPUT PARAMETERS ALONG WITH PSEUDOPOTENTIAL PARAMETERS.

	Metal	Li	Na
Input Parameters	Z [32]	1	1
	Ω_0 (au ³) [33]	114.9	254.5
	M(amu) [32]	6.941	22.989770
	m^* [1]	2.20	1.26
	ω_L (THz) [23]	10.34	4.06
	ω_T (THz) [23]	6.19	2.51
	γ_G [34]	0.89	1.31
	α [22]	4.113	3.499
Pseudopotential Parameters	R(au) [22]	0.342	0.494

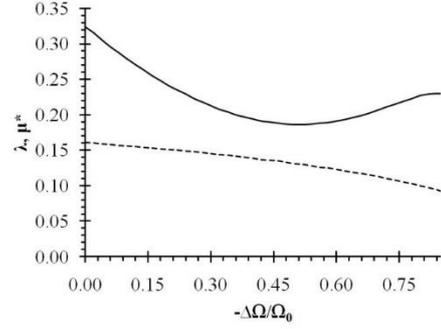


Fig. 1. Electron-phonon coupling strength- λ (solid line) and Coulomb pseudopotential μ^* (broken line) of Li as a function of compressed volume ($-\Delta\Omega/\Omega_0$).

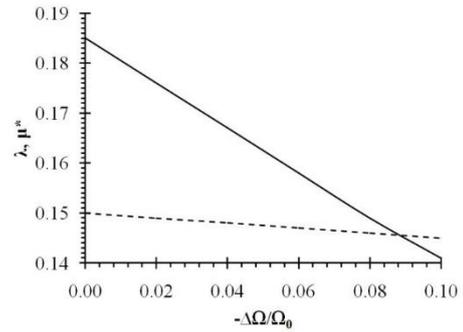


Fig. 2. Electron-phonon coupling strength- λ (solid line) and Coulomb pseudopotential μ^* (broken line) of Na as a function of compressed volume ($-\Delta\Omega/\Omega_0$).

TABLE 2
SUPERCONDUCTING STATE PARAMETERS (SSPs) OF Li AND Na. EXPERIMENTAL RESULTS OF T_C ARE SHOWN IN PARENTHESES.

Metal	SSPs	Present	Others
Li	λ	0.324	0.56[1], 0.53[1], 0.37[1], 0.21[14], 0.45[15], 0.11[16], 0.2630 [17], 0.3892[17], 0.4137[17], 0.4143[17], 0.3495[17]
	μ^*	0.161	0.18[1], 0.17[14], 0.23[15], 0.17[16], 0.1671[17], 0.1876[17], 0.1905[17], 0.1909[17], 0.1804[17]
	T_C (K)	0.007539 (0.08[14], <100X10 ⁻⁶ [8])	1.5[1], 1.1[1], 0.015[1], 1.06 X 10 ⁻²⁶ [14], 0.015[15], 2.68X10 ⁻¹⁹ [16], 0.0000[17], 0.0236[17], 0.0528[17], 0.0526[17], 0.0050[17]
	N_0V	0.126	0.035[14], 0.131[15], -0.05[16], 0.0774[17], 0.1490[17], 0.1622[17], 0.1623[17], 0.1284[17]
	α_I	-0.745	-4.019[17], -0.790[17], -0.602[17], -0.609[17], -1.143[17]
	λ	0.185	0.15[1], 0.19[1], 0.23[1], 0.1608[14], 0.16[15], 0.27[16], 0.2483[17], 0.3970[17], 0.4287[17], 0.4297[17], 0.3470[17]
Na	μ^*	0.150	0.16[1], 0.16[14], 0.18[15], 0.16[16], 0.1621[17],

		0.1825[17], 0.1857[17], 0.1754[17]	0.1853[17], 0.0206[17], 0.0515[17], 0.0517[17], 0.0031[17]
T_C (K)	7.484×10^{-29} (0.0[14])	1.25×10^{-12} [16], 0.0206 [17], 0.0517 [17], 0.0031 [17]	6.88×10^{-08} [17], 0.0515 [17], 0.0031 [17]
N_0V	0.030	0.0007[14], 0.09[16], 0.1576[17], 0.1754[17], 0.1304[17]	-0.017[15], 0.0704[17], 0.1752[17], 0.1304[17]
α_l	-48.801	-4.7344[17], 0.356[17], 0.963[17]	-0.548[17], -0.358[17], -

This reduces the electron density of states at the Fermi surface. It is important to point out that electron-phonon coupling strength decreases under pressure as the lattice becomes stiffer due to decrease in lattice spacing which causes a change in volume and phonon frequencies [2]. Thus, superconductivity must be destroyed in simple metals with application of high pressure. But Li exhibits exceptional behaviour as its superconductivity persists with increasing pressure [2, 9]. Fig. 1 and 2 present electron-phonon coupling strength- λ and Coulomb pseudopotential- μ^* of Li and Na respectively as a function of compressed volume ($-\Delta\Omega/\Omega_0$). From Fig. 1, it seems that λ is more than μ^* for Li in whole compression range and hence pressure cannot destroy its superconductivity. It is also observed for Li (see Fig. 1) that, initially, λ decreases and then starts increasing with increasing pressure and never becomes equal to μ^* . Though, with increasing pressure, due to broadening of energy bands and reduction of energy gaps along with increasing lattice stiffening causes decrease in the electron-phonon coupling strength and hence superconductivity becomes weaker in simple metals [2] but Li shows unusual behaviour possibly due to the following facts. Schilling [2] pointed out that alkali metals Cs and Li behaves like superconductor under sufficiently high pressures. Schilling, in his study, [2] quoted study of Boettger and Trickey [37] who concluded that under strong compression, sizeable *narrowing* of the bands near the Fermi surface occurs. Schilling [2] also noted the exceptional behaviour of Li found in *ab initio* studies [38, 39] which conclude that the Fermi surface of Li becomes increasingly anisotropic at moderate pressure. It is also important to point out that the *d*-bands play no role in Li and only a minor role in Na since they are located relatively far above the Fermi level [2]. As 1s electron core of Li is relatively small, partial overlapping is evident at sufficiently high pressure [2, 40].

But in case of Na, at $-\frac{\Delta\Omega}{\Omega_0} = 0.089$, λ and μ^* are equal and hence superconductivity is destroyed. The compressed volume at which superconductivity destroys is known as critical volume. At critical volume the transition temperature T_C and the effective interaction strength- N_0V which estimates the overall interaction (attractive or repulsive) between pair of electrons becomes zero. Some studies suggests that with increasing pressure, T_C of Li becomes as high as 7 K [41] and 17 K [9] which could not be reproduced in the present study. But the present study confirms that T_C of Li does not reduce to zero with increasing pressure. N_0V of Li as a function of compressed

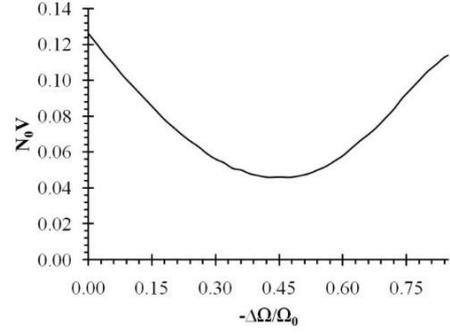


Fig. 3. Effective interaction strength- N_0V of Li as a function of compressed volume ($-\Delta\Omega/\Omega_0$).

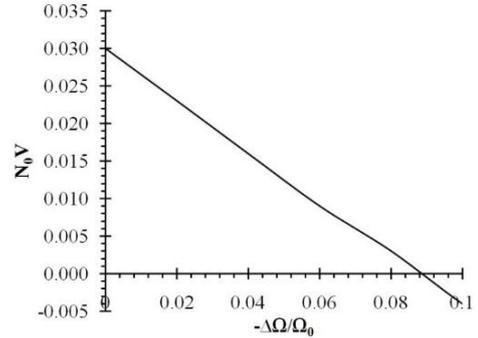


Fig. 4. Effective interaction strength- N_0V of Na as a function of compressed volume ($-\Delta\Omega/\Omega_0$).

volume is shown in Fig. 3 which suggests that N_0V never becomes zero under pressure as attractive potential dominates over repulsive potential in the whole compression range of study.

Volume variation of N_0V of Na is shown in Fig. 4 which suggests that at $-\frac{\Delta\Omega}{\Omega_0} = 0.089$, N_0V becomes zero. The present study also confirms that T_C of Na becomes zero at $-\frac{\Delta\Omega}{\Omega_0} = 0.04$. Critical volumes ($-\frac{\Delta\Omega}{\Omega_0}$) of Na obtained by different approaches used in the present study are 0.089 and 0.04 which are in reasonably good agreement with each other. We could not compare these results due to unavailability of experimental or other theoretical results. Thus, these results may be considered as prediction.

4. CONCLUSION

It is a well-known fact that strong coupling superconductors are well describes by the pseudopotential theory. The present study leads to make a conclusion that the local form of the pseudopotential can also be used successfully to investigate superconducting behavior of weak coupling superconductors not only at ambient pressure but at high pressure also. Present study confirms that the pseudopotential used is transferable to other environment (high pressure) as no fitting or refitting of pseudopotential parameters has been done during course of calculation. Finally, we conclude that present approach may be extended to understand the superconducting properties of remaining metals, metallic alloys and glasses at ambient as well as high pressure.

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