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Superconducting State Parameters for Alkaline Earth Metals Using first Principle Pseudopotentials

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Abstract

In the present communication, comparative study of superconducting state parameters [Electron Phonon coupling strength (λ), Coulomb pseudopotential (μ), Transition temperature (Tc), Isotope effect exponent (α) and Effective interaction strength (N_0V)] have been carried out using Harrison's first principle pseudopotential and non local pseudopotential due to Moriarty for alkaline earth metals (Ca, Sr and Ba). Our computed results are well compared with those obtained from non local as well as local pseudopotentials. It has been observed that for the computation of such parameters, first principle pseudopotentials are necessary and generate accurate results. Both the pseudopotentials used in the present study, are derived from different philosophies and give better understanding in comparison with local ones. The non local pseudopotentials provide better understanding of the highly sensitive physical properties.*

Keywords: First principle pseudopotentials, superconducting state parameters, alkaline earth metals.

Introduction

BCS theory have accomplished all the aims of superconductivity- which is very dynamic and vibrant area in the field of research in condensed matter physics with exploring technology and increasing demand of sophisticated novel materials [1-7]. Though one of the basic aim, i.e. calculation and prediction of superconducting transition temperatures T_C depends sensitively on the normal state properties of materials. The accurate calculations of T_C are not available. In recent years, much has been added to our understanding of these normal state properties & reliable calculations of T_C can now be attempted [1-12]

According to Moriarty [13] the fcc-bcc phase transitions in calcium and strontium can be understood in terms of the generalized pseudopotential theory. Many workers have successfully used pseudopotential theory to calculate SSPs of metals, alloys and metallic glasses and pressure derivative of Tc [1-12]. They have used different forms of pseudopotentials (local & non-local) with different exchange and correlations. During literature survey, we observed that, the comprehensive study of properties (static, dynamic and electronic) of Alkaline Earth metals using local and non-local pseudopotentials is very rare

[8, 9, 10]. Local model pseudopotentials are very easy computationally and contain easily understandable concepts. But at the same time requires lot of adjustable parameters in comparison with first principle or non-local pseudopotentials. Here, in this communication we have used non-local pseudopotentials due to Moriarty to compute SSPs of Alkaline earths (Empty d- band metals) (Ca, Sr and Ba) and we have also computed the same using Harrison's first principle pseudopotential.

Present paper is organized in following manner:

In section-2, we describe theory for computing SSPs with necessary expressions. Section 3 is devoted to results and discussion. Finally, in section-4 we conclude our paper with important remarks.

Theory (Material and Methods)

In the present study, we have used non local pseudopotential due to Moriarty [13] and is given by,

$$\langle k+q|w|k\rangle = \langle k+q|w_0|k\rangle + \sum_{d} \frac{\langle k+q|\Delta|\phi_d\rangle\langle\phi_d|\Delta|k\rangle}{(k^2 - E_d)} \qquad (1)$$

The electron-phonon coupling strength λ is computed using [3]

$$\lambda = \frac{12 m^* Z^*}{M\langle\omega^2\rangle} \int_0^2 x^3 \, |V(x)|^2 \, dx \qquad (2)$$

In above equation, m* is effective mass, M is mass of ion, $x=q/k_f$, where k_f is the Fermi wave vector, V(x)

is a screened pseudopotential form factors and $\langle\omega^2\rangle$ is an averaged square of phonon frequency.

There are two ways to find $\langle w^2\rangle$,

(1) $\langle\omega^2\rangle = (\omega_L+\omega_T)/2$

(2) $\langle\omega^2\rangle=(k_B\Theta_D)^2$. Where, k_B is Boltzmann constant and Θ_D is Debye temperature at zero degree K.

In the present calculation, we have used 2nd approach.

Coulomb pseudopotential is given by [3],

$$\mu^* = \mu \frac{\square}{1+\mu \frac{\ln k_f^2}{k_B\Theta_D}} \tag{3}$$

Where, μ is taken from Gajjar et al [3].

Transition temperature [3],

$$Tc = \frac{\Theta_D}{1}.45 \exp\left[\frac{-1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right] \tag{4}$$

Isotope effect exponent [3],

$$\alpha = \frac{1}{2}\left[1-\left(\frac{\mu^*\ln\Theta_D}{1}.45Tc\right)^2 \frac{1+0.62\lambda}{1.04(1+\lambda)}\right] \tag{5}$$

Effective interaction strength [5],

$$N_0V = \frac{\lambda-\mu^*}{1+\frac{10}{11}\lambda} \tag{6}$$

Results and Discussion

Table: Superconducting state parameters for alkaline earth metals

Metals	SSPs	Moriarty	Harrison	Others
Ca	λ	0.1280	0.1303	0.11[10], 0.22[8], 0.28[8]
	μ*	0.15696	0.15696	0.20[10], 0.16 [8]
	Tc	$321.0841*10^{12}$	$17.32996*10^{-12}$	$5*10^{-5}$ [8]
	α	-9.6354	-9.5882	
	NoV	-25.9414	-23.8821	-0.057[10]
Sr	λ	0.0818		0.19 [8]
	μ*	0.1472		0.16 [8]
	Tc	102.9569		
	α	-1.9124		

	NoV	-0.608732		
Ba	λ	1.12956	0.09365	0.14 [8]
	μ*	0.1269	0.1269	0.15 [8]
	Tc	$399.8436*10^{67}$	$11.0924*10^{-7}$	
	α	-179.5508	-0.4976	
	NoV	2.3797	-30.6413	

Graphs for Ca, Sr and Ba:

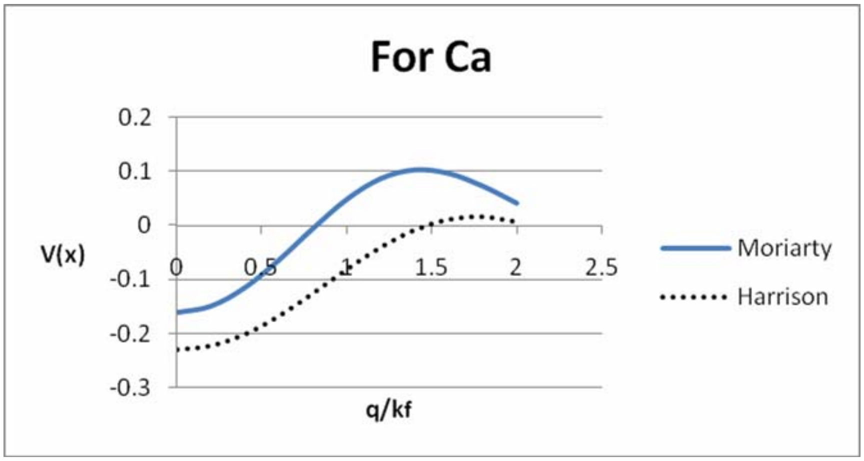

Fig. 1 Comparison of pseudopotential form factors for Ca.

The dotted and continuous lines represent results due to Harrison and Moriarty respectively.

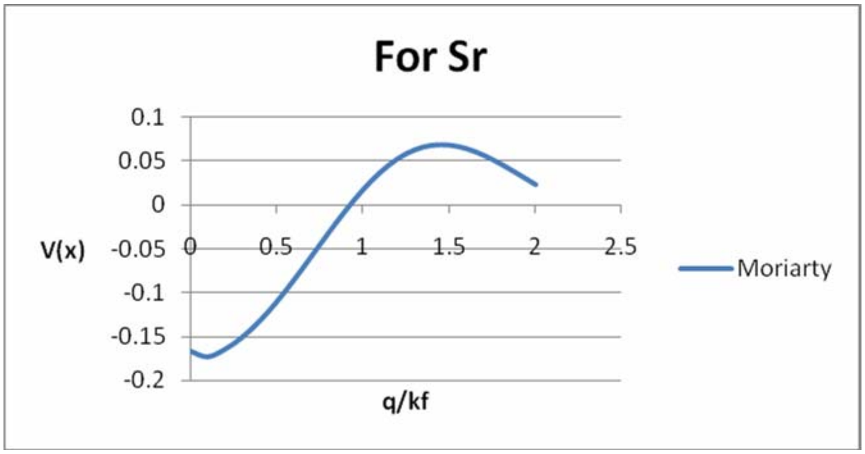

Fig. 2 pseudopotential form factors due to Moriarty for Sr.

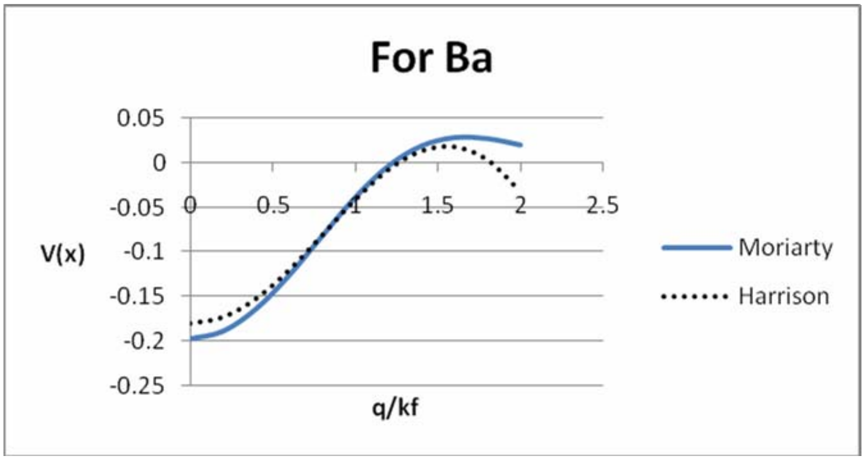

Fig. 3 Same as fig.1 for Ba.

Moriarty [13] has suggested the procedure for constructing much localized d basis states for generalized pseudopotential calculation. In his opinion such d states unlike the d states of free ion or atom, these localized d states do not significantly overlap their neighbors in metal but, also appearing to lead to more accurate estimate of s-p hybridization. Using this concept, he has calculated energy wave number characteristic and pseudopotential form factors which are displayed in figure 1, 2 and 3 with pseudopotential form factor due to Harrison [14]. From the comparison between two types of pseudopotential form factors, we found that, first zero are different. As we know our calculation, based on non-local pseudopotential and the first zero of both the form factors are different, which has serious impact on the calculation of SSPs. In our computation, numerical integrations are evaluated for the values of q, which is smaller than $2k_f$.

Here in the present work both the form factors due to Moriarty and Harrison are generating different numerical values for Ca, they are changing appreciably while in case of Ba for both the form factors the computed values of SSPs are identical. Our computed values for λ for Ca are comparable with Jain and Kachhava [10], while values due to Allen and Cohen [8] are higher, who has used non local empirical pseudopotential. Form factors for Sr are not available due to Harrison so we have calculated using Moriarty only. They are also not comparable with Allen and Cohen [8]. Remaining SSPs for both the sets of pseudopotential form factors are displayed in Table 1. Here, we would also like to point out, how we are differing from other theoretical computations.

Allen and Cohen (1969) have calculated electron- phonon mass enhancement parameter (λ) and superconducting transition temperature (Tc) for 16-simple metals (Li, Na, K, Rb, Cs, Be, Mg, Zn, Cd, Hg, Al, Ga, In, Tl, Sn, Pb) and alkaline earths (Ca, Sr and Ba) using empirical non local pseudopotentials. They have compared calculated values of λ with values of λ extracted from Tc and with values of enhancement of the density of states at the Fermi surface as measured by the low-temperature specific heat. Excellent agreement is found for the divalent hexagonal metals, using empirical nonlocal pseudopotentials. Satisfactory agreement is found for the divalent hexagonal metals, using empirical nonlocal pseudopotentials. Jain and Kachhava [10] have calculated SSPs (λ- the electron-phonon interaction parameter, μ*-Coulomb pseudopotential, Z_0- the quasi-particle mass (or energy) renormalization parameter N_0V- the effective interaction strength, Tc- transition temperature and α- isotope effect exponent) in case of both superconductors and non superconductors (Li, Na, K, Rb, Cs, Mg, Be, Zn, Al, Sn, Pb). He has used Harrison's two parameter (β and r_c) pseudopotential. β and r_c are obtained by fitting the form factors to those obtained by Animalu and Heine (1965) using the model pseudopotential of Heine and Abrenkov.

Conclusion

We would like to conclude present work with following important remarks:

(1) The non-local pseudopotential is providing better understanding in comparison with local pseudopotential for the study of SSPs.

(2) The study of pressure dependence of SSPs for metals as well as metallic glasses should be carried out with nonlocal pseudopotentials. The strong reason behind this is that in case of local pseudopotentials, the parameters adjusted at room temperature may or may not describe pseudopotential form factors accurately at higher pressure. In such circumstances, one cannot justify the use of local pseudopotential and non-local pseudopotentials are more accurate and precise.

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