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Pressure Dependence of the Superconducting State Parameters of Aluminium: A Pseudopotential Approach

N. Vora[1]*, P. Kumar[2], N. K. Bhatt[3], P. R. Vyas[1] and V. B. Gohel[1]

[1]Department of Physics, School of Science, Gujarat University, Ahmedabad - 380009, Gujarat, India.
[2]Department of Science & Humanities, Government Polytechnic, Gandhinagar - 382024, Gujarat, India.
[3]Department of Physics, M. K. Bhavanagar University, Bhavanagar - 364001, Gujarat, India.

ABSTRACT

Comparative study of superconducting state parameters (SSPs), such as electron-phonon coupling strength (λ), Coulomb pseudopotential (μ*), critical temperature (T_c), effective interaction strength (N_0V) and isotopic effect parameter (α) and pressure dependence of SSPs have been carried out in the BCS-Eliashberg-McMillan framework for aluminium by using parameter free form of Ashcroft's empty core (AEC) pseudopotential and energy dependent Ashcroft's empty core (EAEC) pseudopotential. Critical volume is also predicted at which λ=μ* where T_c and N_0V becomes zero. Present results are compared with available experimental as well as other theoretical results and it is found that EAEC pseudopotential is better than AEC pseudopotential for the study of SSPs and their pressure dependence.

KEYWORDS: superconducting state parameters, critical volume, pseudopotential.

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***Corresponding Author**

Nupur Vora

Department of Physics,

School of Science,Gujarat University,

Ahmedabad - 380009,

Gujarat,India.

Email:nupurvora94@gmail.com

INTRODUCTION

Research in Superconductivity has increased many folds during last several years due to increase in demand of novel materials which are required in many sophisticated technological applications. During literature survey, we observed that pseudopotential theory has proven itself a powerful tool to investigate various physical properties of materials successfully[1-3]. Many theoretical studies using different methods have also been reported in literature to investigate SSPs of metals, alloys and metallic glasses[4-12]. Theoretical studies of pressure dependence of SSPs have also been carried out to describe effect of compression in volume[13-14].Encouraged by such studies, in the present study, we have computed superconducting state parameters and their pressure dependence of Al to examine superiority of very simple parameter free form of EAEC pseudopotential over AEC pseudopotential employing BCS-Eliashberg-McMillan formalism.

THEORY

In the present study, we have used very simple Ashcroft's empty core (AEC) pseudopotential along with energy dependent Ashcroft's empty core (EAEC) pseudopotential[15-16] to carry out theoretical study of SSPs and their pressure dependence for Al. Exchange and correlation function due to Taylor[17] has been used to screen the pseudopotential. The pseudopotential parameter r_c(core radius) has been computed by using $r_c = 0.51R_aZ^{-1/3^2}$. Here, R_a is radius of Wigner-Seitz sphere.

The electron phonon coupling strength (λ) is calculated by following equation[5].

$$\lambda = \frac{12m^*Z}{16Mk_B^2\theta_D^2}\int_0^2 x^3|W(x)|^2dx \qquad (1)$$

In equation (1), $W(x)$ is pseudopotential,m^* is specific heat mass, Z is valency, M is ionic mass, k_B is Boltzmaan constant, $\theta_D$is Debye temperature at 0K and $x = q/k_F$. The Coulomb pseudopotential (μ^*) is calculated by following equation[5].

$$\mu^* = \frac{\mu}{1+\mu ln\left(\frac{E_F}{k_B\theta_D}\right)} \qquad (2)$$

E_F, which appears in equation (2) is Fermi energy and μ is given by[4]$\mu = \frac{m_b}{\pi k_F}\int_0^2 \frac{dx}{x\varepsilon(x)}$. The band structure density of mass at Fermi surface has been denoted by m_b. We have computed m_b using the relation[6]$m^* = m_b(1+\lambda)$..

The superconducting transition temperature, T_c is given by[5] $T_C = \frac{\theta_D}{1.4} exp\left[-\left\{\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right\}\right]$.

The effective interaction strength (N_0V) is computed by[4] $N_0V = \frac{\lambda-\mu^*}{1+\frac{10}{11}\lambda}$.

The isotopic effect parameter (α) is calculated by[4] $\alpha = \frac{1}{2}\left[1-\left(\mu^* ln\frac{\theta_D}{1.45T_C}\right)^2 \frac{1+0.62\lambda}{1.04(1+\lambda)}\right]$.

In the next step of calculation, we have studied volume variation of SSPs by calculating explicit volume dependence of physical quantities θ_D, E_F, k_F and $W(q)$. The volume variations of Debye temperature is computed using relation $\theta_D = \theta_{D0}\left(\frac{V}{V_0}\right)^{-\gamma}$. We have computed the Gruneisen constant-γ using equation described in Ref.[14] which is independent of volume-V.Here subscript 0 denotes corresponding variables at normal volume.

RESULT AND DISCUSSION

Presently calculated results of SSPs of Al are compared with experimental and other theoretical results available in literature. Comparison of present results of T_c with experimental result suggests that EAEC pseudopotential is better than AEC pseudopotential. Allen and Cohen[6] have used different pseudopotetials while Vora[7] has used different exchange and correlation functions to calculate SSPs. These theoretical results are tabulated in table 1.Our computed results of SSPs are found to be in good agreement with these results.

Table 1. Comparison of SSPs of Al.

SSP	Present		Other (Theoretical)	Exp.
	AEC	EAEC		
λ	0.454	0.421	0.53[6], 0.52[6], 0.2982[7], 0.4358[7], 0.4542[7], 0.4632[7], 0.3531[7], 0.37[8], 0.38[9], 0.56[10]	
μ*	0.113	0.114	0.14[6], 0.1339[7], 0.1452[7], 0.1468[7], 0.1470[7], 0.1404[7],0.14[10]	
T_c(K)	2.31	1.478	3.0[6],2.6[6], 0.0184[7], 0.7752[7], 1.0044[7], 1.1411[7], 0.1293[7], 0.22[8], 3.653[10]	1.196[6]
N_0V	0.242	0.222	0.1292[7], 0.2081[7], 0.2176[7], 0.2225[7], 0.1610[7], 0.140[8], 0.278[10]	0.175[8]
α	0.373	0.345	-0.238[7], 0.183[7], 0.205[7], 0.218[7], -0.010[7], 0.37[8], 0.255[10]	

Motivated by such good agreement of presently obtained results of SSPs with experimental and other theoretical results, the present model is extended to investigate pressure and hence volume dependence of SSPs. Critical volume is obtained by satisfying condition $\lambda = \mu^*$where T_c and N_0V are

zero. The SSPs $\lambda$and μ^* of Al as a function of compressed volume are shown in figure 1.Intersection of λ and μ^* curves gives critical volume which is shown in table 2. The transition temperatures of Al as a function of compressed volume up to lowest experimentally measurable temperature (of the order of 10^{-3} K[13]) is shown in figure 2.

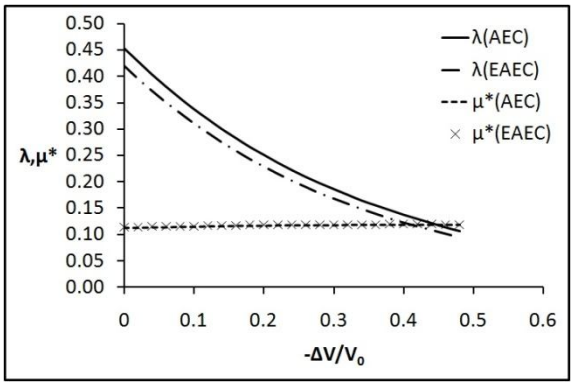

Fig. 1. Volume Variation of λ and μ* for Al.

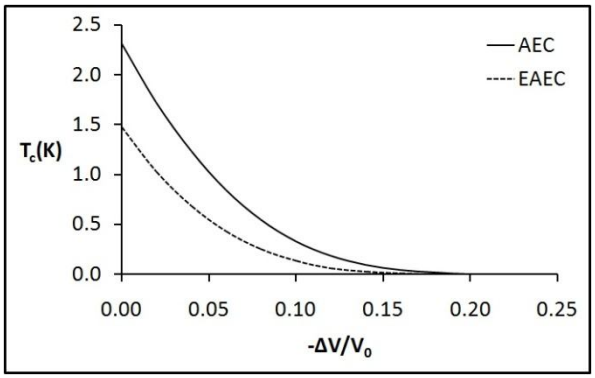

Fig. 2. Volume Variation T_c for Al

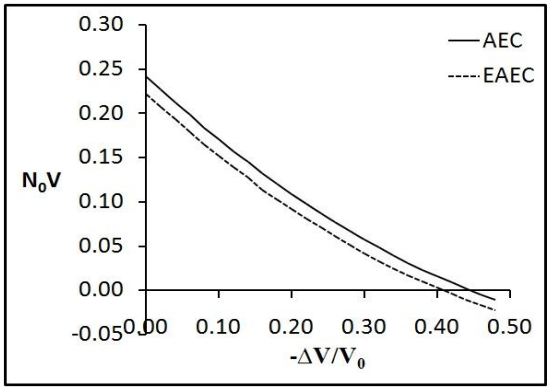

Fig. 3. Volume Variation N_0V for Al

Table 2 Critical Volume of Al

	At which $\lambda = \mu^*$	At which T_c is of the order of 10^{-3} K	At which $T_c = 0$	At which $N_0V = 0$
AEC	0.44	0.22	0.42	0.46
EAEC	0.46	0.18	0.38	0.42
Exp.			0.063[18], 0.163[19]	
Other		0.143[13]	0.329[13]	

Volume corresponding to this temperature is shown in table 2. We have also presented the theoretically computed value of critical volume at which transition temperature becomes zero in table 2. Volume variation of N_0V of Al is presented in figure 3. The volume at which N_0V becomes zero is also tabulated in table 2. It is observed from table 2 that critical volume computed in the present study by different approaches agree well with each other and also with other reported results.

CONCLUSION

Present study confirms that a very simple parameter free form of Energy dependent Ashcroft's empty core (EAEC) pseudopotential is better than Ashcroft's empty core pseudopotential (AEC) for the description of superconducting behavior of metals. From present study we conclude that presently used parameter free form of the pseudopotential can be used to study effect of pressure on the superconducting nature of metallic alloys and glasses.

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REFERENCES

1. Kumar P., Bhatt N. K., Vyas P. R. and Gohel V. B.The Study of AnharmonicProperties and s-p-d Hybridization in Barium at Extreme Environment.Phase Transitions. 2017;90 (12): 1167-1178.
2. Pandya C. V., Vyas P. R., Pandya T. C., Rani N. and Gohel V. B. An Improved Lattice Mechanical Model for FCC Transition Metals. Physica B. 2001; 307: 138-149.
3. Fiolhais C., Perdew J. P., Armster S. Q., MacLaren J. M. and Brajczewska M.Dominant Density Parameter and Local Pseudopotential for Simple Metals. 1995;Phys. Rev. B. 51 (20):14001-14011.
4. Gajjar P. N., Vora A. M. and Jani A. R. Superconducting State Parameters of Metals. Indian J. Phys. 2004; 78 (8):775-780.
5. Yadav J., Rafique S. M. and Kumari S. Impact of Eigenvalues on the pseudopotential calculation of superconducting parameters of metals Ga, Cd and In. Indian J. Phys. 2009; 83 (10):1487-1493.

6. Allen P. B. and Cohen M. L. Pseudopotential Calculation of the Mass Enhancement and Superconducting transition Temperature of Simple Metals. Phys.Rev. 1969; 187(2): 525-538.
7. Vora A. M., Superconducting State Parameters of Amorphous Metals. Physica C. 2007;458: 21-28.
8. Jain S.C. and Kachhava C. M. Pseudopotential Calculation of the Superconducting State Parameters, Transition Temperature and Isotope Effect in Non-Transition Metals. Indian J. Phys. 1981; 55A: 89-95.
9. McMillan W. L. Transition Temperature of Strong-Coupled Superconductors.Phys. Rev. 1968; 167 (2): 331-344.
10. Sharma R.,Sharma K. S. and Daas L. Linearised Screened Pseudopotential and Superconducting State Parameters of a Number of Metals. Phys. Stat. Sol. (b). 1986; 133:701-706.
11. Sharma S., Khan H. and Sharma K. S. Pseudopotential Dependence of Superconducting State Parameters of Be-Al Metallic Glasses. IJPAP. 2003; 41: 301-304.
12. Gajjar P. N., Vora A. M. Patel M. H. and Jani A. R. The Study of Superconducting State Parameters of In-Based Alloys by Pseudopotential. Int. J. Mod. Phys. B.2003; 17 (31&32): 6001-6017.
13. Seiden P. E. Pressure Dependence of the Superconducting Transition Temperature. Phys. Rev. 1969; 179 (2): 458-462.
14. Gupta M., Sharma K. S. and Dass L. Pressure Dependence of the Superconducting State Parameters of Metallic Glass Superconductor $Mg_{70}Zn_{30}$.Pramana J. Phys. 1999;53 (4):765-774.
15. Ashcroft N. W. Electron-Ion Pseudopotentials in Metals. Phys. Lett. 1966; 23 (1): 48-50.
16. Yastrebov L. I. and Katsnelson A. A. Foundations of One-Electron Theory of Solids.Mir Publication: Moscow, 1987.
17. Taylor R. A Simple, Useful Analytical Form of the Static Electron Gas Dielectric Function. J. Phys. 1978; F8 (8): 1699-1702.
18. Smith T. F. and Chu C. W. Will Pressure Destroy Superconductivity?. Phys. Rev. 1967;159(2): 353-358.
19. Brandit N. B. and Ginzburg N. I.Pressure Dependence of the Superconducting Transition Temperature in Zinc. Sov. Phys. JETP. 1966; 23:838-840.