International Journal of Advance Research in Science and Engineering
Volume No 07, Issue No. 01, January 2018
www.ijarse.com
IJARSE
ISSN: 2319 - 8354

Harrison's First Principle pseudopotential approach to study the impact of eigenvalue on electron-phonon coupling strength of alkali metals Li, Na, K and its binary alloys Li-Na, Li-K and Na-K.

Sunil Kumar Chowdhary

T.M. Bhagalpur University, Bhagalpur (Bihar), (india)

ABSTRACT

In this research paper we outlined our findings on impact of the eigenvalue on electron-phonon coupling (e-p coupling) strength of the selected alkali metals Li, Na, K and its binary alloys Li-Na, Li-K and Na-K. In our study we primarily employed Harrison's First Principle [HFP] pseudopotential technique and computed form factors of alkali metals and its binary alloys using different sets of eigenvalue. Further with the help of McMillan formalism the impact of eigenvalues on one of the fundamentally important SSP – e-p couplingstrength, in case of alkali metals Li, Na, Kand its binary alloys Li-Na, Li-K and Na-K, were carried out. Our studies give acceptable results.We also concludes that with choice of suitable eigenvalue the HFP pseudopotential technique can suitably reproduce SSP of metals and alloys.

Key Words-Pseudopotential, SSP, binary-alloy, alkali-metals, electron-phonon.

I.INTRODUCTION

Superconductivity phenomenon is still one of the main themes of solid state physics even after more than one century since its invention. This exciting phenomenon was discovered by H. Kammerlingh Onnes in (1911). With Bardeen, Cooper and Schrieffer (BCS) that bears their name (Bardeen et al., 1957) microscopic theory of superconductivity began. This theory was based on the fundamental theorem (Cooper, 1956) which states that for a system of many electrons at low temperature a weak attraction,which is otherwise negligible, can bind two electrons together with opposite momenta (±k)forming the so called Cooper pair. Eliashberg (1960a, b) was able to derive a full treatment of the pairing interaction and show that phonons do indeed provide the glue which binds a Cooper pair together (at least in a conventional superconductor).

A great number of metals and alloys were discovered that exhibit superconducting property. In addition to recent discoveries of unconventional superconductivity in iron based superconductors Y. Kamihara et al. (2008) K. Ishida et al. (2009) there have been a large number of interesting developments and a surprising large superconducting transition temperature (T_c) of 20K for Li under pressure K Shimizu et al. (2002).The search for new superconductors and their understanding motivate an enormous amount of research work in condensed matter physics either due to the intriguing different mechanisms evolved or the possibility of new technological applications.

All the conventional superconductors are well understood within the BCS theory asphonon mediated pairing of electrons that takes place only between electrons with opposite momenta (±k)and condensation of the resulting Bosonic gas.

The study of e-p interaction has a long and distinguished history but it is only during the past two decades that quantitative and predictive calculation has become possible. First principle calculation of e-p coupling has got an unprecedented verity of application in many areas of condensed matter physics.

The main aim of this paper is to place the study done on impact of eigenvalue on e-p coupling of alkali metals Li, Na and K and its binary alloys Li-Na, Li-K and Na-K. We have used HFP pseudopotential approach Harrison (1966). Also, Faber-Ziman (1965) form-factor for each of the constituents is used to calculate e-p coupling strength by means of HFP pseudopotential technique using well known McMillan formalism (1968).In this studyexchange and correlation of Vaishishta-Singwi (1972) form is employed.

The eigenvalues of the core electrons are one of the basic parameters in HFP pseudopotential theory. The different set of eigenvalues were taken and the influence of eigenvalues on fundamentally important SSP – e-p coupling strength in case of alkali metals Li, Na, K and its binary alloys Li-Na, Li-K and Na-K are studied.

II.THEORY AND FORMALISM

The basis of general quantum theory of superconductivity given by Bardeen, Cooper and Schrieffer (1957). Ziman (1963) suggests that the pseudopotential, originally developed to provide a theory for electronic band structure – a way to find energy eigenvalue ($E_{k)}$, can also be used to describe e-p interaction. McMillan developed BCS theory by the concept of pseudopotential. Allen and Dynes (1975) further developed this concept of pseudopotential for application of binary alloys.

2.1Form Factor:

The form factor w(**k, q**) = <**k**+**q**|w|**k**> is the Fourier transform of crystal potential in the reciprocal lattice. In our present paper the form factor w(**k, q**) of the constituent metals has been derived through the well-known HFP pseudopotential technique.

In fact, the HFP technique has been claimed to be superior to the model potential techniques as no arbitrarily adjustable parameter is introduced and no arbitrary model is proposed. Although the HFP technique is much rigorous than the model potential technique and also free from arbitrariness in choosing a model and its parameter, it lagged behind due to some cumbersome calculations involved. However, this was employed by King and Cutler (1968) and Hafner(1975) along with their co-workers and is still a choice of few researchers.

The non-local screened form factor may be expressed as-

$$w(\boldsymbol{k},\boldsymbol{q}) = \left\{\frac{v_q^{a,b} + v_q^c + v_q^d}{\varepsilon^*(\boldsymbol{q})}\right\} + \left\{\frac{1 - G(\boldsymbol{q})}{\varepsilon^*(\boldsymbol{q})}\right\} v_q^f + W^R \qquad (1)$$

Where, symbols are those of Harrison (1966)viz

$v_q^{a,b}$ = Valance charge and core electron potential

v_q^c = Conduction band – core exchange potential

v_q^d = Conduction electron potential

v_q^f = Screening potential

W^R = Repulsive potential

$\varepsilon^*(q)$ = Dielectric screening function

$$\varepsilon^*(q) = [\{1 - G(q)\}\{\varepsilon(q) - 1\} + 1] \qquad (2)$$

here, $\varepsilon(q)$ is Hartree dielectric function given by

$$\varepsilon(q) = 1 + \frac{2}{\pi k_F \eta^2}\left[1 + \frac{4-\eta^2}{4\eta}\ln\left|\frac{2+\eta}{2-\eta}\right|\right] \qquad (3)$$

Where,

$\eta = q/k_F$ and,

G(q) is the exchange correlation function.

We have used V-S exchange correlation function given as

$$G(q) = A\,[1 - \exp(-B\eta^2)] \qquad (4)$$

V-S exchange correlation satisfies compressibility sum rule and provides a better inter-ionic potential.

Sunil, Sarfraz and, Mehar Khan (2017) has studied the electrical resistivity of Na, K and their alloy for different composition and computed acceptable result in the frame work of optimized model potential theory using Faber-Ziman formulism (1965) and find it quite capable of explaining the electrical resistivity of simple liquid alloys . In our present work also the non-local screened form factor of the alloy is computed by using Faber-Ziman Formalism, given as

$$|w(k,q)|^2 = c_1|w(k,q)_1|^2 + c_2|w(k,q)_2|^2 + 2\,(c_1c_2)^{1/2}\,|w(k,q)_1||w(k,q)_2| \qquad (5)$$

where, c_1 and c_2 are concentration of constituent metals.

2.2e-p coupling strength:

Building on the earlier works of Elieshberg (1960), McMillan (1968) extended the BCS equation.

From McMillan formalism the electron phonon coupling strength is given by –

$$\lambda = \frac{2\int d\omega\alpha^2(\omega)F(\omega)}{\omega}$$

$$= \frac{N(E_F) < I^2 >}{M < \omega^2 >} \qquad (6)$$

Where, F(ω) is the phonon density of state,

M is the atomic mass,

$N(E_F)$ is the spin density of states at E_F

$\alpha^2(\omega)$ is the average of e-p interaction and

$< \omega^2 >$ is the phonon frequency squared averaged McMillan (1968),

and $< I^2 >$ is the electron-phonon matrix element averaged over the Fermi surface.

In pseudopotential approach the average I^2 over the Fermi surface is given by

$$\mathrm{r} < I^2 > = \sum_{v} \int_0^{2k_F} \frac{\left(\in_{qv}, q\right)^2 v_q^2 \; q \, dq}{\int_0^{2k_F} F \; q \, dq}$$

$$= {}^{8}/_{9} \, k_F^2 E_F^2 < V_q^2 > \qquad (7)$$

Where, k_F and E_F are the wave number and Fermi energy, respectively.

A dimensionless average of the pseudopotential is given by

$$< V_q^2 > = \frac{\int_0^{2k_F} v_q^2 q^3 dq}{\int_0^{2k_F} v_0^2 q^3 dq} \qquad (8)$$

From this, the value of λ has been obtained as Sharma et al. (2003)

$$\lambda = \frac{m_b}{4\pi^2 k_F M \, N < \omega^2 >} \int_0^{2k_F} q^3 |w(k,q)|^2 dq \qquad (9)$$

where, w(k, q) is the screened Pseudopotential form factor

M is ionic mass

Z is the valence of the corresponding metallic ions

m_b is the band mass of electron

$< \omega^2 >$ is the average square phonon frequency of metal

q is the momentum transfer

N is the ion number density

We further simplified the expression as below -

As N can be expressed as-

$$N = \frac{1}{\Omega_0} = \frac{k_F^3}{3\pi^2 Z} \qquad (10)$$

Putting the value of N from equation (10) to the equation (9) , we get

$$\lambda = \frac{3 \, m_b \, Z}{4 \, k_F^4 \, M \, < \omega^2 >} \int_0^{2k_F} q^3 \, |w(k,q)|^2 \, dq \qquad (11)$$

Taking , $\eta = \frac{q}{k_F}$ i.e., $q = \eta k_F$ or, $dq = k_F \, d\eta$

As $q = 0$; $\eta = 0$, and, for $q = 2k_F$; $\eta = 2$

Thus, changing the limits, we have

$$\lambda = \frac{3\ m_b\ Z}{4\ \ M\ \ < \omega^2 >} \int_0^2 \eta^3\ |w(k,\eta)|^2\ d\eta \qquad (12)$$

In present work we used this simplified expression for computing the value of λ for alkali metals and alkali-alkali binary alloys.

III.COMPUTATION

The form factor of alkali metals Li, Na, Kof Sunil and Mehar Khan (2017) is used in present work. All the varients with eigenvalue of Herman-Skillman (1963), Hafner (1975) and Clementi (1965) near melting points are used. In this computation exchange and correlation of Vaishishta-Singwi form is employed. Input Values are tabulated in Table-1 below –

Table-1 Input Values

Properties	**Li**	**Na**	**K**
Melting point	453.69 K	373.15	338.15
θ_D	352 K	157 K	59.4 K
Atomic weight (M)	6.94	22.99	39.10
m_b	1.19	1.00	0.94
Z	1	1	1
r_c **a.u**	1.4541	2.0234	2.6370
Atomic volume(Ω_0)	153.3334	278.0259	531.1665
Fermi wave vector(k_F)	0.5780	0.4740	0.3820
Fermi energy(E_F)	4.76	3.20	2.12
V-S constants A	1.00714	1.07783	1.16730
V-S constants B	0.29857	0.28554	0.27051

The form factor of binary alloys Li-Na, Li-K and Na-K is computed from Faber-Ziman (1965) Formalism and plotted below as Fig. 1, 2 and 3 respectively –

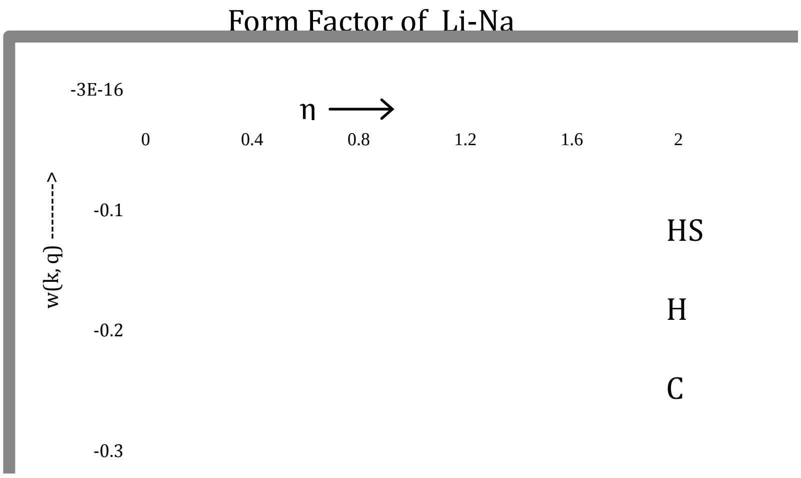

Fig 1: Form Factor of Li-Na with V-S exchange using eigenvalues of Herman-Skillman (HS), Hafner (H) and Clementi (C) near melting point.

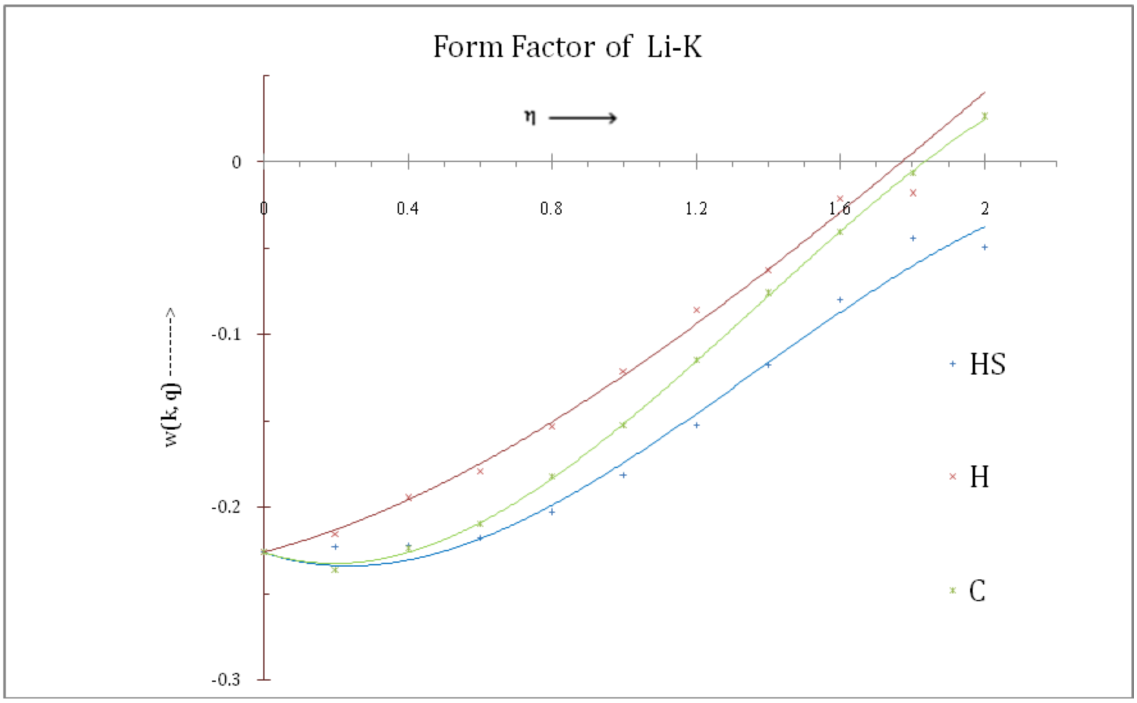

Fig 2: Form Factor of Li-K with V-S exchange using eigenvalues of Herman-Skillman (HS), Hafner (H) and Clementi (C) near melting point.

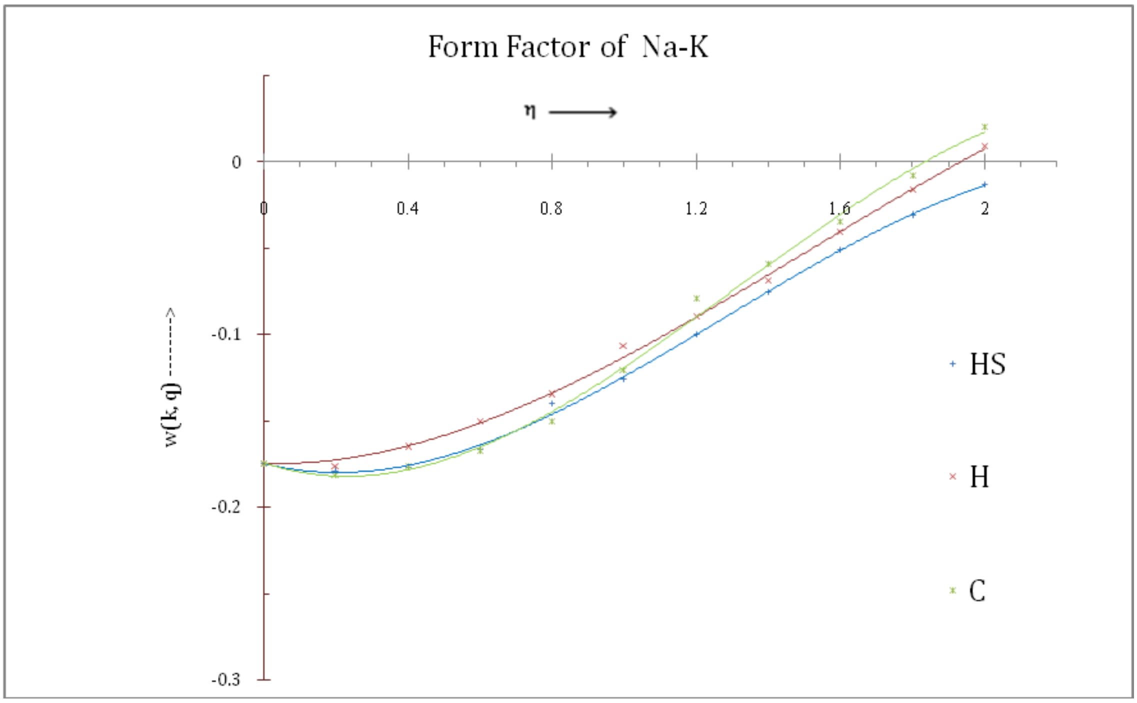

Fig 3: Form Factor of Na-K with V-S exchange using eigenvalues of Herman-Skillman (HS), Hafner (H) and Clementi (C) near melting point.

IV.RESULTS AND DISCUSSIONS

The alkali metals, in particular, are generally believed to be the metals which most closely obey the simple nearly-free-electron model pioneered by Wigner and Seitz (1933). Indeed, their Fermi surfaces are nearly spherical, reflecting the weak electron–ion scattering (pseudopotential). A HFP pseudopotential technique, in terms of electron-ion pseudopotential, is presented for the electron-phonon coupling constant λ. The phonon parameters, needed in the calculation, are characterised by a single average square frequency $<\omega^2>$, which is evaluated after Allen and Cohen (1969). This corresponds to a reduction of $<\omega^2>$ causing an increasing in the electron – phonon coupling strength λ.

We endeavour to discuss the results we obtained for selected alkali metals and the alkali-alkali binary alloys under consideration to the concentration 0f 0.5 for each of the binary constituents i.e., at equal concentration. After which the computed values are compared with the available values from other researchers wherever possible. As stated earlier, Form factor of the alloy is calculated from Faber-Ziman Formalism that has been found fairly suitable, Sunil et al. (2017).

The computed value of λ is placed in Table-2 below. The impact of eigenvalues on the e-p coupling strength can be comprehended from this table. The experimental data of alkali–alkali binary alloys are not available in the literature for further comparison. Also, only little theoretical data for e-p coupling constant for alkali–alkali binary alloys is available. But in the absence of experimental information, such calculations may be considered as one of the guidelines for further investigations either theoretical or experimental.

Table-2: Electron-Phonon Coupling Strength with Eigenvalue of

HS = Herman-Skillman, H = Hafner and C = Clementi

Alkali metals	**Eigenvalue of**	**value of λ**	**Values by other researchers**
Li	**HS**	1.1723	[1.0979, 1.7386, 1.8709, 1.9337, 1.5411]* [0.10, 0.15, 0.45]** [0.11, 0.21] § , [0.37, 0.53, 0.568]##, [1.09, 1.73, 1.87, 1.93, 1.54]#
	H	0.7155	
	C	0.9390	
Na	**HS**	0.3404	[0.2626, 0.4184, 0.4518, 0.4673, 0.3772]* [0.12] *§, [0.27]§, [0.15, 0.19, 0.23, 0.28]¥, [0.26, 0.37, 0.42, 0.45, 0.47]#
	H	0.3435	
	C	0.4160	
K	**HS**	0.4789	[0.3477, 0.5845, 0.6346, 0.6584, 0.5254]* [0.11] §; [0.12, 0.12, 0.145]**; [0.14, 0.22]##; [0.35, 0.53, 0.58, 0.63, 0.66]#
	H	0.3136	
	C	0.3136	
Li-Na	**HS**	1.0376	**Data not available**
	H	0.7819	
	C	0.9712	
Li-K	**HS**	0.8651	**Data not available**
	H	0.5512	
	C	0.6344	
Na-K	**HS**	0.7027	**Data not available**
	H	0.6013	
	C	0.6626	

Vohra (2006) #*Gazzar et al.(2004)* §*Sharma and Sharma (1983)* *§Morel and Anderson (1962)
***Jain et al. (1980)* ##*Allen (1969)* ¥*McMillan(1968)*

V.CONCLUSIONS

HFP pseudopotential technique based on BCS theory and well known McMillan's formalism are used to compute the electron-phonon coupling strength (λ) of alkali metals Li, Na, K and its binary alloys Li-Na, Li-K and Na-K. Different set of eigenvalues is used to observe its impact on the values of λ. As HPF technique and McMillan's formalism are based on various approximation reproduction of exact value is not desired. However, with proper choice of eigenvalues our results are quite acceptable as compared to the values obtained by previous researchers.

Our computation reveals that if the core energy eigenvalues is appropriately chosen the superconducting state parametersare reasonably reproducible by the HFP pseudopotential technique. Similar conclusion has been arrived by other researchers Yadav, Rafique, Prasad and Prasad (2008); Yadav, Rafique and S. Kumari (2009); Chakrabarti (2016); Rafique, Mitra and Shrivastva (1983); Chakrabarti and Shahi (2016) with different superconducting systems.

REFERENCES

[1] H.K. Onnes;*The Superconductivity of Mercury. Leiden Comm.*, 120b, (1911)

[2] J. Bardeen,L.N. cooper and J. R. Schriefeer;*Theory of superconductivity;Phys. Rev., Volume* 108 No. 5 pp. 1175-1186 (1957).

[3] J.M. Ziman; Electrons and Phonons, Oxford Univ Press, London and New York (1963)

[4] G.M. Eliashberg; *JETP*38, 966 (1960a).

[5] G.M. Eliashberg; *JETP*39, 1437 (1960b)

[6] Y. Kamihara, T. Watanabe, M. Hirano and H. Hoson; *J. Am. Chem. Soc.* 130, 3296 (2008)

[7] K. Ishida, Y. Naki and H. Hosono; *J. Phys. Soc. Jpn*. 78, 052001 (2009)

[8] K Shimizu, H Ishikawa, D Takao, T Yagi, K Amaya; *Nature (London)* 419, 597 (2002)

[9] W.A. Harrison; *Pseudopotential in the Theory of Metals, Benjamin, New York* (1966).

[10] T. E. Faber and J. M. Ziman; *Phil. Mag.* 11153 (1965)

[11] Sunil Kr. Chowdhary, M. S. Ahmad, M. Mehar Khan, KIJSET 4(1/A2) 1-16 (2017)

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

[13] P. Vashishta and K.S. Singwi;*Phys. Rev.*, B 6 875 (1972).

[14] P. B. Allen and R. C. Dynes;*Phys. Rev.*, B 12 905 (1975).

[15] G.M. Eliashberg; *JETP*11, 696 (1960).

[16] A. M. Vora; *Supercond.Sci. Technol*. 20, 542 (2007)

[17] Sunil Kr. Chowdhary and M. Mehar Khan, IJARSE6 12 1769-1782 (2017)

[18] F Herman, J Skillman; *Atomic Structure Calculation, Prentice Hall, New Jersey* (1963)

[19] W. F. King and P. H. Cutler, Phys. Lett. A 28, 289 – 290 (1968)

[20] J. Hafner; *J. Phys. F* 5 L150 (1975).

[21] E. Clementi; 1B M. J. Res. and Dev. 9 2 (1965)

[22] P. B. ALLEN and M. L. COHEN, Phys. Rev. 187, 525 (1969)

[23] A. M. Vora; Physica C 450 135–145 (2006)

[24] R. Sharma, K.S. Sharma, Indian J. Pure Appl. Phys. 21 725 (1983)

[25] R. Sharma, K.S. Sharma, Lachhman Dass, Czech. J. Phys. B36 719 (1986)

[26] S.C. Jain, C.M. Kachhava, Indian J. Pure Appl. Phys. 18 489 (1980)

[27] P. Morel, P.W. Anderson, Phys. Rev. 125 1263 (1962)

[28] P.N. Gajjar, A.M. Vora, A.R. Jani, Indian J. Phys. 78 775 (2004)

[29] E. Wigner and F. Seitz, Phys. Rev.43804 (1933).

[30] J. Yadav, S. M. Rafique. U. Prasad, R. S. Prasad; *PCAIJ* 3(2-3) 106 (2008)

[31] J. Yadav, S. M. Rafique. S. Kumari; *Indian J Phys.* 83 1487 (2009)

[32] S. K. Chakrabarti; JOBPCR 3(3) 1-4 (2016)

[33] S. M. Rafique; R.N. Mitra, P.L. Shrivastva; Phys. Stat. Sol. 119 113 (1983)

[34] S. K. Chakrabartiand M. Shahi; SJRMCS 1 36 (2016)