

Theoretical study of pressure dependence of superconducting state parameters of some metals using pseudopotential approach

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In the present theoretical study, we have calculated superconducting state parameters (SSPs) viz; electron-phonon coupling strength (λ), Coulomb pseudopotential (μ^*), critical temperature (T_C), effective interaction strength (N_0V) and isotopic effect parameter (α) of some polyvalent metals (Pb, Ga, In, Sn and Tl) using well-established structured local pseudopotential due to Fiolhais *et al.* (1995). The pseudopotential with its individual set of parameters has been found to be good in predicting transition temperature T_C for all the metals. Looking to such success, we have extended the present model for the theoretical study of pressure dependence of transition temperature T_C using Debye- Gruneisen model. Our predicted critical volumes using different approaches are well agreed with each other and also with other reported findings. Thus, the present model is consistent and better than nonlocal norm conserving pseudopotentials because it is found to be transferable without any kind of adjustment of its parameters along with its simplicity and predictivity.

Keywords: Superconducting state parameters, Pressure dependence, Superconductivity

1 Introduction

Superconductivity is the most complex state of metals. The main aim of study of superconductivity is to understand physics of some metals which behave like superconductor at particular temperature, theoretically or experimentally. It has been observed that valence electrons play a decisive role in the study of transition temperature (T_C)¹⁻³. Theory of superconductivity should explain second order phase transition at critical temperature- T_C . Superconducting transition temperature can be understood with the knowledge of electron energy bands near Fermi-energy, phonon dispersion curves, screened pseudopotential and interaction between electrons.

Multiple phenomenological models have been used to study SSPs (λ , μ^* , T_C , N_0V and α) and their pressure dependence theoretically for metals⁴⁻¹⁵, metallic glasses¹⁶⁻¹⁹ and alloys^{5,13,20-24}. Pseudopotential method, due to its simplicity and predictivity has been used successfully for the comprehensive study of many physical properties in condensed matter physics with good degree of success²⁵⁻²⁷. The pseudopotential has played vital role in the understanding of superconducting behavior of metals⁶⁻¹⁰. Recently,

many researchers have used local form of pseudopotential for the theoretical study of SSPs and hence T_C who have adjusted pseudopotential parameters by different philosophy^{9,10,18}. Such studies are limited to normal volume only. Nonlocal pseudopotentials are more reliable but the study of SSPs using such pseudopotentials is restricted to observed volume (0 K) only^{28,29}. During literature survey, we observed that a few attempts have been made to study pressure dependence of SSPs using pseudopotential. In our opinion, pseudopotential must be determined uniquely in the sense that it can be used at extreme environment (high temperature and high pressure) and also for the comprehensive study of physical properties of metals and alloys. In recent past, such attempts were made by Fiolhais and coworkers^{30,31} who have proposed their local form of the pseudopotential with two sets of parameters called universal and individual. Universal parameters are determined at zero pressure and assuming N_{int} to be its uniform electron gas value. Individual parameters are derived in same way by fitting actual value of N_{int} for each metal. Here N_{int} is the equilibrium number of valence electron in the interstitial region which represents the valency Z and density on the surface of the Weigner-Seitz cell. They have used both sets of parameters for the study of static, electronic and

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lattice mechanical properties with good degree of success. Further, this pseudopotential has been extensively used for the theoretical study of the liquid state properties of alkali and alkaline earth metals³²⁻³⁴. Looking to such success, recently, Bhatt *et al.*³⁵⁻³⁷ have extended this pseudopotential with mean field potential approach to study thermodynamic properties of some simple and polyvalent metals at extreme environment.

Such study encouraged us to use present pseudopotential for the study of SSPs and their pressure dependence. We have carried out study of SSPs using both the sets of parameters. We found that individual set of parameters are better as pointed out by other researchers³⁰⁻³⁷.

2 Theory

We have used following equations for our computational work. Electron-phonon coupling strength, λ is given by⁶:

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

Here m^* is specific heat mass, Z is valancey, M is ionic mass, $\langle\omega^2\rangle$ is average of square of phonon frequency. $V(x)$ is screened ion pseudopotential which is obtained as $\frac{V_{ion}(x)}{\varepsilon(x)}$. Here $\varepsilon(q)$ is dielectric function where electron wave vector q on Fermi-sphere in terms of Fermi-wave vector k_F is given by: $q = xk_F$. The bare ion pseudopotential as suggested by Fiolhais *et al.*³⁰ has following form in q-space:

$$V_{ion}(q) = \left(\frac{8\pi ZR^2}{\Omega} \right) \left[\frac{-1}{[(qR)^2] + \frac{1}{[\alpha^2]}} + \frac{2\alpha\beta}{[(qR)^2 + \alpha^2]^2} + \frac{2A}{[(qR)^2 + 1]^2} \right]$$

Where α and R are pseudopotential parameters. The parameters A and β are written in terms of α as:

$$\beta = \frac{(\alpha^3 - 2\alpha)}{4(\alpha^2 - 1)} \text{ and } A = \left(\frac{\alpha^2}{2} - \alpha\beta \right)$$

There are two different approaches to compute $\langle\omega^2\rangle$. Firstly, $\langle\omega^2\rangle$ can be computed by experimental Debye temperature- θ_D at 0K and secondly $\langle\omega^2\rangle$ is computed by following equation²⁰:

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

Here, ω_L and ω_T are longitudinal and transverse phonon frequencies, respectively. The second input

parameter appearing in Eq. (1) is m^* , the specific heat mass. According to Allen and Cohen⁴, real metals are more complicated because de Hass-van Alphen masses are cyclotron masses which vary from orbit to orbit. Following Allen and Cohen⁴, we have used specific heat mass to compute λ which is defined as the ratio of the linear coefficient of the specific heat to the value would have in a free electron gas of equal density.

Band mass of electron, m_b has been computed using following equation⁴:

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

As pointed out by Allen and Cohen⁴ and also verified by us that band mass of electron (m_b) is not uniquely determined and it is quite sensitive to the choice of the pseudopotential because local and nonlocal pseudopotentials give different values. We have computed m_b using above equation, where m_b is defined as the ratio of the calculated density of states at Fermi-surface to the density of states of the free electron gas.

Coulomb pseudopotential μ^* is calculated by following equation⁶:

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

Here E_F is Fermi-energy, θ_D is Debye temperature, k_B is Boltzmann constant and

$$\mu = \frac{m_b}{\pi k_F} \int_0^2 \frac{dx}{x\varepsilon(x)} \quad \dots (3)$$

In the present study, the equation $\hbar\omega = k_B\theta_D$ is used to calculate Debye temperature θ_D .

Critical temperature, T_C in terms of λ , μ^* and θ_D is defined as⁶:

$$T_C = \frac{\theta_D}{1.4} \exp \left[- \left\{ \frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right\} \right] \quad \dots (4)$$

Following equation is used to calculate effective interaction strength¹⁰, N_0V :

$$N_0V = \frac{\lambda - \mu^*}{1 + \frac{10}{11}\lambda} \quad \dots (5)$$

Isotopic effect parameter, α is written as¹⁰:

$$\alpha = \frac{1}{2} \left[1 - \left(\mu^* \ln \frac{\theta_D}{1.45c} \right)^2 \frac{1+0.62}{1.04(1+\lambda)} \right] \quad \dots (6)$$

Band structure density of states, $N_{b_s}(0)$ is computed by using following equation⁵:

$$N_{bs}(0) = \frac{3\gamma_e}{2\pi^2 k_B^2 (1+\lambda)} \quad \dots (7)$$

Here γ_e is electronic heat capacity coefficient.

Electronic density of states at the Fermi-surface, $N_{fe}(0)$ is obtained by following equation⁵:

$$N_{fe}(0) = \frac{3}{4} \left(\frac{Z}{E_F} \right) \quad \dots (8)$$

Further, we have studied volume variation of SSPs (λ , μ^* and T_C). The Eqs (1) to (6) contain volume dependent quantities (ω , θ_D , E_F , k_F and screened ion pseudopotential $V(q)$). Thus, in order to study pressure dependence (and hence volume dependence) of SSPs, we have calculated explicit volume dependence by calculating volume dependence of physical quantities ω , θ_D , E_F , k_F and $V(q)$. First, using Gruneisen theory by considering Gruneisen parameter γ as independent of volume^{12,14,16,38,39}, the volume variations of phonon frequency and hence Debye temperature are computed using relations $\omega = \omega_0 \left(\frac{\Omega}{\Omega_0} \right)^{-\gamma}$ and $\theta_D = \theta_{D0} \left(\frac{\Omega}{\Omega_0} \right)^{-\gamma}$ respectively. We have computed γ using equation described in Ref. 16. Here subscript 0 denotes corresponding variables at ambient condition.

Now volume variation of λ i.e., $\frac{d\lambda}{d\Omega} = \frac{d\lambda}{dk_F} \cdot \frac{dk_F}{d\Omega}$ can be found by calculating volume variation of Fermi-momentum k_F with respect to volume by using following method. If k_{F0} is the Fermi-momentum at normal volume Ω_0 , then the Fermi-momentum k_F at given volume Ω is given by:

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

In order to calculate volume variation of integrand in Eq. (1), we have calculated volume variation of screened pseudopotential as a product of variation of screened pseudopotential with k_F and volume variation of k_F with respect to volume Ω . Finally, by integrating product of such variations, we get relation between λ (at compressed volume Ω) and λ_0 (at normal volume Ω_0). We have also incorporated the effect of volume dependence of Coulomb pseudopotential μ^* by considering volume variation of Fermi-momentum and Debye temperature with volume. Finally, we obtain Coulomb pseudopotential μ^* at compressed volume (Ω) in terms of Coulomb pseudopotential μ_0^* at normal volume (Ω_0). Using all such volume dependent quantities (λ , μ^* and θ_D),

pressure and hence volume dependence of T_C can be found using following relation:

$$T_C = T_{C0} \left(\frac{\Omega}{\Omega_0} \right)^{-\gamma} \left[\frac{\exp\left[\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right]}{\exp\left[\frac{1.04(1+\lambda_0)}{\lambda_0 - \mu_0^*(1+0.62\lambda_0)} \right]} \right] \quad \dots (10)$$

3 Results and Discussion

Fiolhais *et al.*^{30,31} have computed pseudopotential form factors using both the sets of parameters. It is quite interesting to note here that for each metal, the first zero of pseudopotential form factors for both the sets of parameters are different. The calculation of λ , μ^* and T_C are quite sensitive to the behavior of pseudopotential form factors near first zero and up to $2k_F$. In the present study, we have carried out calculation of SSPs using both the sets of pseudopotential parameters and found that individual set of parameters are better than universal set of parameters because the first zero of pseudopotential form factors for individual set of parameters are close to their conventional values³⁰. Most of the researchers have used experimental Debye temperature- θ_D at 0 K for the calculation of $\langle \omega^2 \rangle$ in Eq. (1). In our opinion, the calculated value of λ using experimental Debye temperature- θ_D does not explain capability of the pseudopotential used. In such circumstances one has to compute theoretical value of Debye temperature- θ_D at 0 K using methods suggested by Raju *et al.*⁴⁰. As we have pointed out $\langle \omega^2 \rangle$ can be found theoretically by calculating longitudinal phonon frequency (ω_L) and transverse phonon frequency (ω_T) at zone boundary using same pseudopotential. In the present calculation, we have used theoretically computed $\langle \omega^2 \rangle$ for all metals⁴¹. In the present communication, we have presented results of SSPs and critical volume obtained by using individual set of parameters.

The computed results of SSPs of Pb, Sn, Ga In and Tl which are in good agreement with available experimental findings and other theoretical results are tabulated in Table 1. Our computed results of T_C for Pb, Ga, In, Sn and Tl are well agreed with experimental results. In order to achieve better agreement with the experimental results, some researchers have used $\mu^* = 0.1$ in Eqs (4), (5) and (6) instead of its actual computed value^{12,13,24}. Such approach is really questionable. Our computed values of $N_{bs}(0)$ alongwith ratio of $N_{bs}(0)$ and $N_{fe}(0)$ are shown in Table 2 which are in excellent agreement with results of McMillan⁵, which further support reliability of our computed results as $N_{bs}(0)$ depends on λ .

Table 1 — The computed values of SSPs of Pb, Sn, Ga, In and Tl along with experimental and other theoretical results. Superscripts *a, b, c, d, e, f, g, h, i* and *j* represent different pseudopotentials used by Allen and Cohen⁴ in their study.

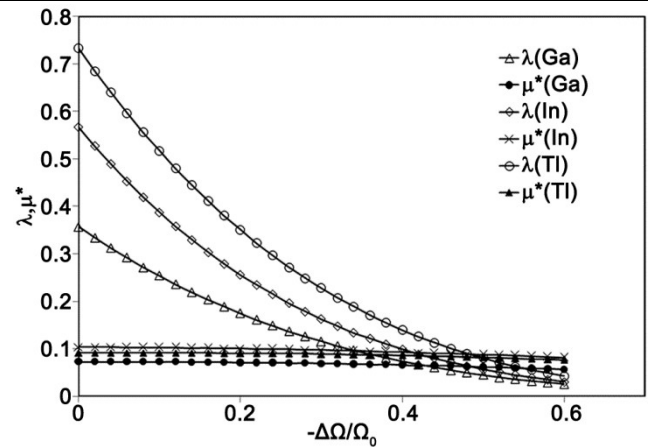
Metal	SSPs	Present	Experimental	Others
Pb	λ	1.239	-	1.34 ^{4a} , 1.32 ^{4b} , 1.12 ⁵ , 1.30 ⁷ , 1.07 ⁸
	μ^*	0.097	-	0.12 ⁴ , 0.14 ⁷ , 0.12 ⁸
	T_c (K)	7.697	7.195 ¹	7.6 ^{4a} , 7.5 ^{4b} , 6.76 ⁷ , 5.61 ⁸
	N_0V	0.537	0.411 ⁸	0.460 ⁷ , 0.482 ⁸
	α	0.483	0.48±0.10 ⁸	0.46 ⁷ , 0.473 ⁸
Sn	λ	0.600	-	0.78 ^{4a} , 0.99 ^{4c} , 0.60 ⁵ , 0.40 ⁷ , 1.07 ⁸
	μ^*	0.105	-	0.12 ⁴ , 0.13 ⁷ , 0.12 ⁸
	T_c (K)	2.620	3.72 ¹	6.2 ^{4a} , 10.2 ^{4c} , 0.30 ⁷ , 11.382 ⁸
	N_0V	0.320	0.263 ⁸	0.160 ⁷ , 0.482 ⁸
	α	0.440	0.47±0.20 ⁸	0.45 ⁷ , 0.429 ⁸
Ga	λ	0.357	-	0.25 ^{4a} , 0.29 ^{4d} , 0.22 ^{4e} , 0.23 ^{4f} , 0.23 ^{4g} , 0.40 ⁵ , 0.24 ⁶ , 0.42 ⁸
	μ^*	0.073	-	0.11 ⁴ , 0.0998 ⁶ , 0.15 ⁸
	T_c (K)	0.626	1.087 ¹	0.006 ^{4a} , 0.05 ^{4d} , 0.0003 ^{4e} , 0.0009 ^{4f} , 0.0005 ^{4g} , 0.90 ⁶ , 0.390 ⁸
	N_0V	0.214	-	0.364 ⁸
	α	0.436	-	0.228 ⁸
In	λ	0.567	-	0.89 ^{4a} , 1.16 ^{4h} , 0.88 ⁴ⁱ , 0.84 ^{4j} , 0.69 ⁵ , 0.90 ⁶ , 0.72 ⁸
	μ^*	0.104	-	0.12 ⁴ , 0.07 ⁶ , 0.12 ⁸
	T_c (K)	2.047	3.39 ¹	4.6 ^{4a} , 7.2 ^{4h} , 4.4 ⁴ⁱ , 4.0 ^{4j} , 5.00 ⁶ , 2.884 ⁸
	N_0V	0.306	-	0.197 ⁸
	α	0.436	-	0.444 ⁸
Tl	λ	0.733	-	1.07 ^{4a} , 0.71 ⁵ , 0.78 ⁸
	μ^*	0.092	-	0.11 ⁴ , 0.15 ⁸
	T_c (K)	2.870	2.38 ¹	4.8 ^{4a} , 2.54 ⁸
	N_0V	0.385	-	0.379 ⁸
	α	0.470	0.50±0.10 ⁸	0.430 ⁸

Table 2 — Band structure density of states $N_{bs}(0)$ and ratio of band structure density of states $N_{bs}(0)$ to electronic density of states $N_{fc}(0)$ at the Fermi-surface. The quantity $N_{bs}(0)$ is in states/eV atom.

Metal	$N_{bs}(0)$ (states/eV atom)		$N_{bs}(0)/N_{fc}(0)$	
	Present	Other ⁵	Present	Other ⁵
Pb	0.282	0.276	0.903	0.87
Sn	0.236	0.238	0.612	0.82
Ga	0.093	0.091	0.434	0.46
In	0.229	0.212	0.879	0.89
Tl	0.180	0.182	0.651	0.66

Further, we have extended the present pseudopotential to study pressure dependence of SSPs and to predict critical volume at which superconductivity quenches for Pb, Ga, In, Sn and Tl. The volume variations of λ and μ^* for Ga, In, and Tl are shown in Fig. 1 and that of for Pb and Sn are shown in Fig. 2.

The electron-phonon coupling strength (λ) favours electron pairing while the Coulomb pseudopotential (μ^*) describes the effects of the electron repulsion which is a measure of depairing correlations. It is found that the variation of μ^* with pressure is very small but λ changes significantly with pressure^{14,22}. It is

Fig. 1 — Volume variation of λ and μ^* for Ga, In and Tl.

also found that the Coulomb pseudopotential changes weakly with pressure^{22,42} because the mode Gruneisen parameter γ is volume independent^{12,14,16,38,39}. Jin *et al.*⁴³ studied Coulomb pseudopotential (μ^*) of Si at a pressure of 14 GPa using a full-dielectric-matrix approach within the local-density functional approximation including all of the screening effects such as the crystal potential, local-field and exchange -

Table 3 — The comparison of predicted values of $-\Delta\Omega/\Omega_0$ with other reported results (shown in parenthesis). Superscripts *a, b, c, d* and *e* represent results obtained by Seiden¹⁴ using different values of Gruneisen parameter

Metal	$-\Delta\Omega/\Omega_0$ (At $\lambda=\mu^*$)	$-\Delta\Omega/\Omega_0$ (T_c of the order of 10^{-3} K)	$-\Delta\Omega/\Omega_0$ ($T_c=0$ K)
Pb	0.72	0.48 (0.425 ^{14a} , 0.387 ^{14b})	0.72 (0.587 ^{14a} , 0.543 ^{14b} , 0.40 ⁴⁵)
Sn	0.46	0.24 (0.297 ^{14c} , 0.269 ^{14d} , 0.30 ¹⁵)	0.44 (0.540 ^{14c} , 0.484 ^{14d} , 0.148 ⁴⁵)
Ga	0.42	0.16	0.42
In	0.42	0.20 (0.429 ^{14e})	0.40 (0.758 ^{14e} , 0.218 ⁴⁵)
Tl	0.50	0.28	0.50

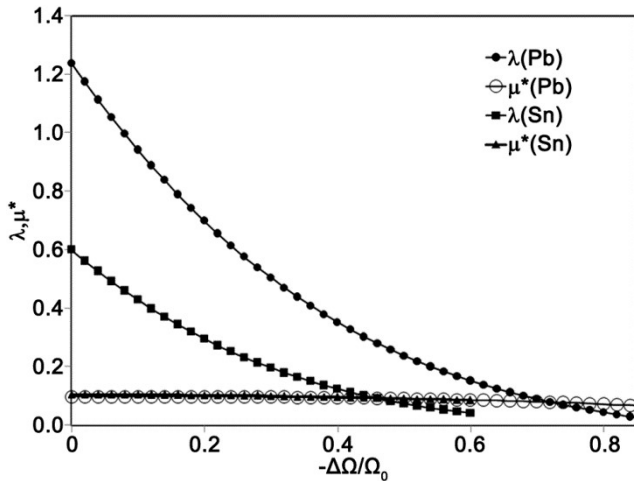


Fig. 2 — Volume variation of λ and μ^* for Pb and Sn.

correlation effects. If only the crystal potential effect is considered, μ^* is found to be very close to that of a free electron gas. Authors concluded that the exchange-correlation effect on the electron dielectric response function decreases the dielectric screening, especially for large wave vectors, giving rise to an increase of μ^* , while the local-field effect which results from directional bonds slightly reduces μ^* . In the present study, μ^* is not found to be constant as a function of compressed volume but a very small change in μ^* is observed. Such small change in μ^* as a function of compressed volume is due to poor volume dependence of dielectric function- $\epsilon(q)$ ⁴⁴.

The intersection of λ and μ^* curves in Figs 1 and 2 give volume at which $\lambda = \mu^*$, so that interaction strength becomes zero and Coulomb repulsion equals the attractive electron phonon interaction. The corresponding pressure at which superconductivity quenches is called critical pressure. In the present study, values of $-\Delta\Omega/\Omega_0$ at critical pressure are shown in Table 3. Here Ω_0 is normal atomic volume and $\Delta\Omega$ is change in atomic volume.

We have computed volume dependence of T_c using McMillan formalism. We have predicted critical volume up to experimentally measurable lowest value

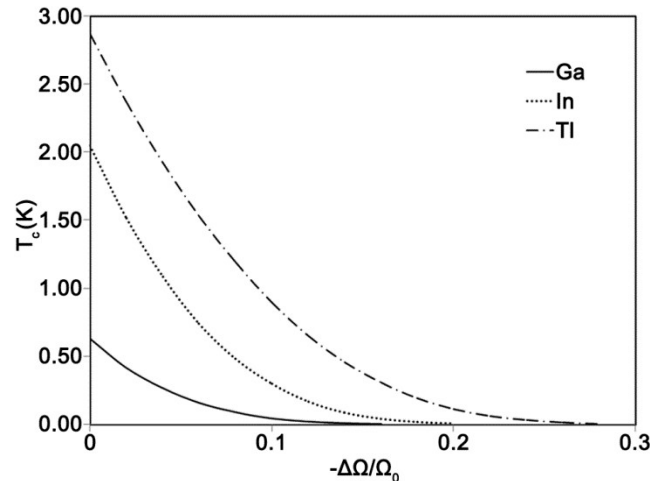


Fig. 3 — Volume dependence of T_c for Ga, In and Tl.

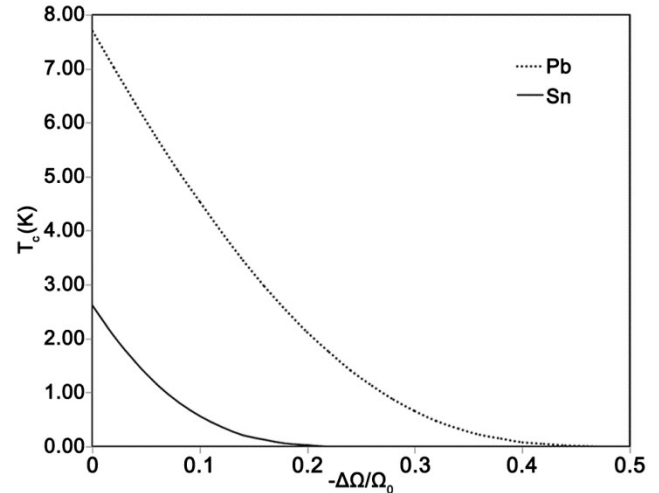


Fig. 4 — Volume dependence of T_c for Pb and Sn.

of T_c which is of the order of 10^{-3} K¹⁴. Such computed critical volumes for all metals are tabulated in Table 3. The volume variations of T_c for these metals up to lowest measurable temperature are shown in Figs 3 and 4. Using our theoretical calculation (curve), one can predict the values of critical volume at which T_c becomes zero as shown in Table 3.

The results of critical volume computed in the present study are well agreed with each other and are

also comparable with other reported results^{14,15,45}. Seiden¹⁴ has used point ion pseudopotential for core repulsion and experimental Debye temperature with jellium phonon spectrum. The author has used different values of Gruneisen constant (γ) to study volume dependence of T_C . The present model is better in the sense that it is free from any kind of adjustment of any parameter. Our results of T_C are nonlinear for the higher compressions. Such trend is also observed by Seiden¹⁴.

Present study confirms that the local form of the pseudopotential proposed by Fiolhais *et al.*^{30,31} which is continuous in r -space as well as analytic in r & q -space is found to be successful for the description of pressure dependence of SSPs and prediction of critical volume. They derived structured local electron-ion pseudopotential and found that computed results of static properties (binding energies, bulk moduli and pressure derivatives of bulk moduli) are in good agreement with experimental results. They have also noted that computed results of bulk moduli are better than those obtained by first principle nonlocal norm-conserving pseudopotentials. They have also pointed out in their research paper that the local form of the pseudopotential proposed by them alongwith method used to determine pseudopotential parameters can be used as a proxy to the nonlocal norm-conserving pseudopotentials. This fact has been verified by many researchers by carrying out study of thermophysical properties at extreme environment³⁵⁻³⁷ and for the liquid state properties³². The nonlocal form of the pseudopotential is better for the description of physical properties of a system but at the same time it is computationally lengthy, conceptually difficult and physically less transparent in comparison with local one. Very recently, Szczesniak and Durajski⁴⁶ pointed out that computation of μ^* and hence other SSPs are very difficult using ab-initio methods. The reason for difficulties arose in the use of density functional theory (DFT) can be understood as follows. In such approach the interacting system of fermions is described by knowing its density instead of its many body interaction using nonlocal norm conserving pseudopotentials.

4 Conclusions

The transition temperature T_C and critical volume for Pb, Ga, In, Sn and Tl are in good agreement with experimental and other theoretical results. The present study confirms that the pseudopotential proposed by

Fiolhais *et al.*³⁰⁻³¹ with its individual set of parameters is found to be good working for the study of pressure dependence of SSPs without any readjustment of pseudopotential parameters. The reasons for the variation of our computed value of T_C with experimental value may be the use of theoretical value of $\langle\omega^2\rangle$ in the calculation of SSPs. The result of pressure dependence of T_C can be improved by accounting pressure dependence of Gruneisen parameter. But experimental studies show that Gruneisen parameter has poor volume dependence³⁸. We have not considered pressure dependence of c/a for hcp metal (Tl). One can improve results by considering pressure dependence of c/a . In the present study, we have found that local pseudopotential method is simple, transparent and mathematically tractable alongwith its predictivity. Looking to such success, we would like to extend present pseudopotential for the study of pressure dependence of SSPs of alloys and metallic glasses.

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