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Pressure effects on $Ca_{60}Al_{40}$ metallic glass superconductors

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Abstract
Theoretical computation of the pressure dependence superconducting state parameters of binary $Ca_{60}Al_{40}$ is reported using model potential formalism. Explicit expressions have been derived for the volume dependence of the electron–phonon coupling strength λ and the Coulomb pseudopotential μ^* considering the variation of Fermi momentum k_F and Debye temperature θ_D with volume. Well known Ashcroft's empty core model pseudopotential and five different types of the local field correction functions viz. Hartree, Taylor, Ichimaru-Utsumi, Farid *et al.* and Sarkar *et al.* have been used for obtaining pressure dependence of transition temperature T_C and the logarithmic volume derivative Φ of the effective interaction strength N_OV for metallic glass superconductor. It has been observed that T_C of $Ca_{60}Al_{40}$ metallic glass decreases rapidly with increase of pressure upto 60% decrease of volume, for which the μ^* and Φ curves show a linear nature. The superconducting phase disappears at about 60% decrease of volume.

Keywords: pseudopotential, metallic glass, pressure dependence superconducting state parameters, local field correction functions

1. Introduction

With the advent of high pressure technique, it has been possible in the recent years to explore a wide spectrum of solid state phenomena under high pressure by using different kinds of diagnostic tools, earlier used only at ambient pressure. When solids are subjected to high pressure, we can in general expect metal-insulator, magnetic-nonmagnetic and crystal structure transitions in the solids. Thus, the high pressure technique provides a unique possibility of investigating the same material in different forms or phases. Further, the high pressure technique enables us to produce an often small but well controlled variation of the pertinent electronic properties viz. density of states, exchange interactions, electron-phonon coupling etc., which can provide a feasible route to critically assess the predications of the theoretical models [1].

The question whether the application of sufficient pressure to a superconductor can eventually inhibit the transition to the superconducting state down to absolute zero has existed since the early discovery [2] that the application of pressure could lower the transition temperature T_C of a superconductor. There have been various experimental investigations [3–8] of the behaviour of the superconducting transition temperature T_C, as well as a number of phenomenological analyses [7–9] have been tried to describe the behaviour of T_C with variation of pressure in metals. Attempts have also been made to study the pressure dependence by consideration of the various interactions involved [10–14] and also from a semi-emperical point of view. However, there has been no serious attempt, to our knowledge, to try to understand theoretically the pressure dependence of superconducting state parameters viz. electron–phonon coupling strength λ and the Coulomb pseudopotential μ^*, the superconducting transition temperature T_C and the effective interaction strength N_OV and in metallic glass superconductors.

In this paper we have, therefore, attempted to discuss the pressure dependence of these parameters of $Ca_{60}Al_{40}$ metallic glass from the variation of the electron-phonon coupling strength λ and the Coulomb pseudopotential μ^* with volume for the first time. Either experimental or theoretical data are not available of the glass in the literature. We employ Ashcroft's empty core (EMC) model pseudopotential [15], which has been found to explain successfully the superconductivity in a number of metallic superconductors [16–18]. Recently we have reported pressure dependence superconducting state parameters of some metallic superconductors [16]. Five different types of the local field correction functions proposed by Hartree (H) [19], Taylor (T) [20], Ichimaru-Utsumi (IU) [21], Farid *et al.* (F) [22] and Sarkar *et al.* (S) [23] are used in the present investigation to study the screening influence on the aforesaid properties. The variations of Fermi momentum k_F and the Debye temperature θ_D with volume have been explicitly considered and thus the variation of λ, μ^*, T_C and Φ with volume have been derived for $Ca_{60}Al_{40}$ metallic glass superconductor. An expression for volume dependence of T_C was derived by Sharma *et al.* [24] for metals. The same has been extended for metallic glasses in the present work. For studying the volume dependence of the effective interaction strength $N_O V$, we define a quantity $\Phi = \partial \ln(N_O V)/\partial \ln \Omega$, and the value of Φ has been worked out for $Ca_{60}Al_{40}$ metallic glass. Gupta *et al.* [14] have derived explicit expression for the electron-phonon coupling strength λ for $Mg_{70}Zn_{30}$ metallic glass with some modifications and for the sake of simplicity. Also, they have not introduced screening effects in their computation. But, in the present article we have applied here only general expression of electron-phonon coupling strength λ, which is very useful to various readers. Also, we have applied here screening effects in the computation.

2. Computational technique

In the present investigation for binary metallic glass, the electron-phonon coupling strength λ is computed using the relation [16-18]

$$\lambda = \frac{12\, m_b\, Z}{M\, \langle \omega^2 \rangle} \int_0^1 X^3 \left| W(X) \right|^2 dX \ , \ X = q/2k_F \quad (1)$$

Here m_b is the band mass, M the ionic mass, Ω_O the atomic volume, k_F the Fermi momentum, $W(X)$ the EMC pseudopotential [15], $\langle \omega^2 \rangle$ the averaged square phonon frequency and Z the valence of the binary glassy alloy, respectively. The averaged square phonon frequency $\langle \omega^2 \rangle$ is calculated using the relation given by Butler [25], $\langle \omega^2 \rangle^{1/2} = 0.69\,\theta_D$, where θ_D is the Debye temperature of the metallic glass.

The well known Ashcroft's empty core (EMC) model potential [15] used in the present computations of the SSP of binary metallic glass is of the form,

$$W(X) = \frac{-2\pi Z}{\Omega_O X^2 k_F^2 \varepsilon(X)} \cos(2k_F X r_C), \quad (2)$$

here r_C is the parameter of the model potential of binary metallic glass. The Ashcroft's empty core (EMC) model potential is a simple one-parameter model potential [15], which has been successfully found for various metallic complexes [16-18].

Also, $\varepsilon(X)$ the modified Hartree dielectric function, which is written as [19]

$$\varepsilon(X) = 1 + (\varepsilon_H(X) - 1)(1 - f(X)). \quad (3)$$

Here $\varepsilon_H(X)$ is the static Hartree dielectric function and the expression of is given by [19],

$$\varepsilon_H(X) = 1 + \frac{m e^2}{2\pi k_F \hbar^2 \eta^2} \left(\frac{1-\eta^2}{2\eta} ln \left| \frac{1+\eta}{1-\eta} \right| + 1 \right); \ \eta = \frac{q}{2k_F} \quad (4)$$

While $f(X)$ is the local field correction function. In the present investigation, the local field correction functions due to H [19], T [20], IU [21], F [22] and S [23] are incorporated to see the impact of exchange and correlation effects. The details of all the local field corrections are below.

The Hartree (H) [19] screening function is purely static, and it does not include the exchange and correlation effects. While, Taylor (T) [20] has introduced an analytical expression for the local field correction function, which satisfies the compressibility sum rule exactly. This is the most commonly used local field correction function and covers the overall features of the various local field correction functions proposed before 1972. According to Taylor (T) [20],

$$f(X) = \frac{q^2}{4k_F^2} \left[1 + \frac{0.1534}{\pi k_F^2} \right]. \quad (5)$$

The Ichimaru-Utsumi (IU) [21] local field correction function is a fitting formula for the dielectric screening function of the degenerate electron liquids at metallic and lower densities, which accurately reproduces the Monte-Carlo results as well as it also, satisfies the self consistency condition in the compressibility sum rule and short range correlations. The fitting formula is

$$\begin{aligned} f(X) &= A_{IU} Q^4 + B_{IU} Q^2 + C_{IU} \\ &+ \left[A_{IU} Q^4 + \left(B_{IU} + \frac{8A_{IU}}{3} \right) Q^2 - C_{IU} \right] \\ &\times \left\{ \frac{4-Q^2}{4Q} \ln \left| \frac{2+Q}{2-Q} \right| \right\}. \end{aligned} \quad (6)$$

On the basis of Ichimaru-Utsumi (IU) [21] local field correction function, Farid *et al.* (F) [22] have given a local field correction function of the form

$$\begin{aligned} f(X) &= A_F Q^4 + B_F Q^2 + C_F \\ &+ \left[A_F Q^4 + D_F Q^2 - C_F \right] \\ &\times \left\{ \frac{4-Q^2}{4Q} \ln \left| \frac{2+Q}{2-Q} \right| \right\}. \end{aligned} \quad (7)$$

Based on eqs. (8-9), Sarkar *et al.* (S) [23] have proposed a simple form of local field correction function, which is of the form

$$f(X)=A_S\left\{1-\left(1+B_SQ^4\right)\exp\left(-C_SQ^2\right)\right\}, \quad (8)$$

where $Q = 2X$. The parameters A_{IU} , B_{IU} , C_{IU} , A_F , B_F , C_F , D_F , A_S , B_S and C_S are the atomic volume dependent parameters of IU, F and S-local field correction functions. The mathematical expressions of these parameters are narrated in the respective papers of the local field correction functions [21-23]. For the volume dependence of θ_D , we will assume that the Gruneisen constant [1, 14, 16].

$$\gamma_G = -\partial \ln\theta_D / \partial \ln\Omega , \quad (9)$$

is volume independent [10, 11, 14, 16, 26, 27]. Thus we obtain expression for the Debye temperature as

$$\theta_D = \theta_{DO}\left(\Omega/\Omega_O\right)^{-\gamma_G} , \quad (10)$$

here, θ_{DO} corresponds to Debye temperature for the normal volume respectively and $\Delta\Omega$ is the change in volume. Using eqs. (1-10), we obtain an explicit expression for volume dependence of the electron-phonon coupling strength λ as

$$\lambda = \lambda_O\left(\frac{\Omega}{\Omega_O}\right)^{-2\gamma_G}\frac{\int_0^1 X^3\left|W(X)\right|^2 dX}{\int_0^1 X_O{}^3\left|W(X_O)\right|^2 dX_O} . \quad (11)$$

Here λ_O and $X_O = q/2k_{FO}$ is the electron–phonon coupling strength and Fermi momentum at normal volume. The pressure derivative of the electron-phonon coupling strength λ is given by

$$\frac{\partial\ln\lambda}{\partial\ln\Omega} = 2\gamma_G - \left(\frac{4\pi^2Z^2}{\lambda^2}\right)\int_0^1\left[\frac{\cos^2\left(2k_FXr_C\right)}{X\varepsilon(X)}\right]dX . \quad (12)$$

The expression is certainly an improvement over the expressions obtained by Seiden [10], Sharma *et al.* [24], Jain and Kachhava [27] and Olsen *et al.* [28].

In the present work, we have also incorporated the effects of volume dependence of the Coulomb pseudopotential μ^*, by considering the variation of the Fermi momentum and the Debye temperature with volume. The expression for Coulomb pseudopotential μ^* derived in the present work is as follows [14, 16]

$$\mu^* = \frac{\dfrac{3m_b}{\pi k_{FO}\left(4-\Omega/\Omega_O\right)}\displaystyle\int_0^1\frac{dX}{X\varepsilon(X)}}{1+\dfrac{3m_b}{\pi k_{FO}\left(4-\Omega/\Omega_O\right)}\ln\left[\dfrac{k_{FO}^2\left(4-\Omega/\Omega_O\right)^2}{180\theta_{DO}\left(\Omega/\Omega_O\right)^{-\gamma_G}}\right]\displaystyle\int_0^1\frac{dX}{X\varepsilon(X)}} . \quad (13)$$

The volume dependence of the Coulomb pseudopotential μ^* plays an important role, near the point of quenching.

Teble 1. Input parameters and other constants.

Constants	Values
Z	2.4
Ω_O (au)	220.6
M (amu)	34.84
r_c (au)	2.1125
θ_D (K)	303.77
γ_G	1.04
μ^*_O	0.13

All the eqs. (11-13) are derived from taking the pressure derivates of the main expressions of the superconducting properties available in the standard literature.

The volume dependence of superconducting transition temperature T_C may be obtained from volume dependence of the electron-phonon coupling strength λ and the Coulomb pseudopotential μ^* by using Eqs. (10). Thus we obtain [16]

$$T_C = T_{CO}\left(\frac{\Omega}{\Omega_O}\right)^{-\gamma_G}\left\{\frac{exp\left[\dfrac{-1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right]}{exp\left[\dfrac{-1.04(1+\lambda_O)}{\lambda_O-\mu_O^*(1+0.62\lambda_O)}\right]}\right\} , \quad (14)$$

where T_C and T_{CO} are the values of superconducting transition temperature at volumes Ω and Ω_O, respectively. Here, $\mu_O^* = 0.13$ according to McMillan [29].

In the present theory, the effective interaction strength N_OV , is approximately [10, 16, 29]

$$N_OV \cong \frac{\lambda-\mu^*}{1+\lambda} , \quad (15)$$

Now, the logarithmic volume derivative Φ of the effective interaction strength N_OV is defined by [1, 16, 24]

$$\Phi = \frac{\partial\ln(N_OV)}{\partial\ln\Omega} = \frac{\lambda\left(1+\mu^*\right)}{(1+\lambda)\left(\lambda-\mu^*\right)}\frac{\partial\ln\lambda}{\partial\ln\Omega} \quad (16)$$

Substituting for $\partial\ln(N_OV)/\partial\ln\Omega$ from (15), we get the value of the logarithmic volume derivative of the effective interaction strength N_OV . Similarly for the expression the electron-phonon coupling strength λ , the present expression for Φ is also qualitatively different than the results of Seiden [10], Sharma *et al.* [24], Jain and Kachhava [27] and Olsen *et al.* [28].

3. Results and discussion

The input parameters and other constants used in the present computation are taken from our earlier paper [18] and narrated in table 1. The pressure dependence superconducting state parameters are displayed in figures 1-5.

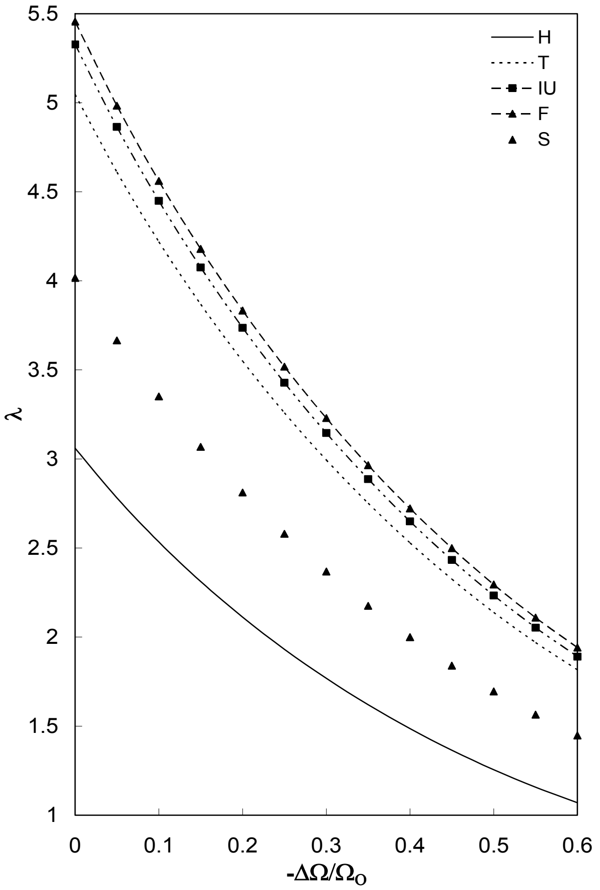

Figure 1. Variation of electron-phonon coupling strength (λ) with change in volume.

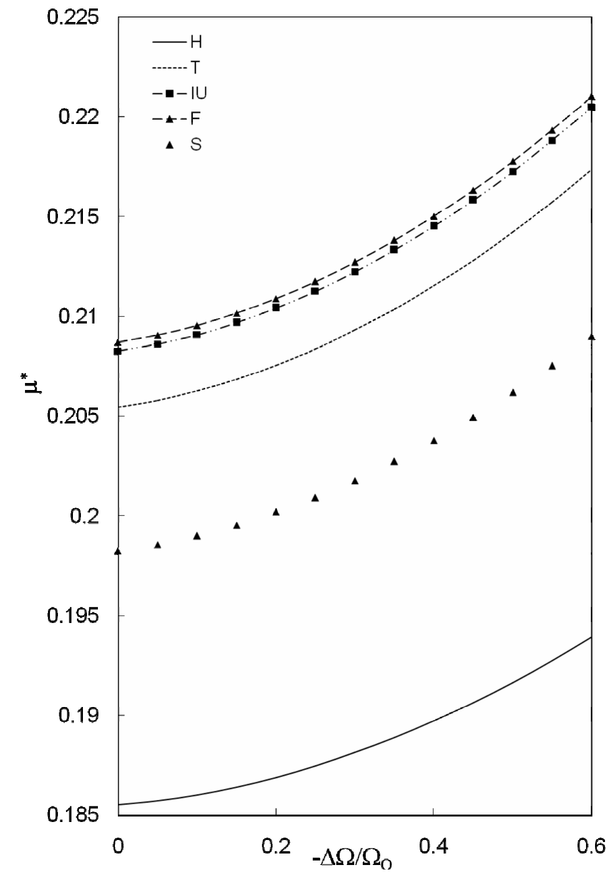

Figure 2. Variation of Coulomb pseudopotential (μ^*) with change in volume.

The pressure dependence of the electron-phonon coupling strength λ has been evaluated by employing eq. (11), upto 60% changes in the volume. The variation of λ with volume on using EMC model potential is shown in figure 1. It is noticed from the Figure 1 that, λ vales are quite sensitive to the local field correction functions. Also, the H-screening yields lowest values of λ , whereas those obtained from the F-function are the highest. It is also observed from the present study that, the percentile influence of the various local field correction functions with respect to the static H-screening function on the electron-phonon coupling strength λ is 31.26%-81.34%, which shows the screening nature of other local field correction functions.

The variation of the Coulomb pseudopotential μ^* with volume is shown in figure 2, which gives a graphically increasing nature with volume. Also, it shows that the direct Coulomb repulsive interaction between the electrons becomes weakest at this volume, so that the electron-phonon interaction may be most effective during the volume dependent process. It is observed that the μ^* lies between 0.1855 and 0.2210, which is not in accordance with McMillan [29]. The weak screening influence shows on the computed values of the μ^* . The percentile influence of the various local field correction functions with respect to the static H-screening function on μ^* for $Ca_{60}Al_{40}$ metallic glass superconductor is observed in the range of 6.85%-13.97%. Again the H-screening function yields lowest values of the μ^* , while the values obtained from the F-function are the highest.

The values showing volume dependence of the superconducting transition or critical temperature T_C obtained from the present formulation have been assembled in Figure 3. It is seen that T_C is quite sensitive to the local field correction functions. It is also observed that the static H-screening function yields lowest T_C whereas the F-function yields highest values of T_C . The percentile influence of the various local field correction functions with respect to the static H-screening function on the superconducting transition or critical temperature T_C is 11.03%-34.68%. It has been observed that T_C of $Ca_{60}Al_{40}$ metallic glass decreases rapidly with increase of pressure upto 60% decrease of volume, for which the μ^* and Φ curves show a linear nature. Also Fig. 3 shows that, the T_c is never reached zero value in any pressure.

In the expression of electron-phonon coupling

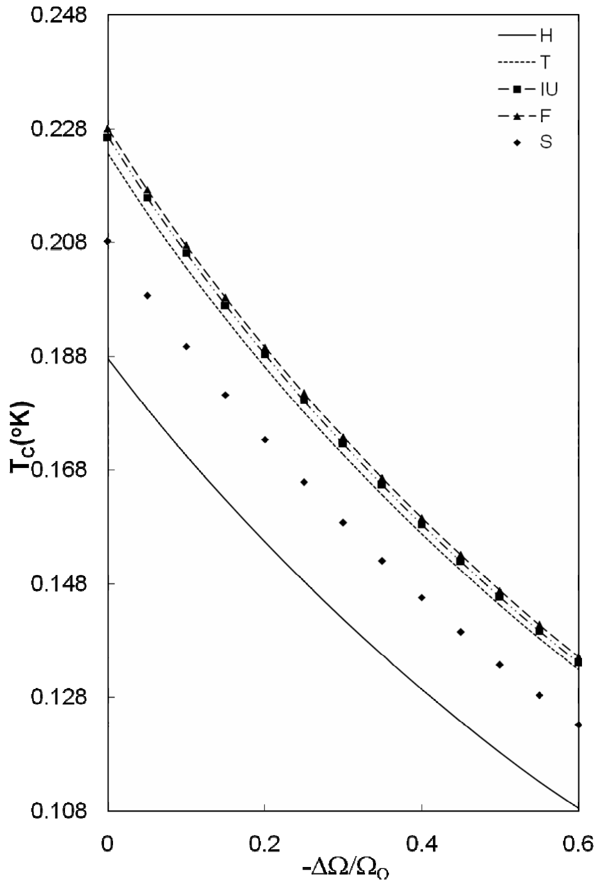

Figure 3. Variation of transition temperature (T_C) with change in volume.

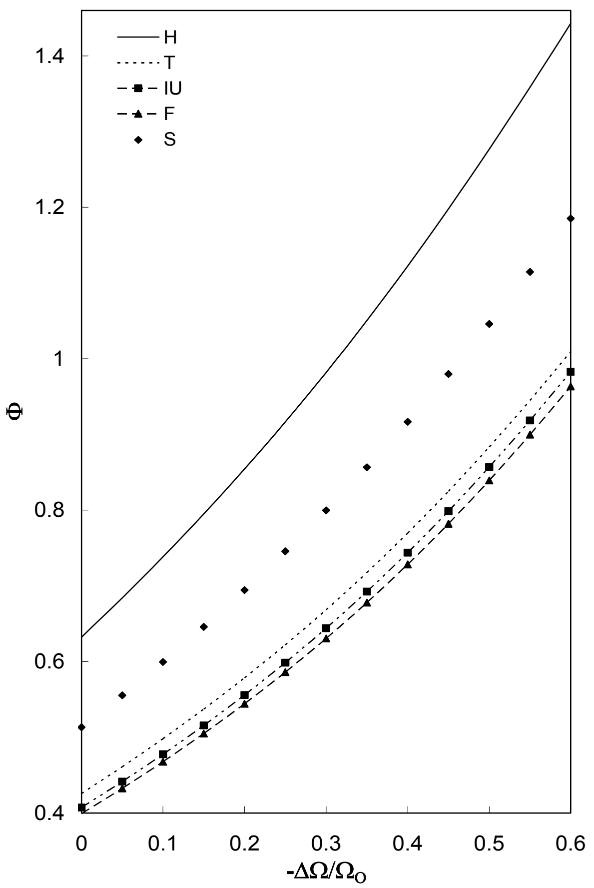

Figure 4. Variation of logarithmic volume derivative (Φ) with change in volume.

strength λ, effect of the model potential is directly involved in the computations. Therefore, it shows larger value in the computation. Also, this parameter is also related to phonon frequency. If phonon frequencies are low then the λ shows higher values. Also, in the expression of superconducting transition or critical temperature T_C shows that the effect of λ is negligible because it is available in the nominator and denominator terms in the exponential factor. Therefore, the theoretical values of the transition temperature T_C shows much lower values then the theoretical values of the electron-phonon coupling strength λ.

The experimental or theoretical values of the λ for 'Ca' metal are 0.05 [17] and 027 [17]. And those for the superconducting transition or critical temperature T_C is 4.3 [1]. The value of the T_C for 'Al' metal is 1.140 [17]. From these values of the pure metals we can say that 'Ca' metals having larger T_C values then the 'Al' metal. The main role plays a "Ca" metal in the construction of $Ca_{60}Al_{40}$ metallic glass superconductors. When, this metallic glass put in the pressure condition at that time reverse nature is observed because of phase transition in the values of λ and T_C i.e. λ goes higher and T_C becomes lower.

Figure 4 shows the variation of logarithmic volume derivative Φ of the effective interaction strength N_OV with volume. It is seen that Φ is quite sensitive to the local field correction functions. It is also observed that the static H-screening function yields lowest Φ whereas the F-function yields highest values of Φ. The percentile influence of the various local field correction functions with respect to the static H-screening function on the superconducting transition or critical temperature Φ is 17.86%-36.88%. It is observed that the magnitude of Φ shows that the metallic glass under investigation lie in the range of weak coupling superconductors.

The effect of local field correction functions plays an important role in the computation of λ and μ^*, which makes drastic variation on T_C and Φ. The local field correction functions due to IU, F and S are able to generate consistent results regarding the pressure dependence SSP of the $Ca_{60}Al_{40}$ metallic glass superconductors as those obtained from more commonly employed H and T functions. Thus, the use of these more promising local field correction functions is established successfully.

In the present work, we have restricted the pressure effect upto 60% for the sake of simplicity from reducing the volume content and practically it is possible. In conclusion we may add that the present theory provides overall satisfactory answer to the problems related with the effect of pressure on superconductivity, particularly in view of the fact that reliable experimental values of γ_G at low temperatures are not available. Moreover, the present results can be improved if uncertainties involved in the values of μ^* and γ_G are removed. The experimentally observed values of the dependence SSP are not available in the literature for $Ca_{60}Al_{40}$ metallic glass superconductors therefore it is difficult to drew any special remarks. However, the comparison with theoretical data supports the applicability of the EMC model potential and different forms of the local field correction functions.

4. Conclusion

We conclude from the present study, the transition temperature T_C of $Ca_{60}Al_{40}$ metallic glass decreases rapidly with increase of pressure upto 60% decrease of volume, for which the μ^* and Φ curves show a linear nature. Such study on pressure dependence SSP of other such metallic glasses is in progress, which will be communicated in near future.

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