PRESSURE DEPENDENCE OF THE SUPERCONDUCTING STATE PARAMETERS OF BINARY METALLIC GLASS SUPERCONDUCTOR 
\[ \text{Ca}_{70}\text{Zn}_{30} \]

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Theoretical computation of the pressure dependence superconducting state parameters of binary \( \text{Ca}_{70}\text{Zn}_{30} \) is reported using model potential formalism. Explicit expressions have been derived for the volume dependence of the electron-phonon coupling strength \( \lambda \) and the Coulomb pseudopotential \( \mu^* \) considering the variation of Fermi momentum \( k_F \) and Debye temperature \( \theta_D \) with volume, if glasses in the considered system are superconducting or not in normal conditions. Well known Ashcroft's empty core (EMC) model pseudopotential and five different types of the local field correction functions viz. Hartree (H), Taylor (T), Ichimaru-Utsumi (IU), Farid \textit{et al.} (F) and Sarkar \textit{et al.} (S) have been used for obtaining pressure dependence of transition temperature \( T_c \) and the logarithmic volume derivative \( \Phi \) of the effective interaction strength \( N_f \rho^V \) for metallic glass superconductor.

Key words: pseudopotential; metallic glass; pressure dependence superconducting state parameters; local field correction functions.
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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. In solids subjected to high pressure, one can in general expect metal-insulator, magnetic-nonmagnetic and crystal structure transitions and, thus, the technique provides a unique possibility of investigating one and the same phase material in different forms or phases. Further, the technique enables one to produce an often small but well controlled variation of the pertinent electronic properties like the
density of states, exchange interactions, electron-phonon coupling, which can be provide a feasible route to critically assess the predications of the theoretical models. Broadly speaking, with the application of external pressure one changes the ionic separations in solids, which in principle can also be achieved by chemical processes leading to lattice pressure. However, as the latter involves interlinked parameters the results obtained invariably tend to be ambiguous. Also, the pressure effects on superconductivity are equally fascinating. A normal metal or non-metal can be superconducting, while a superconductor can be non-superconducting under pressure. The effect of pressure on superconducting properties has been a subject of considerable interest since long and to-date numerous superconducting elements have been investigated. The study of pressure effects on superconductors was once thought to be the most effective for revealing the underlying mechanism of superconductivity. However, the data generated have been so diverse and puzzling that the effect of pressure on superconductivity has become a challenging area in its own right. In this article, we attempt to review the present understanding of pressure effects in glass superconductor. As will be seen, the pressure studies reveal several unresolved anomalies, but, nevertheless, it seems that at least some of them may be satisfactorily answered if one can invokes the possible creative role of exchange interactions in the conduction band in the occurrence of superconductivity [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-empirical 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 $\lambda$ and the Coulomb pseudopotential $\mu^*$, the superconducting transition temperature $T_c$ and the effective interaction strength $N_oV$ and in metallic glass superconductors, if glasses in the considered system are superconducting or not in normal conditions. Very recently, we have reported pressure dependence superconducting state parameter of some binary metallic glass superconductors [15].

In this paper we have, therefore, attempted to discuss the pressure dependence of these parameters of Ca$_{70}$Zn$_{30}$ metallic glass superconductors from
the variation of the electron-phonon coupling strength $\lambda$ and the Coulomb pseudopotential $\mu^*$ with volume. In the present investigations, we employ Ashcroft’s empty core (EMC) model pseudopotential [17], which has been found to explain successfully the superconductivity in a number of metallic superconductors [17, 18]. 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 the Fermi momentum $k_F$ and the Debye temperature $\Theta_D$ with volume have been explicitly considered and thus the variation of $\lambda$, $\mu^*$, $T_c$ and $\Phi$ with volume have been derived for Ca$_{70}$Zn$_{30}$ metallic glass superconductor. An expression for volume dependence of $T_c$ was derived by Sharma et al. [24] for metals. The same expression has been extended for metallic glasses in the present work. For studying the volume dependence of the effective interaction strength $V_{NO}$, we define a quantity

$$\Phi = \partial \ln \left( N_p V \right) / \partial \ln \Omega,$$

and the value of $\Phi$ has been worked out for Ca$_{70}$Zn$_{30}$ metallic glass if glasses in the considered system are superconducting or not in normal conditions. Gupta et al. [14] have derived explicit expression for the electron-phonon coupling strength $\lambda$ for Ca$_{70}$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 $\lambda$, which is very useful to various readers. Also, we have applied here screening effects in the present computation. The theoretical work related to pressure dependence superconducting state parameters of Ca$_{70}$Zn$_{30}$ metallic glass are available in the literature. Hence, we have decided the work on this glassy material. Such types of the theoretical analysis are very useful for further study either experimentally or theoretically.

2. COMPUTATIONAL TECHNIQUE

In the present investigation for binary metallic glass, the electron-phonon coupling strength $\lambda$ is computed using the relation [17, 18]

$$\lambda = \frac{m_b k_F \Omega_0}{4 \pi^2 k_F M \langle \omega^2 \rangle} \int_0^{2k_F} q^3 |V(q)|^2 dq.$$  

Here $m_b$ is the band mass, $M$ the ionic mass, $\Omega_0$ the atomic volume, $k_F$ the Fermi momentum, $V(q)$ the pseudopotential and $\langle \omega^2 \rangle$ the averaged square
The averaged square phonon frequency \( \left\langle \omega^2 \right\rangle \) is calculated using the relation given by Butler [25],
\[
\left\langle \omega^2 \right\rangle^{1/2} = 0.69 \theta_D,
\]
where \( \theta_D \) is the Debye temperature of the metallic glass.

Using \( X = q/2k_F \) and \( \Omega_o = 3\pi^2Z/(k_F)^3 \), we get Eq. (1) in the following form,
\[
\lambda = \frac{12m_bZ^2}{M\langle \omega^2 \rangle} \int X^3 \left| W(X) \right|^2 dX,
\tag{2}
\]
where \( Z \), \( W(X) \) are the valence of the metallic glass and the EMC pseudopotential [16] for binary mixture, respectively.

The well known Ashcroft’s empty core (EMC) model potential [16] used in the present computations of the SSP of binary metallic glass is of the form,
\[
W(X) = \frac{-2\pi Z}{\Omega_o X^2 k_F^2 \epsilon(X)} \cos(2k_F X r_C),
\tag{3}
\]
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 [16], which has been successfully found for various metallic complexes [17, 18].

Also, \( \epsilon(X) \) the modified Hartree dielectric function, which is written as [19]
\[
\epsilon(X) = 1 + (\epsilon_{II}(X) - 1)(1 - f(X)).
\tag{4}
\]
Here \( \epsilon_{II}(X) \) is the static Hartree dielectric function and the expression of it is given by [19],
\[
\epsilon_{II}(X) = 1 + \frac{m \epsilon^2}{2\pi k_F \hbar^2 \eta^2} \left( 1 - \eta^2 \ln \frac{1 + \eta}{1 - \eta} + 1 \right); \quad \eta = \frac{q}{2k_F}
\tag{5}
\]
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. The expression of it is,
\[
f(X) = 0.
\tag{6}
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],

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

(7)

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

\[ f(X) = A_{IU}Q^4 + B_{IU}Q^2 + C_{IU} + \left[ A_{IU}Q^4 + \left( B_{IU} + \frac{8A_{IU}}{3} \right)Q^2 - C_{IU} \right] \left\{ \frac{4-Q^2}{4Q} \ln \left[ \frac{2+Q}{2-Q} \right] \right\}. \]  

(8)

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

\[ f(X) = A_FQ^4 + B_FQ^2 + C_F + \left[ A_FQ^4 + D_FQ^2 - C_F \right] \left\{ \frac{4-Q^2}{4Q} \ln \left[ \frac{2+Q}{2-Q} \right] \right\}. \]  

(9)

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

\[ f(X) = A_S \left\{ 1 - \left( 1 + B_SQ^4 \right) \exp \left( -C_SQ^2 \right) \right\}. \]  

(10)

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 \( \theta_D \), we will assume that the Gruneisen constant \([1, 14, 15]\)

\[ \gamma_G = -\partial \ln \theta_D / \partial \ln \Omega, \]  

(11)

is volume independent \([10, 11, 14, 15, 26, 27, 28]\). Thus we obtain expression for the Debye temperature as
The variation of the Fermi momentum $k_F$ with volume can be calculated from the relation $k_F = k_{FO} \left(1 - \Delta \Omega/3 \Omega_O \right)$, putting $\Delta \Omega = \Omega - \Omega_O$, we obtain

$$k_F = \left( k_{FO} / 3 \right) \left( 4 - \Omega / \Omega_O \right),$$

(13)

In Eqs. (12) and (13), $\theta_{DO}$ and $k_{FO}$ correspond to Debye temperature and Fermi momentum for the normal volume respectively and $\Delta \Omega$ is the change in volume. Using Eqs. (1-13), we obtain an explicit expression for volume dependence of the electron-phonon coupling strength $\lambda$ as

$$\lambda = \lambda_O \left( \frac{\Omega}{\Omega_O} \right)^{-2\gamma_G} \int_0^1 \left[ X^2 \left| W(X) \right|^2 \right] dX.$$

(14)

Here $\lambda_O$ and $X_O = q/2k_{FO}$ is the electron-phonon coupling strength and Fermi momentum at normal volume. From the use of (13) and (14) and carrying out the required differentiation, we get following relation

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

(15)

The expression is certainly an improvement over the expressions obtained by Seiden [10], Sharma et al. [24], Jain and Kachhava [26] and Olsen et al. [28].

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

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

(16)

At the volume where $\lambda = \mu^\ast$, the superconductivity must disappear and for the exact determination of this transition, the consideration of the volume dependence
of the Coulomb pseudopotential $\mu^*$ plays an important role, near the point of quenching.

Since superconducting transition temperature $T_c$ depends on $\theta_D$, $\lambda$, and $\mu^*$, hence for finding volume dependence of $T_c$, we take into account the volume dependence of the electron-phonon coupling strength $\lambda$, the Coulomb pseudopotential $\mu^*$ and the Debye temperature $\theta_D$. The expression for superconducting transition temperature $T_c$ is given by [16-18, 29]

$$T_c = \frac{\theta_D}{1.45} \exp\left[\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right], \quad (17)$$

The volume dependence of superconducting transition temperature $T_c$ may be obtained from volume dependence of the electron-phonon coupling strength $\lambda$ and the Coulomb pseudopotential $\mu^*$ by using (12). Thus we obtain [15]

$$T_c = T_{CO} \left(\frac{\Omega}{\Omega_O}\right)^{-\gamma_o} \left\{ \frac{\exp\left[\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right]}{\exp\left[\frac{-1.04(1+\lambda_o)}{\lambda_o - \mu_o^*(1+0.62\lambda_o)}\right]} \right\}, \quad (18)$$

where $T_c$ and $T_{CO}$ are the values of superconducting transition temperature at volumes $\Omega$ and $\Omega_O$, respectively. Here, $\mu^*_o = 0.13$ according to McMillan [29]. In the present theory, the effective interaction strength $N_oV$, is approximately [10, 29]

$$N_oV \approx \frac{\lambda - \mu^*}{1+\lambda}, \quad (19)$$

Now, the logarithmic volume derivative $\Phi$ of the effective interaction strength $N_oV$ is defined by [1, 15, 24]

$$\Phi = \frac{\partial \ln (N_oV)}{\partial \ln \Omega}. \quad (20)$$

Taking the logarithmic volume derivative of Eq. (20), we have

$$\Phi = \frac{\lambda(1+\mu^*)}{(1+\lambda)(\lambda - \mu^*)} \frac{\partial \ln \lambda}{\partial \ln \Omega}. \quad (21)$$
Substituting for $\partial \ln (N_0 V)/\partial \ln \Omega$ from (15), we get the value of the logarithmic volume derivative of the effective interaction strength $N_0 V$. Similarly for the expression the electron-phonon coupling strength $\lambda$, the present expression for $\Phi$ is also qualitatively different than the results of Seiden [10], Sharma et al. [24], Jain and Kachhava [26] 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]. The required value of Gruneisen constant is taken as $\gamma_G=1.04$. The pressure dependence superconducting state parameters are displayed in Figures 1–5.

The pressure dependence of the electron-phonon coupling strength $\lambda$ has been evaluated by employing (14), upto 60% changes in the volume. The variation of $\lambda$ with volume on using EMC model potential is shown in Figure 1. It is noticed from the Figure 1 that, $\lambda$ values are quite sensitive to the local field correction functions. Also, the H-screening yields lowest values of $\lambda$, whereas the values 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 $\lambda$ is 35.86%-90.82%.

The variation of the Coulomb pseudopotential $\mu^*$ with volume is shown in Figure 2. A minimum is observed in this graph at $-\Delta \Omega/\Omega_G \approx 0.3$, which shows that the direct Coulomb repulsive interaction between the electrons becomes weakest at this pressure, so that the electron–phonon interaction may be most effective at this value. It is observed that the $\mu^*$ lies between 0.1974 and 0.2375, which is in accordance with McMillan [29], who suggested $\mu^* \approx 0.13$ for transition metals. The weak screening influence shows on the computed values of the $\mu^*$. The percentile influence of the various local field correction functions with respect to the static H-screening function on $\mu^*$ for Ca$_{70}$Zn$_{30}$ metallic glass superconductor is observed in the range of 7.71%-15.49%. Again the H-screening function yields lowest values of the $\mu^*$, 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 43.24%-109.46%. It has been observed that $T_c$ of Ca$_{70}$Zn$_{30}$ metallic glass decreases rapidly with increase of pressure upto 60% decrease of volume, for which the $\mu^*$ and $\Phi$ curves show a linear nature.

Figure 4 shows the variation of logarithmic volume derivative $\Phi$ of the effective interaction strength $N_p V$ with volume. It is seen that $\Phi$ is quite sensitive to the local field correction functions. It is also observed that the static H-screening function yields lowest $\Phi$ whereas the F-function yields highest values of $\Phi$. 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 $\Phi$ is 17.65%-38.36%. It is observed that the magnitude of $\Phi$ shows that the metallic glass under investigation lie in the range of weak coupling superconductors.

In Figure 5 variation of $\mu^*$ with volume has been shown on the same graph. The point of intersection of the $\mu^*$ curve with the $\lambda$ curve gives us the volume at which $\lambda = \mu^*$, so that the interaction strength tends to be zero and $\Phi$ tends to be infinity at this volume. From equation (17) of the transition temperature $T_c$, we can write approximately that $\lambda = \mu^*(1+0.62 \lambda)$, but near the point of quenching, the factor $(1+0.62 \lambda)$ is nearly tends to unity. Therefore, at that point we have taken only $\lambda = \mu^*$. The corresponding pressure may be called as the critical pressure, since the superconductivity will quench at this pressure. In the present work, the value for $-\Delta \Omega / \Omega_o$ at the critical pressure is found to be 0.35, 0.15, 0.15, 0.15 and 0.15 for H, T, IU, F and S-local field correction functions, respectively. These values show good agreement with $-\Delta \Omega / \Omega_o \cong 0.35, 0.15, 0.15, 0.15$ and 0.15 for H, T, IU, F and S-local field correction functions, respectively obtained from $\mu^*$ curve.

The effect of local field correction functions plays an important role in the computation of $\lambda$ and $\mu^*$, which makes drastic variation on $T_c$ and $\Phi$. 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$_{70}$Zn$_{30}$ 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.
Fig. 1 – Variation of electron-phonon coupling strength ($\lambda$) with change in volume.
Fig. 2 – Variation of Coulomb pseudopotential ($\mu^*$) with change in volume.
Fig. 3 – Variation of transition temperature ($T_c$) with change in volume.
Fig. 4 – Variation of logarithmic volume derivative (Φ) with change in volume.
Fig. 5 – Variation of electron-phonon coupling strength ($\lambda$) and Coulomb pseudopotential ($\mu^*$) with change in volume.
4. CONCLUSION

In conclusion we may add that the present theory provides overall satisfactory answer to the problems related with the effect of pressure on superconductivity if glasses in the considered system are superconducting or not in normal conditions, particularly in view of the fact that reliable experimental values of $\gamma_G$ at low temperatures are not available. Moreover, the present results can be improved if uncertainties involved in the values of $\mu^*$ and $\gamma_G$ are removed. The experimentally observed values of the dependence SSP are not available in the literature for Ca$_{70}$Zn$_{30}$ 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. Such study on pressure dependence SSP of other such metallic glasses is in progress.

REFERENCES

1. A. V. Narlikar and S. N. Ekbote, Superconductivity and superconducting materials (South Asian Publishers, New Delhi, Madras, 1983).