Theoretical Investigation of Superconducting State Parameters of \((Ni_{33}Zr_{67})_{1-x}Co_x\) Bulk Metallic Glasses

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ABSTRACT
In the present article, the study of the superconducting state parameters (SSP) viz. electron-phonon coupling strength \(\lambda\), Coulomb pseudopotential \(\mu^*\), transition temperature \(T_C\), isotope effect exponent \(\alpha\) and effective interaction strength \(N_0V\) of some bulk metallic glasses using Ashcroft’s empty core (EMC) model potential. Five different types of the local field correction functions due to Hartree (H), Taylor (T), Ichimaru-Utsumi (IU), Farid et al. (F) and Sarkar et al. (S) are used in the present investigation to see the screening effects on the aforesaid properties. Presently obtained \(T_C\) from Sarkar et al. (S) local field correction function is found an excellent agreement with available theoretical data. Quadratic equation has been proposed, which provide successfully the values of bulk metallic glasses under consideration. Also, the present results are found in qualitative agreement with other such earlier reported data, which confirms the superconducting phase in the glassy superconductors.

Keywords: pseudopotential, superconducting state parameters (SSP), bulk metallic glasses

1. INTRODUCTION
During last several years, the superconductivity remains a dynamic area of research in condensed matter physics with continual discoveries of novel materials and with an increasing demand for novel devices for sophisticated technological applications. Stable ternary glasses can be formed on addition of third element \((M)\) to binary metallic glasses. There are of interest since third element can modify the physical properties of binary metallic glasses and it can also be used as a probe to study the host. Influence of third element on the electronic and electron transport properties of binary metallic glasses and liquid metals and their alloys have been studied extensively [1-6] but its effect on superconducting properties has been given lesser attention. Only few researchers studied the superconducting properties of bulk metallic glasses using model potential formalism [6-13].

The study of the superconducting state parameters (SSP) of the bulk metallic glasses may be of great help in deciding their applications; the study of the dependence of the transition temperature \(T_C\) on the composition of metallic elements is helpful in finding new superconductors with high \(T_C\).
The application of pseudopotential to bulk metallic glasses involves the assumption of pseudoions with average properties, which are assumed to replace three types of ions in the ternary systems, and a gas of free electrons is assumed to permeate through them. The electron-pseudoion is accounted by the pseudopotential and the electron-electron interaction is involved through a dielectric screening function. For successful prediction of the superconducting properties of the alloying systems, the proper selection of the pseudopotential and screening function is very essential [6-13].

Therefore, it is decided to investigate the superconducting behaviour of \((Ni_{33}Zr_{67})_{1-x}Co_x\) \((x = 0, 0.05, 0.1)\) bulk metallic glasses. In this paper, well known McMillan’s theory [14] of the superconductivity is used for predicting the superconducting state parameters (SSP) of bulk metallic glasses. The Ashcroft’s empty core (EMC) model potential [15] is used to study the electron-phonon coupling strength \(\lambda\), Coulomb pseudopotential \(\mu^*\), transition temperature \(T_C\), isotope effect exponent \(\alpha\) and effective interaction strength \(NOV\) for the first time. To see the impact of various exchange and correlation functions on the aforesaid properties, five different types of local field correction functions proposed by Hartree (H) [16], Taylor (T) [17], Ichimaru-Utsumi (IU) [18], Farid et al. (F) [19] and Sarkar et al. (S) [20] are employed. More advanced local field correction functions due to IU [18], F [19] and S [20] with EMC model potential in the present computation of the superconducting state parameters (SSP) for bulk metallic glasses are used for the first time. Actually, our main aim of the present study is to check the validity of the appropriate local field correction functions. Therefore, various types of the local field correction functions are taken in the present computation.

In the present work, the pseudo-alloy-alloy atom (PAA) model was used to explain electron-ion interaction for alloying systems [7-11]. It is well known that the pseudo-alloy-alloy atom (PAA) model is a more meaningful approach to explain such kind of interactions in alloying systems. In the PAA approach a hypothetical monoatomic crystal is supposed to be composed of pseudo-alloy-atoms, which occupy the lattice sites and form a perfect lattice in the same way as pure metals. In this model the hypothetical crystal made up of PAA is supposed to have the same properties as the actual disordered alloy material and the pseudopotential theory is then applied to studying various properties of an alloy and metallic glass. The complete miscibility in the alloy systems is considered as a rare case. Therefore, in such alloying systems the atomic matrix elements in the pure states are affected by the characteristics of alloys such as lattice distortion effects and charging effects. In the PAA model, such effects are involved implicitly. In addition to this it also takes into account the self-consistent treatment implicitly. Looking to the advantage of the PAA model, propose use of PAA model for the first time to investigate the superconducting state parameters (SSP) of bulk metallic glasses.

2. THEORETICAL METHODOLOGY

The mathematical expressions used for the present investigation of \(\lambda\), \(\mu^*\), \(T_C\), \(\alpha\) and \(NOV\) are [7-12]

\[
\lambda = \frac{12m_e Z^2}{M(\sigma^2)} \int[X^\alpha][W][X] \, dX, 
\]

\[
\mu^* = \left[ \frac{m_e}{\pi\hbar^2} \int 0^\infty \frac{dx}{X^\alpha} \{X^\alpha + \ln \left( \frac{2\pi\hbar^2}{2m_e}\right) \} \right]^{1/2}, 
\]

\[
T_C = \frac{\alpha_D}{1.45} \exp \left[ \frac{-1.04 (1 + \lambda)}{\lambda - \mu^*(1 + 0.62 \lambda)} \right]. 
\]
Here is the band mass, $M$ the ionic mass, $\Omega$ the atomic volume, the Fermi wave vector and $<\omega^2>$ the averaged square phonon frequency, which is calculated using the relation given by Butler [21], $<\omega^2>^{1/2} = 0.69 \theta_D$, where $\theta_D$ is the Debye temperature of the $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x (x = 0, 0.05, 0.1)$ bulk metallic glasses, respectively. The well known screened Ashcroft’s empty core (EMC) model potential [15] used in the present computations of the SSP of $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x (x = 0, 0.05, 0.1)$ bulk metallic glasses, respectively. The well known screened Ashcroft’s empty core (EMC) model potential [15] used in the present computations of the SSP of $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x (x = 0, 0.05, 0.1)$ bulk metallic glasses is of the form,

$$w(x) = \frac{-\pi \lambda}{\Omega_O X^2 k_F^2} \cos(2k_F X r_C)$$

Where $\lambda$ is the parameter of the model potential of $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x (x = 0, 0.05, 0.1)$ amorphous superconductors and $\varepsilon/Xt$ he modified Hartree dielectric function [16]. 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 [7-12]. When used with a suitable form of dialectic screening functions, this potential has also been found to yield good results in computing the SSP of $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x (x = 0, 0.05, 0.1)$ bulk metallic glasses. As such we decided to employ this EMC form in the present work. Here the parameter $r_C$ is adjusted such that the calculated values of $T_C$ agree well with the experimental value of $T_C$ as close as possible.

3. RESULTS AND DISCUSSION

The values of the input parameters for the $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x (x = 0, 0.05, 0.1)$ bulk metallic glasses under investigation are assembled in Table 1. To determine the input parameters and various constants for PAA model [7-11], the following definition

$$A_{1-x}B_x (A = \text{Ni}_{33}\text{Zr}_{67}; B = \text{Co})$$

$Z = (1-x)(Z_A) + x(Z_B)$,

$M = (1-x)(M_A) + x(M_B)$,

$\Omega = (1-x)(\Omega_A) + x(\Omega_B)$,

$\theta_D = (1-x)(\theta_D) + x(\theta_D)$.

Where $x$ is the concentration factor of the ‘Co’ content. The input parameters such as $Z$, $\Omega$ and $M$ of the pure metallic components are taken from the literature [12]. The presently calculated results of the superconducting state parameters (SSP) are tabulated in Table 2 with other such theoretical [12] and experimental [4] findings. The graphical representation of the model potential parameter $r_C$ with the concentration $(x)$ of ‘Co’ are plotted in Figure 1. Also, the graphical analyses of the superconducting state parameters (SSP) of $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x (x = 0, 0.05, 0.1)$ bulk metallic glasses are also plotted in Figures 2-6.

The calculated values of the electron-phonon coupling strength $\lambda$ for $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x (x = 0, 0.05, 0.1)$ bulk metallic glasses, using five different types of the local field correction functions with EMC model potential, are shown in Table 2 with other theoretical data [12]. The graphical nature of $\lambda$ is also displayed in Figure 2. It is noticed 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 18.17%-52.45% for $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x (x = 0, 0.05, 0.1)$ bulk metallic glasses, respectively. It is also observed from the Table 2 that, $\lambda$ goes decreasing from the values of 0.7302→0.4571 as the concentration ‘$x$’ of ‘Co’ is increased from 0.0→0.15. The decrease in $\lambda$ with concentration ‘$x$’ of ‘Co’ shows a gradual transition from weak coupling behaviour to intermediate coupling behaviour of electrons and phonons, which may be attributed to an increase of the hybridization of sp-d electrons of ‘Co’ with increasing concentration ($Z$). This may also be attributed to the increase role of ionic vibrations in the Co-rich region. Presently computed $\lambda$ from S-local field correction function is found an excellent agreement with available theoretical data [12].

The computed values of the Coulomb pseudopotential $\mu^*$, which accounts for the Coulomb interaction between the conduction electrons, obtained from the various forms of the local field correction functions are tabulated in Table 2 with other theoretical data [12]. It is observed from the Table 2 that for $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x (x = 0, 0.05, 0.1)$ bulk metallic glasses, $\mu^*$ lies between 0.14

<table>
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<tr>
<th>Superconductors</th>
<th>SSP</th>
<th>Present results</th>
<th>Others</th>
<th>Expt.</th>
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<td>$(\text{Ni}<em>{33}\text{Zr}</em>{67})_{1-x}\text{Co}_x$</td>
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<td>$\mu^*$</td>
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<tr>
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<tr>
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<tr>
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<tr>
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and 0.16, which is in accordance with McMillan [14], who suggested $\mu^* \approx 0.13$ for transition metals. The graphs of $\mu^*$ versus concentration ($x$) for different local field correction functions are plotted in Figure 3, which shows the weak dependence of $\mu^*$ on the local field correction functions. The weak screening influence shows on the computed values of $\mu^*$. The percentile influence of the various local field correction functions with respect to the static H-screening function on $\mu^*$ for the superconductors is observed in the range of 5.26%-10.70%.

Table 2 contains calculated values of the transition temperature $T_C$ for $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x$ ($x = 0, 0.05, 0.1$) bulk metallic glasses computed from the various forms of the local field correction functions along with theoretical [12] and experimental [4] findings. The present results obtained from the S-local field correction functions are found in good agreement with available theoretical [12] and experimental [4] data. The calculated results of the transition temperature $T_C$ for $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x$ ($x = 0, 0.05, 0.1$) bulk metallic glasses deviate in the range of 0.02%-166.07% from the experimental findings [4], respectively. The variation of the computed values of the transition temperature $T_C$ for $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x$ ($x = 0, 0.05, 0.1$) bulk metallic glasses with the atomic concentration ($x$) of ‘Co’, using five different types of the local field correction functions with EMC potential are shown in Figure 4. The graph also includes the experimental findings [4]. It is seen that $T_C$ is quite sensitive to the local field.
correction functions, and the results of $T_C$ by using S-screening are in best agreement with experimental data [4] for the \((\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x\) \((x = 0, 0.05, 0.1)\) bulk metallic glasses under investigation, as the relevant curves for S-screening almost overlaps the theoretical curves. It is also seen from the graphical nature, $T_C$ decreases considerably with increasing Co-concentration \((x)\). The composition dependence can be described by polynomial regression of the data obtained for S-screening for different values of the concentration ‘\(x\)’, which yields

$$T_C (K) = -4.0x^2 - 5.4x + 2.68 \quad (11)$$

The graph of the fitted $T_C$ equation is displayed in Figure 4, which indicates that $T_C$ decreases considerably with increasing ‘Co’ content with a slope \(dT_C/dx = 5.4\). Wide extrapolation predicts a $T_C = 2.68K$ for the hypothetical case of ‘amorphous pure Ni$_{33}$Zr$_{67}$’ alloy. The linear $T_C$ Eq. (18) obtained in the present study closely resembles the linear $T_C$ equations

$$T_C (K) = -9.1800x^2 - 4.713x + 2.6734, \quad (12)$$

suggested by Sharma et al. [12] on the basis of experimental data for the system.

The presently computed values of the $T_C$ are found in the range, which is suitable for further exploring the applications of the superconductors for usage like lossless transmission line for cryogenic applications. While alloying elements show good elasticity and could be drawn in the form of wires as such they have good chances of being used as superconducting transmission lines at low temperature of the order of 7K.

The values of the isotope effect exponent \(\alpha\) for \((\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x\) \((x = 0, 0.05, 0.1)\) bulk metallic glasses are tabulated in Table 2. Figure 5 depicts the variation of \(\alpha\) with Cu-concentration \((x)\) decreases. The computed values of \(\alpha\) show a weak dependence on the dielectric screening function. Since the experimental value of has not been reported in the literature so far, the present data of \(\alpha\) may be used for the study of ionic vibrations in the superconductivity of alloying substances. Since S-local field correction function yields the best results for \(\alpha\) and \(T_C\), it may be observed that values obtained from this screening provide the best account for the role of the ionic vibrations in superconducting behaviour of

![Figure 4. Variation of transition temperature \((T_C)\) with Co-concentration \(x\) (at %).](image)

![Figure 5. Variation of isotope effect exponent \((\alpha)\) with Co-concentration \(x\) (at %).](image)
this system. The values of the effective interaction strength are listed in Table 2 and depicted in Figure 6 for different local field correction functions. It is observed that the magnitude of shows that the (0, 0.05, 0.1) bulk metallic glasses under investigation lie in the range of weak to intermediate superconductors.

The main difference of the local field correction functions are played in important role in the production of the superconducting state parameters (SSP) of (0, 0.05, 0.1) bulk metallic glasses. The Hartree (H) dielectric function [16] is purely static and it does not include the exchange and correlation effects. Taylor (T) [17] has introduced an analytical expression for the local field correction function, which satisfies the compressibility sum rule exactly. The Ichimaru-Utsumi (IU) local field correction function [18] 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. On the basis of Ichimaru-Utsumi (IU) local field correction function [18], Farid et al. (F) [19] and Sarkar et al. (S) [20] have given a local field correction function. Hence, Ichimaru-Utsumi (IU) [18] and Farid et al. (F) [19] functions represent same characteristic nature. Also, the superconducting state parameters (SSP) computed from Sarkar et al. (S) [20] local field correction are found in qualitative agreement with available theoretical data [12].

From the overall study of the superconducting properties, one can be observed that, the Hartree (H) screening function [16] yields lowest values, whereas the values obtained from the Farid et al. (F) [19] function are the highest, which suggested that the Sarkar et al. (S) screening function [20] found suitable in the present case than the other screening functions. Thus, the use of these more promising local field correction functions is established successfully. After introducing the screening effects in the pseudopotential, the results of the superconducting state parameters (SSP) are more affected due to nature of the local field correction functions.

The effect of local field correction functions is played an important role in the computation of and , which makes drastic variation on , and . The local field correction functions due to IU, F and S are able to generate consistent results regarding the superconducting state parameters (SSP) of (0, 0.05, 0.1) bulk metallic glasses as those obtained from more commonly employed Hartree (H) and Taylor (T) functions. The computed results of and are not showing any abnormal values for the (0, 0.05, 0.1) bulk metallic glasses.

It is observed that this simple methodology successfully explains superconducting behaviour of bulk metallic glasses without requiring the solution of
the Dirac equation for many body problem or estimation of various interactions as required in ab-initio pseudopotential theory. In the present work superconducting properties of bulk metallic glasses have been determined in the BCS-Eliashberg-McMillan framework. It is observed that addition of ‘Co’ as the third element (M) to a binary metallic systems (Ni_{33}Zr_{67}) causes the parameters $\lambda$, $T_C$, $\alpha$ and $NOV$ to decrease, and the Coulomb pseudopotential ($\mu^*$) to increase with concentration of the third element (M), showing that the presence of the third element (M) causes suppression of superconducting behaviour of the alloy. The decrease in with increasing concentration of the third element (M) may be attributed to the modifications in the density of states at the Fermi level $N(E_F)$, and probable changes in the band structure of the alloy due to addition of the third element (M) [12]. Both specific heat measurements and band structure calculation [1-4] reveal the decrease in density of states at $E_F$ with the addition of the third element (M). Since, is related to the modifications of density of states (DOS) at $E_F$, $N(E_F)$, decrease in $T_C$ can be related to the modifications of DOS at the Fermi level, $N(E_F)$ [12].

It is also observed that superconductivity persists only for small values of x (i.e. $x \leq 0.10$) which is because the third element (M) considered here are all 3d-transition metals which have smaller band width and stronger localized character than Zr, thus they causes narrowing of bands in ternary system [12]. These narrow bands have magnetic instabilities which prevent superconductivity as suggested by Allen and Dynes [22].

According to Matthias rules [23, 24], the bulk metallic glasses having $Z > 2$ do exhibit superconducting nature. Hence, $(Ni_{33}Zr_{67})_{1-x}Co_x \ (x = 0, 0.05, 0.1)$ bulk metallic glasses are exhibiting superconducting nature in the present case. When we go from $Z=3.21$ to $Z=3.34$, the electron-phonon coupling strength $\lambda$ changes with lattice spacing “a”. Similar trends are also observed in the values of $T_C$ for all bulk metallic glasses. Hence, a strong dependency of the superconducting state parameters (SSP) of the bulk metallic glasses on the valence ‘Z’ is found.

Lastly, it would like to emphasize the importance of involving a precise form for the pseudopotential. It must be confessed that although the effect of pseudopotential in strong coupling superconductor is large, yet it plays a decisive role in weak coupling superconductors i.e. those substances which are at the boundary dividing the superconducting and nonsuperconducting region. In other words, a small variation in the value of electron-ion interaction may lead to an abrupt change in the superconducting properties of the material under consideration. In this connection we may realize the importance of an accurate form for the pseudopotential.

4. CONCLUSIONS

Lastly, the H-local field corrections when used with EMC model potential provide the best explanation for superconductivity in $(Ni_{33}Zr_{67})_{1-x}Co_x \ (x = 0, 0.05, 0.1)$ bulk metallic glasses. The values of $\lambda$ and $T_C$ show an appreciable dependence on the local field correction function, whereas for $\mu^*$, $\alpha$ and $NOV$ a weak dependence is observed. The magnitude of $\lambda$, $\alpha$ and $NOV$ values shows that, the bulk metallic glasses are weak to intermediate superconductors. Quadratic $T_C$ equation has been proposed, which provide successfully the $T_C$ values of the bulk metallic glasses under
consideration. In the absence of experimental data for $\alpha$ and $\text{NOV}$, the presently computed values may be considered to form reliable data for these ternary systems, as they lie within the theoretical limits of the Eliashberg-McMillan formulation. The comparisons of presently computed results of the superconducting state parameters (SSP) of the $(\text{Ni}_{33}\text{Zr}_{67})_{1-x}\text{Co}_x$ ($x = 0, 0.05, 0.1$) bulk metallic glasses with available experimental findings are highly encouraging, which confirms the applicability of the EMC model potential and different forms of the local field correction functions. Such study on superconducting state parameters (SSP) of other multi component metallic alloys is in progress.

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