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Superconducting State Parameters of Be-Zr Glassy Alloys

Aditya M. VORA

Parmeshwari 165, Vijaynagar Area, Hospital Road, Bhuj-Kutch, 370 001, Gujarat-INDIA e-mail: voraam@yahoo.com

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Abstract

The theoretical investigation of the superconducting state parameters (SSP) viz. electron-phonon coupling strength λ , Coulomb pseudopotential μ^* , transition temperature T_C , isotope effect exponent α and effective interaction strength N_OV of Be_cZr_{1-c} (c=0.30, 0.35, 0.40 and 0.45) metallic glasses have been reported using Ashcroft's empty core (EMC) model potential for the first time. Five local field correction functions proposed by Hartree (H), Taylor (T), Ichimaru-Utsumi (IU), Farid et al. (F) and Sarkar et al. (S) are used in the present investigation to study the screening influence on the aforesaid properties. It is observed that the electron-phonon coupling strength λ and the transition temperature T_C are quite sensitive to the selection of the local field correction functions, whereas the Coulomb pseudopotential μ^* , isotope effect exponent α and effective interaction strength N_OV show weak dependences on the local field correction functions. The T_C obtained from H-local field correction function are found an excellent agreement with available theoretical or experimental data. Also, the present results are found in qualitative agreement with other such earlier reported data, which confirms the superconducting phase in the metallic glasses.

Key Words: Pseudopotential, superconducting state parameters, Be-Zr metallic glasses.

1. Introduction

The field of electron correlation in condensed matter, especially superconductivity, is one of the dynamic areas in condensed matter physics which involves discoveries of new and existing phenomena, novel materials and devices for sophisticated technological applications. During the last few years, superconducting metallic glasses based on various simple as well as transition metals have been obtained and studied by various researchers. The study of the SSP of the 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 glass is helpful in finding new superconductors with high T_C . Experiments also show that the superconducting transition temperature T_C is grater for amorphous metals than for crystals, which also depends on the composition of the metallic elements in the crystalline as well as amorphous phases [1–10]. Though the pseudopotential theory is found very successful in studying the various properties of the metallic glasses, there are very few scattered attempts to study the superconducting state parameters (SSP) of metallic glasses based on model potential [7–20]. The application of pseudopotential to a metallic glass involves the assumption of pseudoions with average properties, which are assumed to replace two types of ions in the binary systems, and a gas of free electrons is assumed to permeate through them. The electron-pseudoion is accounted for by

the pseudopotential and the electron-electron interaction is involved through a dielectric screening function. For successful prediction of the superconducting properties of the metallic glasses, the proper selection of the pseudopotential and screening function is very essential [4–20].

Out of very large numbers of the metallic glasses, the SSP of only few metallic glasses are reported based on the pseudopotential, so far. Recently, Vora et al. [4–11] have studied the SSP of some metals, Inbased binary alloys, alkali-alkali binary alloys, large number of metallic glasses, Cu-Zr metallic glasses using single parametric model potential formalism. The SSP of $Ca_{0.70}Mg_{0.30}$ metallic glass has been reported by Gupta et al. [18] and Sharma et al. [19]. The study on SSP of $Mg_{0.70}Zn_{0.30}$ glass was made by Agarwal et al. [20] and Gupta et al. [21]. They have used Ashcroft's empty core (EMC) model potential [22] in the computation of the SSP. The screening dependence of the SSP of $Ca_{0.70}Mg_{0.30}$ metallic glass has been studied by Sharma and Sharma [21] using Ashcroft's empty core (EMC) model potential [22], Sharma and Kachhava's linear potential [23] and Veljkovic and Slavic [24] model potential. The theoretical investigation of the SSP of Be_cAl_{1-c} metallic glasses i.e. $Be_{0.90}Al_{0.10}$ and $Be_{0.70}Al_{0.30}$ has been reported by Sharma et al. [16]. Experimental studies on the superconducting properties of Be_cZr_{1-c} (c = 0.30, 0.35, 0.40 and 0.45 at.%) metallic glasses have been reported by Hasegawa and Tanner [25].

In most of these studied, Ashcroft's empty core (EMC) model potential [22] is adopted in the calculation. But, nobody has used Hartree (H) [26], Taylor (T) [27], Ichimaru-Utsumi (IU) [28], Farid et al. (F) [29] and Sarkar et al. (S) [30] local field correction functions in their computation of the SSP. Also, Be and Zr being a good conductor and exhibits superconducting nature, this class of glasses may be quite suitable for industrial applications. Hence, in the present article, we decided to study the SSP viz. electron-phonon coupling strength λ , Coulomb pseudopotential μ^* , transition temperature T_C , isotope effect exponent α and effective interaction strength $N_O V$ of $Be_c Zr_{1-c}$ (c = 0.30, 0.35, 0.40 and 0.45 at.%) metallic glasses on the basis of Ashcroft's empty core (EMC) potential [22].

2. Computational Methodology

In the present investigation for Be_cZr_{1-c} metallic glasses, the electron-phonon coupling strength λ is computed using the relation [4–11]

$$\lambda = \frac{m_b \,\Omega_0}{4\pi^2 \,k_F \,M \,\langle\omega^2\rangle} \int_0^{2k_F} q^3 \,\left|V\left(q\right)\right|^2 \,dq. \tag{1}$$

Here m_b is the band mass, M the ionic mass, Ω_O the atomic volume, k_F the Fermi wave vector, V(q) the screened pseudopotential and $\langle \omega^2 \rangle$ the averaged square phonon frequency, of the binary glassy alloy, respectively. The effective averaged square phonon frequency $\langle \omega^2 \rangle$ is calculated using the relation given by Butler [31], $\langle \omega^2 \rangle^{1/2} = 0.69 \theta_D$, where θ_D is the Debye temperature of the metallic glasses.

Using $X = q/2k_F$ and $\Omega_O = 3\pi^2 Z/(k_F)^3$, we get equation (2) in the form,

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

where Z and W(X) are the valence of the metallic glasses and the screened Ashcroft's empty core pseudopotential [22] of the metallic glasses, respectively.

The well known screened Ashcroft's empty core (EMC) model potential [22] used in the present computations of the SSP of metallic glasses is of the form,

$$W(X) = \frac{-2\pi Z}{\Omega_O X^2 k_F^2 \varepsilon(X)} \cos\left(2k_F X r_C\right), \qquad (3)$$

where r_C is the parameter of the model potential of metallic glasses. The Ashcroft's empty core (EMC) model potential is a simple one-parameter model potential [22], which has been successfully found for various metallic complexes [10–21]. When used with a suitable form of dielectric screening functions, this potential has also been found to yield good results in computing the SSP of metallic glasses [10–21]. Therefore, in the present work we use Ashcroft's empty core (EMC) model potential with more advanced IU, F and S-local field correction functions for the first time. The model potential parameter r_C may be obtained by fitting either to some experimental data or to realistic form factors or other data relevant to the properties to be investigated. In the present work, r_C is fitted in such a way that, the presently computed values of the transition temperature T_C of the metallic glasses obtained from all local field correction functions are found as close as possible with the experimental data of T_C for metallic glasses whichever are available in the literature. After fitting the model potential parameter r_C , same r_C is then used in the computation of the SSP of binary metallic glasses.

The Coulomb pseudopotential μ^* is given by [4–11]

$$\mu^* = \frac{\frac{m_b}{\pi \, k_F} \int\limits_0^1 \frac{dX}{\varepsilon(X)}}{1 + \frac{m_b}{\pi \, k_F} \ln\left(\frac{E_F}{10 \, \theta_D}\right) \int\limits_0^1 \frac{dX}{\varepsilon(X)}},\tag{4}$$

where E_F is the Fermi energy and $\varepsilon(X)$ the modified Hartree dielectric function, which is written as [4–11]

$$\varepsilon(X) = 1 + (\varepsilon_H(X) - 1) (1 - f(X)).$$
(5)

 $\varepsilon_H(X)$ is the static Hartree dielectric function [4–11] and f(X) the local field correction function. In the present investigation, the local field correction functions due to H [26], T [27], IU [28], F [29] and S [30] are incorporated to see the impact of exchange and correlation effects. The details of all the local field corrections are below.

The H-screening function [26] is purely static, and it does not include the exchange and correlation effects and is thus expressed as

$$f(X) = 0. (6)$$

Taylor (T) [27] 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 T [27],

$$f(X) = \frac{q^2}{4k_F^2} \left[1 + \frac{0.1534}{\pi k_F^2} \right].$$
 (7)

The Ichimaru-Utsumi (IU)-local field correction function [28] 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 IU [28] local field correction function, Farid et al. (F) [29] have given a local field correction function of the form

$$f(X) = A_F Q^4 + B_F Q^2 + C_F + \left[A_F Q^4 + D_F Q^2 - C_F\right] \left\{\frac{4 - Q^2}{4Q} \ln \left|\frac{2 + Q}{2 - Q}\right|\right\}.$$
(9)

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Based on equations (8)-(9), Sarkar et al. (S) [30] have proposed a simple form of local field correction function, which is of the form

$$f(X) = A_S \left\{ 1 - \left(1 + B_S Q^4 \right) \exp \left(-C_S Q^2 \right) \right\}.$$
 (10)

where Q = 2X. 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 [28–30].

After evaluating λ and μ^* , the transition temperature T_C and isotope effect exponent α are investigated from the McMillan's formula [4–11]

$$T_C = \frac{\theta_D}{1.45} \exp\left[\frac{-1.04 \ (1+\lambda)}{\lambda - \mu^* \ (1+0.62\lambda)}\right],\tag{11}$$

$$\alpha = \frac{1}{2} \left[1 - \left(\mu^* \ln \frac{\theta_D}{1.45T_C} \right)^2 \frac{1 + 0.62\lambda}{1.04 \left(1 + \lambda \right)} \right].$$
(12)

The expression for the effective interaction strength $N_O V$ is studied using [4–11]

$$N_O V = \frac{\lambda - \mu^*}{1 + \frac{10}{11}\lambda}.$$
 (13)

3. Results and Discussion

The input parameters are other constants used in the present computation of the SSP of Be_cZr_{1-c} metallic glasses are shown in Table 1. The presently calculated results of the SSP are tabulated in Table 2 with the experimental [25] findings.

Metallic glass	Ζ	r_C	Ω_O	M	θ_D	$\left\langle \omega^2 \right\rangle^2 (\mathrm{au})^2 \times 10^{-6}$
		(au)	$(au)^3$	(amu)	(K)	
$\mathrm{Be}_{0.45}\mathrm{Zr}_{0.55}$	3.10	0.8786	113.54	54.23	785.55	1.8412
$\mathrm{Be}_{0.40}\mathrm{Zr}_{0.60}$	3.20	0.8781	117.75	58.34	730.60	2.1816
$\mathrm{Be}_{0.35}\mathrm{Zr}_{0.65}$	3.30	0.9040	123.81	62.45	675.65	2.5509
${\rm Be}_{0.30}{\rm Zr}_{0.70}$	3.40	0.9457	129.67	66.56	620.70	2.9490

Table 1. Input parameters and other constants.

The calculated values of the electron-phonon coupling strength λ for Be_cZr_{1-c} metallic glasses, using five different types of the local field correction functions with EMC model potential, are shown in Table 2 with other experimental data [25]. It is noticed from the Table 1 that, λ vales are quite sensitive to the local field correction functions. 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 21.30%-40.40%, 21.38%-40.53%, 21.40%-39.91% and 21.22%-38.62% for Be_{0.45}Zr_{0.55}, Be_{0.40}Zr_{0.60}, Be_{0.35}Zr_{0.65} and Be_{0.30}Zr_{0.70} metallic glasses, respectively. Also, the H-screening yields lowest values of λ , whereas the values obtained from the F-function are the highest. It is also observed from the Table 2 that, λ goes on increasing from the values of 0.4173 \rightarrow 0.6849 as the concentration c of Zr is increased from 0.10-0.30. The increase in λ with concentration c of Zr shows a gradual transition from weak coupling behavior to intermediate coupling behavior of electrons and phonons, which may be attributed to an increase of the hybridization of sp-d electrons of Zr with increasing concentration c, as was also observed by Minnigerode and Samwer [32]. This may also be attributed to the increase role of ionic vibrations in the Zr-rich region [16]. The calculated results of the electron-phonon coupling strength λ for Be_{0.40}Zr_{0.60},

Be_{0.35}Zr_{0.65} and Be_{0.30}Zr_{0.70} metallic glasses deviate in the range of 40.84%-48.90%, 43.67%-59.74% and 54.34%-67.06% from the experimental findings [25], respectively. The presently computed values of the electron-phonon coupling strength λ are found in the qualitative agreement with the available experimental data [25].

Glass	SSP		Evot [23]				
		Н	Т	IU	F	S	Expt. [25]
$\mathrm{Be}_{0.45}\mathrm{Zr}_{0.55}$	λ	0.4173	0.5601	0.5848	0.5859	0.5062	-
	μ^*	0.1454	0.1588	0.1607	0.1610	0.1530	0.13
	T_C (K)	1.0020	4.9874	5.9899	6.0097	3.1961	≤ 1.0
	α	0.1423	0.2698	0.2834	0.2829	0.2413	-
	N_0V	0.1971	0.2659	0.2769	0.2772	0.2419	-
${ m Be}_{0.40}{ m Zr}_{0.60}$	λ	0.4631	0.6221	0.6496	0.6508	0.5621	1.1
	μ^*	0.1441	0.1572	0.1590	0.1593	0.1515	0.13
	T_C (K)	2.1018	7.7616	9.0308	9.0582	5.3736	2.10
	α	0.2365	0.3233	0.3329	0.3325	0.3036	-
	N_0V	0.2245	0.2969	0.3085	0.3088	0.2717	-
Be _{0.35} Zr _{0.65}	λ	0.4831	0.6468	0.6748	0.6759	0.5865	1.2
	μ^*	0.1430	0.1559	0.1577	0.1580	0.1504	0.13
	T_C (K)	2.6012	8.5481	9.8081	9.8286	6.1643	2.60
	α	0.2682	0.3410	0.3490	0.3486	0.3252	-
	N_0V	0.2363	0.3091	0.3205	0.3208	0.2845	-
${ m Be}_{0.30}{ m Zr}_{0.70}$	λ	0.4941	0.6570	0.6839	0.6849	0.5990	1.5
	μ^*	0.1417	0.1544	0.1562	0.1565	0.1490	0.13
	T_C (K)	2.8027	8.4972	9.6286	9.6428	6.3322	2.80
	α	0.2866	0.3504	0.3572	0.3568	0.3375	-
	N_0V	0.2432	0.3146	0.3254	0.3257	0.2913	-

Table 2. Superconducting state parameters of the Be-Zr metallic glasses.

The computed values of the Coulomb pseudopotential μ^* , 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 experimental data [25]. It is observed from the Table 2 that for all metallic glasses, the μ^* lies between 0.15 and 0.18, which is in accordance with Mcmillan [33], who suggested $\mu^* \approx 0.13$ for simple and transition metals. Hasegawa and Tanner [25] have also been taken $\mu^* = 0.13$ in their study of Be-Zr metallic glasses. 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 the metallic glasses is observed in the range of 5.23%-10.73%, 5.14%-10.55%, 5.14%-10.50% and 5.14%-10.43% for Be_{0.45}Zr_{0.55}, Be_{0.40}Zr_{0.60}, Be_{0.35}Zr_{0.65} and Be_{0.30}Zr_{0.70} metallic glasses, respectively. Again the H-screening function yields lowest values of the μ^* , while the values obtained from the F-function are the highest. The present results are found in good agreement with the available experimental data [25]. Here also, as the concentration c of Zr (in at.%) increases the present results of μ^* decreases.

Table 2 contains calculated values of the transition temperature T_C for $Be_c Zr_{1-c}$ metallic glasses computed from the various forms of the local field correction functions along with the experimental [25]. From the Table 2 it can be noted that, the static H-screening function yields lowest T_C whereas the F-function yields highest values of T_C . The present results obtained from the H-local field correction functions are found in good agreement with available experimental data [25]. It is seen that T_C is quite sensitive to the local field correction functions, and the results of T_C by using H-screening are in best agreement with the experimental data for the $Be_c Zr_{1-c}$ metallic glasses under investigation. The percentile influence of the various local field correction functions with respect to the static H-screening function on T_C for the metallic glasses is

observed in the range of 218.79%-499.77%, 155.67%-330.97%, 136.98%-277.85% and 125.93%-244.05% for $Be_{0.45}Zr_{0.55}$, $Be_{0.40}Zr_{0.60}$, $Be_{0.35}Zr_{0.65}$ and $Be_{0.30}Zr_{0.70}$ metallic glasses, respectively. The calculated results of the transition temperature T_C for $Be_{0.45}Zr_{0.55}$, $Be_{0.40}Zr_{0.60}$, $Be_{0.35}Zr_{0.65}$ and $Be_{0.30}Zr_{0.70}$ metallic glasses deviate in the range of 0.2%-500.97%, 0.09%-331.34%, 0.05%-278.02% and 0.10%-244.39% from the experimental findings [25], respectively. Also, the above observations indicate that simple metallic glasses having high valence (more than two) tend to have higher T_C . Perhaps only exception is divalent Be-Zr metallic glasses where high T_C is likely to be due to unusually high Debye temperature. The higher values of T_C may be due to the electron transfer between the transition metal and other metallic element. The increase in T_C has also been attributed to the excitonic mechanism resulting from the granular structure separated by semiconducting or insulating materials [2].

The subtle difference of the shift among the glassy Be-Zr alloys may be reflected in the values of the electron-phonon coupling strength λ . Since both the density and the values of the electron-phonon coupling strength λ are larger for Be_{0.30}Zr_{0.70} alloys than those for the Be_{0.40}Zr_{0.60} alloy, a larger shift of the centre of gravity of the phonon spectrum toward lower phonon energy for the former than the latter alloy may be expected. If such a trend toward a softer phonon spectrum is related to the degree of the disorder increases as Be content decreases in the Be-Zr glassy system, which was reported by Hasegawa and Tanner [25] from the glass transition temperature T_g . From this, we may thus conclude that the increase of T_C or λ with decreasing Be in the Be-Zr glassy system is due to the increase of the degree of structural disorder as was noted by Hasegawa and Tanner [25].

The presently computed values of the T_C are found in the range, which is suitable for further exploring the applications of the metallic glasses for usage like lossless transmission line for cryogenic applications. While metallic glasses 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 7 K.

The values of the isotope effect exponent α for Be_cZr_{1-c} metallic glasses are tabulated in Table 2. The computed values of the α show a weak dependence on the dielectric screening, its value is being lowest for the H-screening function and highest for the F-function. The negative value of the α is observed in the case of metallic glasses, which indicates that the electron-phonon coupling in these metallic complexes do not fully explain all the features regarding their superconducting behaviour. Since the experimental or theoretical values of α has not been reported in the literature so far, the present data of α may be used for the study of ionic vibrations in the superconductivity of amorphous substances. Since H-local field correction function yields the best results for λ and T_C , it may be observed that α values obtained from this screening provide the best account for the role of the ionic vibrations in superconducting behaviour of this system. The most important feature noted here is that as the concentration c of Zr (in at.%) increases the present results of α increases sharply.

The values of the effective interaction strength $N_O V$ are listed in Table 2 for different local field correction functions. It is observed that the magnitude of $N_O V$ shows that the metallic glasses under investigation lie in the range of weak coupling superconductors. The values of the $N_O V$ also show a feeble dependence on dielectric screening, its value being lowest for the H-screening function and highest for the F-screening function. The variation of present values of the $N_O V$ show that, the metallic glasses under consideration fall in the range of weak coupling superconductors. Here also, as the concentration c of Zr (in at.%) increases the present results of $N_O V$ increases.

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 , α and N_OV . The local field correction functions due to IU, F and S are able to generate consistent results regarding the SSP of the metallic glasses 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. The computed results of α and N_OV are not showing any abnormal values for $Be_c Zr_{1-c}$ metallic glasses.

Lastly, we 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 we concluded that, the H, T, IU, F and S-local field corrections when used with EMC model potential provide the best explanation for superconductivity in the Be_cZr_{1-c} system. The values of the electron-phonon coupling strength λ and the transition temperature T_C show an appreciable dependence on the local field correction function, whereas for the Coulomb pseudopotential μ^* , isotope effect exponent α and effective interaction strength N_OV a weak dependence is observed. The magnitude of the λ , α and N_OV values shows that Be_cZr_{1-c} metallic glasses are weak to intermediate superconductors. In the absence of experimental data for α and N_OV , the presently computed values of these parameters may be considered to form reliable data for Be_cZr_{1-c} metallic glasses, as they lie within the theoretical limits of the Eliashberg-McMillan formulation. It is also concluded that, the Be_cZr_{1-c} metallic glasses are favored superconductors. The comparisons of presently computed results of the SSP of Be_cZr_{1-c} metallic glasses with available theoretical and experimental findings are highly encouraging, which confirms the applicability of the EMC model potential and different forms of the local field correction functions.

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