STUDY OF SUPERCONDUCTING STATE PARAMETERS OF AMORPHOUS ALLOYS

A. M. Vora

Humanities and Social Science Department, STBS College of Diploma Engineering, Opp. Spinning Mill,

Varachha Road, Surat 395006, Gujarat, INDIA

PACS number: 74.70.-b

Abstract

Theoretical study of superconducting state parameters (SSP) viz. the electron-phonon coupling strength λ , Coulomb pseudopotential μ^* , transition temperature T_c , isotope effect exponent α , and effective interaction strength N_0V of five Mg_{0.70}Zn_{0.30-x}Ga_x (x = 0.0, 0.06, 0.10, 0.15 and 0.20) ternary amorphous alloys is carried out using the Ashcroft's empty core (EMC) model potential. Five local-field correction functions due to Hartree (H), Taylor (T), Ichimaru–Utsumi (IU), Farid et al. (F) and Sarkar et al. (S) are used to study the screening influence. 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_0V show weak dependences on the local-field correction functions. The value of T_c obtained from H-local-field correction function are found in excellent agreement with available experimental data. Also, the present results are found in qualitative agreement with other such earlier reported data, which confirms the superconducting phase in the ternary amorphous alloys.

Keywords: Pseudopotential; superconducting state parameters; ternary amorphous alloys. PACS Numbers: 61.43.Dq; 71.15.Dx; 74.20.–z; 74.70.Ad

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. A large number of metals and amorphous alloys are superconductors, with critical temperature T_C ranging from 1 to 18K [1–11]. The pseudopotential theory has been used successfully in explaining the superconducting state parameters (SSP) for metallic complexes by many workers [1–11]. Many of them have used well-known model pseudopotential in the calculation of the SSP for the metallic complexes. Recently, Vora et al. [3–11] have studied the SSP of some metals, In-based binary alloys, alkali-alkali binary alloys and large number of metallic glasses using single parametric model potential formalism. The study of SSP of the ternary alloy-based superconductors 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 ternary amorphous alloys 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 interaction is accounted for by the pseudopotential and the electron–electron interaction is involved through a dielectric screening function. For successful prediction of superconducting properties of the alloying systems, the proper selection of the pseudopotential and screening function is very essential [3–11].

The possible technological applications of metals with high superconducting transition temperature T_c have generated great interest in the study of the group VB transition metals, V, Nb and Ta, which exhibit high T_c in general [12]. Therefore, in the present work, we have used the well-known McMillan's theory [13] of superconductivity for predicting the SSP of five Mg_{0.70}Zn_{0.30}Ga_{0.00}, Mg_{0.70}Zn_{0.24}Ga_{0.06}, Mg_{0.70}Zn_{0.20}Ga_{0.10}, Mg_{0.70}Zn_{0.15}Ga_{0.15} and Mg_{0.70}Zn_{0.10}Ga_{0.20} ternary amorphous alloys. We have incorporated here the Ashcroft's empty core (EMC) model potential [13] for studying the electron–phonon coupling strength λ , Coulomb pseudopotential μ^* , transition temperature T_c , isotope effect exponent α , and effective interaction strength N_0V . To reveal the impact of various exchange and correlation functions on the aforesaid properties, we have employed here five different types of local-field correction functions proposed by Hartree (H) [14], Taylor (T) [15], Ichimaru–Utsumi (IU) [16], Farid et al. (F) [17], and Sarkar et al. (S) [18].

In the present work, the pseudo-alloy-atom (PAA) model was used to explain the electron-ion interaction for alloying systems [3-11]. It is well known that the 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 a 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 the 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, we propose a use of PAA model for the first time to investigate the SSP of metallic glasses.

2. Computational Methodology

In the present investigation for ternary amorphous alloys, the electron–phonon coupling strength λ is computed using the relation [3-11]

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$$\lambda = \frac{m_{\rm b} \,\Omega_0}{4\pi^2 \,k_{\rm F} \,M\langle\omega^2\rangle} \int_0^{2k_{\rm F}} q^3 \left| V(q) \right|^2 \mathrm{d}q \,. \tag{1}$$

Here m_b is the band mass, M the ionic mass, Ω_0 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 ternary amorphous alloys. The effective averaged square phonon frequency $\langle \omega^2 \rangle$ is calculated using the relation given by Butler [19], $\langle \omega^2 \rangle^{1/2} = 0.69 \theta_D$, where θ_D is the Debye temperature of the ternary amorphous alloy.

Using $X = q/2k_F$ and $\Omega_0 = 3\pi^2 Z/(k_F)^3$, we get Eq. (1) in the following form,

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

where Z and W(X) are the valence and the screened EMC pseudopotential [13] of the ternary amorphous alloys, respectively.

The well-known screened Ashcroft's empty core (EMC) model potential [13] used in the present computations is of the form

$$W(X) = \frac{-2\pi Z}{\Omega_0 X^2 k_F^2 \varepsilon(X)} \cos(2k_F X r_C), \qquad (3)$$

where r_c is the parameter of the model potential of ternary amorphous alloys. The Ashcroft's EMC model potential is a simple one-parameter model potential [13], which has been successfully found for various metallic complexes [5–8]. 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 complexes [5–8]. 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 with experimental T_c of the ternary amorphous alloys for most of the local-field correction functions.

The Coulomb pseudopotential μ^* is given by the formula [3–11]

$$\mu^{*} = \frac{\frac{m_{b}}{\pi k_{F}} \int_{0}^{1} \frac{dX}{\epsilon(X)}}{1 + \frac{m_{b}}{\pi k_{F}} \ln\left(\frac{E_{F}}{10\theta_{D}}\right) \int_{0}^{1} \frac{dX}{\epsilon(X)}},$$
(4)

where E_F is the Fermi energy, m_b the band mass of the electron, θ_D the Debye temperature and $\varepsilon(X)$ the modified Hartree dielectric function, which is written as [14]

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$$\varepsilon(\mathbf{X}) = 1 + (\varepsilon_{\mathrm{H}}(\mathbf{X}) - 1)(1 - f(\mathbf{X})), \tag{5}$$

 $\varepsilon_{\rm H}(X)$ is the static Hartree dielectric function [14], and f(X) the local-field correction function. In the present investigation, the local-field correction functions due to H, T, IU, F and S are incorporated to see the impact of exchange and correlation effects.

The H-screening function [14] is purely static, and does not include the exchange and correlation effects. The expression of it is

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

Taylor (T) [15] 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) [15],

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

The Ichimaru–Utsumi (IU) local-field correction function [16] 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 satisfies the self-consistency condition in the compressibility sum rule and short-range correlations. The fitting formula has the form

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

On the basis of Ichimaru–Utsumi (IU) local-field correction function [16], Farid et al. (F) [17] have given a local-field correction function of the form

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

Based on Eqs. (8) and (9), Sarkar et al. (S) [18] have proposed a simple form of the local-field correction function, which is of the form

$$f(q) = A_s \left\{ 1 - \left(1 + B_s Q^4\right) \exp\left(-C_s Q^2\right) \right\}$$

where $Q = q/k_F$. 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 [16–18].

After evaluating λ and μ^* , the transition temperature T_c and isotope effect exponent α are determined from the McMillan's formula [3–11, 12]

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$$T_{\rm C} = \frac{\theta_{\rm D}}{1.45} \exp\left[\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right],$$
(11)

$$\alpha = \frac{1}{2} \left[1 - \left(\mu^* \ln \frac{\theta_{\rm D}}{1.45 {\rm T}_{\rm C}} \right)^2 \frac{1 + 0.62 \lambda}{1.04 (1 + \lambda)} \right].$$
(12)

The expression for the effective interaction strength N_0V is studied using the expression [3–11]

$$N_{0}V = \frac{\lambda - \mu^{*}}{1 + \frac{10}{11}\lambda}.$$
(13)

3. Results and discussion

The values of the input parameters for the ternary amorphous alloys under investigation are assembled in Table 1. To determine the input parameters and various constants for the PAA model [3–11], the following definitions fA + gB + hC are adopted,

$$Z = fZ_A + g Z_B + hZ_C, \qquad (14)$$

$$M = fM_A + gM_B + hM_C, (15)$$

$$\Omega_o = f \Omega_{OA} + g \Omega_{OB} + h \Omega_{OC} \,. \tag{16}$$

where *A*, *B* and *C* are denoted the first, second and third pure metallic components. *f*, *g* and *h* the concentration factor of the first, second and third metallic components. The input parameters such as *Z*, Ω_o and *M* of the pure metallic components are taken from the literature [7, 8]. The values of the Debye temperature θ_D of the ternary glassy alloys are directly obtained from [12]. The presently calculated results of the SSP are tabulated in Table 2 with the other such experimental findings [12].

Table 1. Input parameters and other constants.

Superconductors	Ζ	<i>r_c</i> , a.u.	$\Omega_0, (a.u.)^3$	<i>M</i> , a.m.u.	θ_D, K	$\left< \omega^2 \right>^2$, a.u. ² ×10 ⁻⁶
Mg _{0.70} Zn _{0.30} Ga _{0.00}	2.00	1.0446	139.73	36.63	308	1.82409
Mg _{0.70} Zn _{0.24} Ga _{0.06}	2.06	1.0523	141.49	36.89	307	1.81226
Mg _{0.70} Zn _{0.20} Ga _{0.10}	2.10	1.0551	142.67	37.06	307	1.81226
Mg _{0.70} Zn _{0.15} Ga _{0.15}	2.15	1.0870	144.14	37.28	294	1.66203
Mg _{0.70} Zn _{0.10} Ga _{0.20}	2.20	1.0776	145.61	37.50	294	1.66203

The calculated values of the electron-phonon coupling strength λ are shown in Table 2 with available experimental data [12]. 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 λ is

27.66%–51.07%, 27.38%–50.18%, 27.21%–49.70%, 26.66%–47.76% and 26.62%–47.83% for Mg_{0.70}Zn_{0.30}Ga_{0.00}, Mg_{0.70}Zn_{0.24}Ga_{0.06}, Mg_{0.70}Zn_{0.20}Ga_{0.10}, Mg_{0.70}Zn_{0.15}Ga_{0.15} and Mg_{0.70}Zn_{0.10}Ga_{0.20}, respectively. Also, the H-screening yields the lowest values of λ , whereas the values obtained from the F-function are the highest. It is also observed from Table 2 that λ goes increasing from the values of 0.3631 \rightarrow 0.5884 as the concentration *h* of Ga is increased from 0.0 \rightarrow 0.20. The increase in λ with the concentration *h* of Ga shows a gradual transition from a weak coupling behavior to an intermediate coupling behavior of electrons and phonons, which may be attributed to an increase in the hybridization of sp-d electrons of Ga with increasing concentration *h*. This may also be attributed to the increasing role of ionic vibrations in the Ga-rich region. The present results are found in qualitative agreement with the available experimental data [12].

The computed values of the Coulomb pseudopotential μ^* , which accounts for the Coulomb interaction between the conduction electrons, are presented in Table 2. It is observed from Table 2 that μ^* lies between 0.13 and 0.16, which is in accordance with McMillan [20], who suggested $\mu^* \approx 0.13$ for simple and non-simple metals. The weak screening influence shows on the computed values of μ^* . The percentile influence of the various local-field correction functions with respect to the static H-screening function on μ^* for the ternary amorphous alloys is observed in the range of 6.03%–11.158%, 5.99%–11.12%, 5.98%–11.11%, 5.91%–10.99% and 5.87%–10.93% for Mg_{0.70}Zn_{0.30}Ga_{0.00}, Mg_{0.70}Zn_{0.24}Ga_{0.06}, Mg_{0.70}Zn_{0.20}Ga_{0.10}, Mg_{0.70}Zn_{0.15}Ga_{0.15} and Mg_{0.70}Zn_{0.10}Ga_{0.20} ternary amorphous alloys, respectively. Again the H-screening function yields the lowest values of μ^* , while the values obtained from the F-function are the highest.

Table 2 contains calculated values of the transition temperature T_c along with the experimental findings [12]. It can be noted that the static H-screening function yields lowest T_c whereas the F-function yields the 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 [12]. The theoretical data of T_c for five Mg_{0.70}Zn_{0.30-x}Ga_x ternary amorphous alloys are not available in the literature. The calculated results of the transition temperature T_c for Mg_{0.70}Zn_{0.30}Ga_{0.00}, Mg_{0.70}Zn_{0.24}Ga_{0.06}, Mg_{0.70}Zn_{0.20}Ga_{0.10}, Mg_{0.70}Zn_{0.15}Ga_{0.15} and Mg_{0.70}Zn_{0.10}Ga_{0.20} ternary amorphous alloys deviate in the range of 80.56%–100.00%, 75.51%–130.03%, 72.54%–124.47%, 62.40%–106.08% and 94.89%–95.58% from the experimental findings, respectively.

The presently computed values of T_c are found in the range, which is suitable for further exploring the applications of the ternary amorphous alloys for usage like lossless transmission line for cryogenic applications. While alloying elements show good elasticity and could be drawn in the

form of wires because they have good chances of being used as superconducting transmission lines at low temperature of the order of 7K.

Amorphous alloys	SSP		Exp.,				
		Н	Т	IU	F	S	[12]
Mg _{0.70} Zn _{0.30} Ga _{0.00}	λ	0.3631	0.5176	0.5471	0.5485	0.4635	0.297
	μ*	0.1432	0.1570	0.1589	0.1592	0.1518	_
	<i>T_C</i> , K	0.1112	1.3120	1.7254	1.7395	0.7266	0.111, 0.1125
	α	-0.0059	0.2331	0.2566	0.2565	0.1857	-
	N_0V	0.1653	0.2452	0.2593	0.2598	0.2193	_
Mg _{0.70} Zn _{0.24} Ga _{0.06}	λ	0.3676	0.5216	0.5507	0.5521	0.4682	0.302
	μ^{*}	0.1427	0.1564	0.1583	0.1586	0.1512	_
	<i>T_C</i> , K	0.1303	1.3858	1.8041	1.8163	0.7896	0.130, 0.11
	α	0.0194	0.2414	0.2635	0.2633	0.1978	_
	N_0V	0.1686	0.2478	0.2615	0.2620	0.2223	-
Mg _{0.70} Zn _{0.20} Ga _{0.10}	λ	0.3711	0.5252	0.5543	0.5556	0.4721	0.305
	μ^{*}	0.1424	0.1560	0.1579	0.1582	0.1509	_
	<i>T_C</i> , K	0.1461	1.4527	1.8784	1.8899	0.8420	0.146
	α	0.0364	0.2475	0.2687	0.2684	0.2062	_
	N_0V	0.1710	0.2499	0.2636	0.2640	0.2247	_
Mg _{0.70} Zn _{0.15} Ga _{0.15}	λ	0.3815	0.5345	0.5627	0.5637	0.4832	0.317
	μ^{*}	0.1412	0.1546	0.1564	0.1567	0.1495	_
	<i>T_C</i> , K	0.1950	1.5787	1.9963	2.0033	0.9721	0.195
	α	0.0857	0.2651	0.2832	0.2828	0.2313	_
	N_0V	0.1784	0.2557	0.2688	0.2691	0.2318	-
Mg _{0.70} Zn _{0.10} Ga _{0.20}	λ	0.3980	0.5577	0.5873	0.5884	0.5039	0.333
	μ^{*}	0.1409	0.1542	0.1560	0.1563	0.1492	_
	<i>T_C</i> , K	0.2931	1.9873	2.4689	2.4777	1.2668	0.293, 0.306
	α	0.1359	0.2888	0.3046	0.3042	0.2595	_
	N_0V	0.1888	0.2678	0.2812	0.2815	0.2433	-

Table 2. Superconducting state parameters of $Mg_{0.70}Zn_{0.30-x}Ga_x$ amorphous alloys.

The values of the isotope effect exponent α for five $Mg_{0.70}Zn_{0.30-x}Ga_x$ ternary amorphous alloys are given in Table 2. The computed values of 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 Mg_{0.70}Zn_{0.30}Ga_{0.00} ternary alloy, which indicates that the electron–phonon coupling in these metallic complexes does not fully explain all the features regarding their superconducting behaviour. Since the experimental value 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 alloying 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 ionic vibrations in superconducting behavior of this system.

The values of the effective interaction strength N_0V are listed in Table 2 for different local field correction functions. It is observed that the magnitude of N_0V shows that the five $Mg_{0.70}Zn_{0.30-x}Ga_x$ ternary amorphous alloys under investigation lie in the range of weak coupling superconductors. The values of N_0V 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 main difference of the local-field correction functions plays an important role in the calculation of the SSP of ternary amorphous alloys. On the basis of Ichimaru–Utsumi (IU) local-field correction function [16], Farid et al. (F) [17] and Sarkar et al. [18] have given a local-field correction functions. Hence, F-function represents the same characteristic nature. Also, the SSP computed from Sarkar et al. [18] local-field correction are found in qualitative agreement with the available experimental data [12]. Our main aim in the present study is to check the applicability of the local-field correction functions with respect to the Hartree (H) dielectric function [14].

The numerical values of the aforesaid properties are found to be quite sensitive to the selection of the local-field correction function and show a significant variation with the change in the function. The local-field correction functions due to IU, F and S are able to generate consistent results of the SSP of ternary amorphous alloys 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 theoretical data for SSP for ternary superconductors are not available in the literature for detailed comparison, but the comparison with other such theoretical values is encouraging, which confirms the applicability of EMC model potential in explaining the superconducting state parameters of ternary alloys.

According to Matthias rules [21] the alloys having Z > 2 exhibit a superconducting nature. Hence, the presently computed ternary amorphous alloys are the superconductors. Also when we go from Z = 2.00 to Z = 20, the electron–phonon coupling strength λ changes with the lattice constant a. Similar trends are also observed in the values of the transition temperature T_c . Hence, a strong dependence of the SSP of the ternary amorphous alloys on the valence Z is found, which is shown in Figure. Also from the presently computed results of the SSP of ternary amorphous alloys, we observe that as the atomic volume Ω_0 increases the SSP increases.



Superconducting temperature versus the valence of the ternary amorphous alloys

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 superconductors 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 conclude that the H-local-field corrections when used with the EMC model potential provides the best explanation for superconductivity in the ternary systems. The values of λ and T_c show an appreciable dependence on the local-field correction functions, whereas for μ^* , α and N_0V a weak dependence is observed. The values of λ , α and N_0V show that ternary amorphous alloys are weak to intermediate superconductors. In the absence of experimental data for α and N_0V , the presently computed values of these parameters may be considered to form reliable data for these ternary systems, as they lie within the theoretical limits of the Eliashberg– McMillan formulation. The comparison of presently computed results of the SSP with available experimental findings is highly encouraging, which confirms the applicability of the EMC model potential and different forms of the local-field correction functions. Such study on SSP of other multicomponent metallic alloys is in progress.

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