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RESEARCH ARTICLE

Aditya M. VORA

Superconducting state parameters of Cu_CZr_{100-C} metallic glasses

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_0V of ten Cu_CZr_{100-C} metallic glasses have been reported using Ashcroft's empty core (EMC) model potential. Three local field correction functions proposed by Hartree (H), Taylor (T) and Ichimaru-Utsumi (IU) are used in the current 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_0V show weak dependences on local field correction functions. The T_c obtained from IU-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 metallic glasses.

Keywords pseudopotential, superconducting state parameters, Cu-Zr metallic glasses

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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 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 greater for amorphous metals than for crystals, which also depends on the composition of the metallic elements in the crystalline as well as amorphous phases [1−19]. Though the pseudopotential theory is found very successful in studying the various properties of metallic glasses, there are very few scattered attempts to study the superconducting state parameters (SSP) of metallic glasses based on model potential [1−19]. The application of pseudopotential to a metallic glass involves the assumption of pseudo-ions 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. For successful prediction of the superconducting properties of metallic glasses, the proper selection of the pseudopotential and screening function is very essential [4–19].

Out of very large numbers of metallic glasses, the SSP of only few metallic glasses are reported based on the pseudopotential, so far. Recently, Vora *et al.* [4–9] 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 SSP of $Ca_{70}Mg_{30}$ metallic glass has been reported by Gupta *et al.* [15] and Sharma *et al.* [16]. The study on SSP of $Mg_{70}Zn_{30}$

Aditya M. VORA (✉)
Parmeshwari 165, Vijaynagar Area, Hospital Road, Bhuj-Kutch
370 001, Gujarat, India
E-mail: voraam@yahoo.com

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glass was made by Agarwal *et al.* [17] and Gupta *et al.* [18]. They have used Ashcroft's empty core (EMC) model potential [20] in the computation of the SSP. The screening dependence of the SSP of $Ca_{70}Mg_{30}$ metallic glass has been studied by Sharma *et al.* [19] using Ashcroft's empty core (EMC) model potential [20], Sharma and Kachhava's linear potential [21] and Veljkovic and Slavic [22] model potential.

The theoretical investigation of the SSP of Cu_CZr_{100-C} metallic glasses has been reported by Sharma *et al.* [10–12]. In most of these studied, Ashcroft's empty core (EMC) model potential [20] is adopted in the calculation. But, nobody has used Hartree (H) [23], Taylor (T) [24] and Ichimaru-Utsumi (IU) [25] local field correction functions in their computation of the SSP. Also, Cu being a good conductor and exhibits conditional superconducting nature and Zr being a transition metal and also exhibiting non-superconducting nature in normal condition, 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_0V of ten Cu_CZr_{100-C} (C = 0.25, 0.30, 0.33, 0.35, 0.40, 0.45, 0.50, 0.55, 0.57 and 0.60) metallic glasses on the basis of Ashcroft's empty core (EMC) potential [20].

2 Computational methodology

In the present investigation for Cu_CZr_{100-C} metallic glasses, the electron-phonon coupling strength λ is computed using the relation [4–9]:

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

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 binary glassy alloy, respectively. The effective averaged square phonon frequency $\langle\omega^2\rangle$ is calculated using the relation given by Butler [26], $\langle\omega^2\rangle^{1/2} = 0.69\,\theta_D$, where θ_D is the Debye temperature of the metallic glasses.

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

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

where Z and $W(X)$ are the valence and the screened EMC pseudopotential [20] of the metallic glasses, respectively.

The well known screened Ashcroft's empty core (EMC) model potential [20] used in the present computations of the SSP of metallic glasses is of the form:

$$W(X) = \frac{-2\pi Z}{\Omega_0 X^2 k_F^2 \varepsilon(X)}\cos\left(2k_F X r_c\right) \tag{3}$$

here 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 [20], which has been successfully found for various metallic complexes [10–19]. 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 [10–19]. Therefore, in the present work we use Ashcroft's empty core (EMC) model potential with more advanced Ichimaru-Utsumi (IU) [25] local field correction functions for the first time.

The Coulomb pseudopotential μ^* is given by [4–9]:

$$\mu^* = \frac{\dfrac{m_b}{\pi k_F}\displaystyle\int_0^1\frac{dX}{\varepsilon(X)}}{1+\dfrac{m_b}{\pi k_F}\ln\dfrac{E_F}{10\theta_D}\displaystyle\int_0^1\frac{dX}{\varepsilon(X)}} \tag{4}$$

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 [4–9]:

$$\varepsilon(X) = 1+[\varepsilon_H(X) - 1]\,[1 - f(X)] \tag{5}$$

$\varepsilon_H(X)$ is the static Hartree dielectric function [4–9] and $f(X)$ the local field correction function. In the present investigation, the local field correction functions due to H [23], T [24] and IU [25] are incorporated to see the impact of exchange and correlation effects.

After evaluating λ and μ^*, the transition temperature T_c and isotope effect exponent α are investigated from the McMillan's formula [4–9]:

$$T_c = \frac{\theta_D}{1.45}\exp\left[\frac{-1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right] \tag{6}$$

$$\alpha = \frac{1}{2}\left[1-\left(\mu^*\ln\frac{\theta_D}{1.45T_c}\right)^2\frac{1+0.62\lambda}{1.04(1+\lambda)}\right] \tag{7}$$

The expression for the effective interaction strength N_0V is studied using [4–9]

$$N_0V = \frac{\lambda-\mu^*}{1+\dfrac{10}{11}\lambda} \tag{8}$$

3 Results and discussion

The input parameters are other constants used in the present computation of the SSP of $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ metallic glasses are shown in Table 1. The presently calculated results of the SSP are tabulated in Table 2 with the experimental [27] and other such theoretical findings [9, 12].

The calculated values of the electron-phonon coupling strength λ for ten $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ 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 [9−12]. It is noticed from the Table 1 that, λ vales are quite sensitive to the local field correction functions. 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 λ is 19.57 %–58.99 %. Also, the H-screening yields the lowest values of λ, whereas the values obtained from the IU-function are the highest. It is also observed from the Table 2 that, λ goes on increasing from the values of 0.2789 to 0.6055 as the concentration *C* of Zr is increased from 0.40–0.75. The increase in λ with concentration *C* of Zr 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 Zr with increasing concentration (*C*), as was also observed by Minnigerode and Samwer [28]. This may also be attributed to the increase role of ionic vibrations in the Zr rich region [11, 12]. The most important feature noted here is that in the series of $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ metallic glasses, as the concentration (*C*) of Cu (in at %) increases the present results of λ decreases.

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 theoretical data [9, 12]. It is observed from the Table 2 that for all metallic glasses, the μ^* lies between 0.13 and 0.16, 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 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 4.65 %–10.19 %. Again the H-screening function yields lowest values of the μ^*, while the values obtained from the IU-function are the highest. The present results are found in congruent with the available theoretical data [8−19]. Here also, as the concentration (C) of Cu (in at %) increases the present results of μ^* decreases.

Table 2 contains calculated values of the transition temperature T_c for $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ metallic glasses computed from the various forms of the local field correction functions along with the experimental [27] and theoretical findings [9, 12]. From Table 2 it can be noted that, the static H-screening function yields the lowest T_c whereas the IU-function yields the highest values of T_c. The present results obtained from the IU-local field correction functions are found in good agreement with the available experimental [27] and theoretical data [9, 12]. The experimental data of T_c for $\mathrm{Cu}_{57}\mathrm{Zr}_{43}$ metallic glass is not available in literature. It is seen that T_c is quite sensitive to the local field correction functions, and the results of T_c by using IU-screening are in best agreement with the experimental data for the $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ metallic glasses under investigation, as the relevant curves for IU-screening almost overlaps the experimental curves. It is also observed that the static H-screening function yields lowest T_c whereas the IU-function yields highest values of T_c. The calculated results of the transition temperature T_c for $\mathrm{Cu}_{60}\mathrm{Zr}_{40}$, $\mathrm{Cu}_{55}\mathrm{Zr}_{45}$, $\mathrm{Cu}_{50}\mathrm{Zr}_{50}$, $\mathrm{Cu}_{45}\mathrm{Zr}_{55}$, $\mathrm{Cu}_{40}\mathrm{Zr}_{60}$, $\mathrm{Cu}_{35}\mathrm{Zr}_{65}$, $\mathrm{Cu}_{33}\mathrm{Zr}_{67}$, $\mathrm{Cu}_{30}\mathrm{Zr}_{70}$ and $\mathrm{Cu}_{25}\mathrm{Zr}_{75}$ metallic glasses deviate in the range of 0 % −100 %, 0 %−97 %, 0 %−97 %, 0 %−95%, 0 %−93%, 0 % −87 %, 0 %−86 %, 0 %−84 % and 0 %−81% from the experimental findings, respectively.

Table 1 Input parameters and other constants.

Metallic glass	Z	r_c /a.u.	Ω_0 /(a.u.)^3	M /amu	θ_D /K
$\mathrm{Cu}_{60}\mathrm{Zr}_{40}$	2.20	1.5006	110.71	74.62	322.20
$\mathrm{Cu}_{57}\mathrm{Zr}_{43}$	2.29	1.5135	112.57	75.45	320.64
$\mathrm{Cu}_{55}\mathrm{Zr}_{45}$	2.35	0.9187	114.59	76.00	319.60
$\mathrm{Cu}_{50}\mathrm{Zr}_{50}$	2.50	1.4564	118.47	77.39	317.00
$\mathrm{Cu}_{45}\mathrm{Zr}_{55}$	2.65	1.4320	122.34	78.77	314.40
$\mathrm{Cu}_{40}\mathrm{Zr}_{60}$	2.80	1.4149	126.22	80.15	311.80
$\mathrm{Cu}_{35}\mathrm{Zr}_{65}$	2.95	0.9277	130.10	81.54	309.20
$\mathrm{Cu}_{33}\mathrm{Zr}_{67}$	3.01	0.9307	131.65	82.09	308.16
$\mathrm{Cu}_{30}\mathrm{Zr}_{70}$	3.10	0.9296	133.98	82.92	306.60
$\mathrm{Cu}_{25}\mathrm{Zr}_{75}$	3.25	0.9355	137.86	84.30	304.00

Table 2 Superconducting state parameters of the Cu-Zr metallic glasses (The value in the parenthesis gives the deviation from experimental value in percentage).

Glass	SSP	Present results			Expt. [27]	Others
		H	T	IU		
$Cu_{60}Zr_{40}$	λ	0.2789	0.4077	0.4222	–	0.44[12], 0.40[12], 0.39[12], 0.39[12], 0.39[12]
	μ^*	0.1428	0.1547	0.1564	–	0.15[12], 0.14[12], 0.14[12], 0.14[12], 0.14[12]
	T_c /K	0.0015 (100)	0.2364 (24)	0.3095 (0)	0.31	0.52[12], 0.31[12], 0.31[12], 0.30[12], 0.27[12]
	α	−0.780	0.020	0.049	–	0.16[12], 0.12[12], 0.14[12], 0.14[12], 0.14[12]
	N_0V	0.1086	0.1846	0.1921	–	0.21[12], 0.19[12], 0.19[12], 0.19[12], 0.18[12]
$Cu_{57}Zr_{43}$	λ	0.3138	0.4599	0.4767	–	0.6911[9]
	μ^*	0.1421	0.1539	0.1555	–	0.2052[9]
	T_c /K	0.0168	0.6744	0.4510	–	2.6834[9]
	α	−0.293	0.1636	0.1823	–	0.1662[9]
	N_0V	0.1336	0.2158	0.2241	–	0.2984[9]
$Cu_{55}Zr_{45}$	λ	0.3158	0.4378	0.4601	–	0.47[12], 0.44[12], 0.43[12], 0.43[12], 0.42[12]
	μ^*	0.1418	0.1536	0.1552	–	0.15[12], 0.14[12], 0.14[12], 0.14[12], 0.14[12]
	T_c /K	0.0190 (97)	0.4629 (29)	0.6505 (0)	0.65	0.98[12], 0.65[12], 0.63[12], 0.61[12], 0.57[12]
	α	−0.270	0.119	0.154	–	0.23[12], 0.20[12], 0.21[12], 0.22[12], 0.22[12]
	N_0V	0.1352	0.2033	0.2150	–	0.23[12], 0.21[12], 0.21[12], 0.21[12], 0.21[12]
$Cu_{50}Zr_{50}$	λ	0.3223	0.4659	0.4818	–	0.50[12], 0.46[12], 0.45[12], 0.45[12], 0.44[12]
	μ^*	0.1410	0.1525	0.1541	–	0.15[12], 0.14[12], 0.14[12], 0.14[12], 0.14[12]
	T_c /K	0.0275 (97)	0.7605 (17)	0.9190 (0)	0.92	1.33[12], 0.92[12], 0.88[12], 0.86[12], 0.81[12]
	α	−0.199	0.185	0.200	–	0.26[12], 0.24[12], 0.25[12], 0.25[12], 0.25[12]
	N_0V	0.1402	0.2201	0.2279	–	0.24[12], 0.22[12], 0.22[12], 0.22[12], 0.22[12]
$Cu_{45}Zr_{55}$	λ	0.3398	0.4882	0.5044	–	0.52[12], 0.48[12], 0.47[12], 0.47[12], 0.46[12]
	μ^*	0.1402	0.1516	0.1531	–	0.14[12], 0.14[12], 0.14[12], 0.13[12], 0.13[12]
	T_c /K	0.0601 (95)	1.0577 (15)	1.2492 (0)	1.25	1.74[12], 1.25[12], 1.18[12], 1.15[12], 1.09[12]
	α	−0.073	0.226	0.238	–	0.29[12], 0.27[12], 0.28[12], 0.28[12], 0.28[12]
	N_0V	0.1525	0.2332	0.2409	–	0.25[12], 0.24[12], 0.23[12], 0.23[12], 0.23[12]
$Cu_{40}Zr_{60}$	λ	0.3617	0.5174	0.5343	–	0.55[12], 0.51[12], 0.50[12], 0.49[12], 0.49[12]
	μ^*	0.1394	0.1507	0.1522	–	0.14[12], 0.14[12], 0.14[12], 0.13[12], 0.13[12]
	T_c /K	0.1296 (93)	1.5137 (14)	1.7506 (0)	1.75	2.34[12], 1.75[12], 1.65[12], 1.61[12], 1.53[12]
	α	0.038	0.267	0.276	–	0.32[12], 0.31[12], 0.31[12], 0.31[12], 0.31[12]
	N_0V	0.1673	0.2494	0.2572	–	0.27[12], 0.25[12], 0.25[12], 0.25[12], 0.25[12]
$Cu_{35}Zr_{65}$	λ	0.3929	0.5353	0.5607	–	0.58[12], 0.54[12], 0.52[12], 0.52[12], 0.51[12]
	μ^*	0.1387	0.1499	0.1514	–	0.14[12], 0.14[12], 0.13[12], 0.13[12], 0.13[12]
	T_c /K	0.2977 (87)	1.8340 (18)	2.2521 (0)	2.25	2.93[12], 2.25[12], 2.11[12], 2.07[12], 1.98[12]
	α	0.143	0.288	0.303	–	0.34[12], 0.33[12], 0.34[12], 0.34[12], 0.34[12]
	N_0V	0.1873	0.2593	0.2711	–	0.28[12], 0.27[12], 0.26[12], 0.26[12], 0.26[12]
$Cu_{33}Zr_{67}$	λ	0.3983	0.5416	0.5670	–	0.58[12], 0.54[12], 0.53[12], 0.52[12], 0.52[12]
	μ^*	0.1385	0.1495	0.1510	–	0.14[12], 0.14[12], 0.13[12], 0.13[12], 0.13[12]
	T_c /K	0.3374 (86)	1.9531 (18)	2.3821 (0)	2.38	3.09[12], 2.39[12], 2.23[12], 2.19[12], 2.10[12]
	α	0.159	0.295	0.309	–	0.35[12], 0.34[12], 0.35[12], 0.35[12], 0.35[12]
	N_0V	0.1907	0.2627	0.2745	–	0.29[12], 0.27[12], 0.27[12], 0.26[12], 0.26[12]
$Cu_{30}Zr_{70}$	λ	0.4125	0.5601	0.5862	–	0.47[12], 0.44[12], 0.43[12], 0.43[12], 0.42[12]
	μ^*	0.1381	0.1491	0.1506	–	0.14[12], 0.14[12], 0.13[12], 0.13[12], 0.13[12]
	T_c /K	0.4537 (84)	2.3114 (17)	2.7814 (0)	2.78	2.53[12], 2.78[12], 2.60[12], 2.56[12], 2.46[12]
	α	0.192	0.312	0.324	–	0.36[12], 0.35[12], 0.35[12], 0.35[12], 0.35[12]
	N_0V	0.1996	0.2724	0.2842	–	0.30[12], 0.28[12], 0.28[12], 0.27[12], 0.27[12]
$Cu_{25}Zr_{75}$	λ	0.4275	0.5782	0.6045	–	0.62[12], 0.58[12], 0.56[12], 0.55[12], 0.55[12]
	μ^*	0.1375	0.1484	0.1498	–	0.14[12], 0.14[12], 0.13[12], 0.13[12], 0.13[12]
	T_c /K	0.6011 (81)	2.6848 (16)	3.1837 (0)	3.18	3.98[12], 3.18[12], 2.97[12], 2.92[12], 2.81[12]
	α	0.224	0.327	0.338	–	0.37[12], 0.36[12], 0.36[12], 0.36[12], 0.36[12]
	N_0V	0.2089	0.2817	0.2934	–	0.31[12], 0.29[12], 0.28[12], 0.28[12], 0.28[12]

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 $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ 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 IU-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. The comparisons of present results with other such theoretical data [9, 12] are highly encouraging. 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 amorphous substances. Since IU-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 Cu (in at %) increases the present results of α decreases sharply.

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 metallic glasses under investigation lie in the range of weak coupling superconductors. The values of the N_0V also show a feeble dependence on dielectric screening, its value being lowest for the H-screening function and highest for the IU-screening function. The present outcomes are found qualitative agreement with the available theoretical data [9, 12]. The variation of present values of the N_0V show that, the metallic glasses under consideration fall in the range of weak coupling superconductors. Also, as the concentration (C) of Cu (in at %) increases the present results of N_0V decreases.

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_0V. 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_0V are not showing any abnormal values for $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ metallic glasses.

4 Conclusion

Lastly we concluded that, the IU-local field correction when used with EMC model potential provides the best explanation for superconductivity in the $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ 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_0V a weak dependence is observed. The magnitude of the λ, α and N_0V values shows that $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ metallic glasses 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 $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ metallic glasses, as they lie within the theoretical limits of the Eliashberg-McMillan formulation. It is also concluded that, the $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ metallic glasses are favoured superconductors. The comparisons of presently computed results of the SSP of $\mathrm{Cu}_C\mathrm{Zr}_{100-C}$ 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. Such study on SSP of other multi component metallic glasses is in progress.

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