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SUPERCONDUCTING STATE PARAMETERS OF $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) TERNARY AMORPHOUS SUPERCONDUCTORS

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A well known empty core (EMC) model potential of Ashcroft is used to investigate 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_0 of $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors. Five different types of 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. The T_C values obtained from the Sarkar et al. (S) local field correction function are found in excellent agreement with available theoretical data. Quadratic T_C equation has been proposed, which provides successfully the T_C values of ternary amorphous alloys under consideration. Also, the present results are found to be in qualitative agreement with earlier reported data, which confirms the superconducting phase in the superconductors.

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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 a third element (M) to binary metallic glasses. They are of interest since the 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 the third element on the electronic and electron

transport properties of binary metallic glasses have been studied extensively [1 – 4], but its effect on superconducting properties has been given lesser attention. Only few researchers studied the superconducting properties of ternary amorphous superconductors using model potential formalism [4 – 12].

The study of the superconducting state parameters (SSP) of the ternary amorphous 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 superconductors 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 by the pseudopotential and the electron-electron interaction is involved through a dielectric screening function. For successful predictions of the superconducting properties of the alloying systems, the proper selection of the pseudopotential and screening function is essential [6 – 11].

Therefore, we decided to investigate the superconducting behaviour of $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors. In this paper, we used the well known McMillan's theory [13] of the superconductivity for predicting the superconducting state parameters (SSP) of ternary amorphous superconductors. We used Ashcroft's empty core (EMC) model potential [14] 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 for the first time. To see the impact of various exchange and correlation functions on the aforesaid properties, we employed here five different types of local field correction functions proposed by Hartree (H) [15], Taylor (T) [16], Ichimaru-Utsumi (IU) [17], Farid et al. (F) [18] and Sarkar et al. (S) [19]. We have incorporated for the first time more advanced local field correction functions due to IU [17], F [18] and S [19] with EMC model potential. Actually, our main aim of the present study is to check the validity of the appropriate local field correction functions. Therefore, we used various types of the local field correction functions in the present computation.

In the present work, the pseudo-alloy-atom (PAA) model was used to explain electron-ion interaction for alloying systems [6 – 10]. It is well known that the pseudo-alloyatom (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, we propose a use of PAA model for the first time to investigate the superconducting state parameters (SSP) of ternary amorphous alloys.

2. Computational methodology

The well known screened Ashcroft's empty core (EMC) model potential [14], used in the present computations of the superconducting state parameters (SSP) of ternary amorphous alloys, is of the form,

$$W(X) = \frac{-2\pi Z}{\Omega_0 X^2 k_F^2 \epsilon(X)} \cos(2k_F X r_C)\,. \tag{1}$$

Here r_C is the parameter of the model potential of ternary amorphous alloys. The Ashcroft's empty core (EMC) model potential is a simple one-parameter model potential [15], which has been successfully applied for various metallic complexes with various forms of the screening functions [3 – 12]. Therefore, in the present work, we use Ashcroft's empty core (EMC) model potential with more advanced Ichimaru-Utsumi (IU) [18], Farid et al. (F) [19] and Sarkar et al. (S) [20] local field correction functions for the first time in the present case. 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 to the experimental T_C of the ternary amorphous alloys for most of the local field correction functions.

In the present investigation for $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors, the electron-phonon coupling strength λ is computed using the relation [3 – 12]

$$\lambda = \frac{m_b \Omega_0}{4\pi^2 k_F M \langle\omega^2\rangle} \int_0^{2k_F} q^3 |W(q)|^2 \mathrm{d}q\,. \tag{2}$$

Here m_b is the band mass, which is taken unity for the sake of simplicity, M is the ionic mass, Ω_0 is the atomic volume, k_F is the Fermi wave vector, $W(q)$ the screened pseudopotential and $\langle\omega^2\rangle$ is the phonon frequency of the ternary amorphous alloys, which is calculated using the relation given by Butler [20], $\langle\omega^2\rangle^{1/2} = 0.69\,\theta_D$, where θ_D is the Debye temperature of the ternary amorphous alloys.

Using $X = q/2k_F$ and $\Omega_0 = 3\pi^2 Z/(k_F)^3$, we obtain Eq. (2) as

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

where Z and $W(X)$ are the valence and the screened EMC pseudopotential [14] of the ternary amorphous alloys, respectively.

The BCS theory gives the relation $T_C \approx \theta_D \exp(-1/N(0)V)$ for the superconducting transition temperature T_C in terms of the Debye temperature θ_D. The electron-electron interaction V consists of the attractive electron-phonon-induced interaction minus the repulsive Coulomb interaction. The used notation is $\lambda = N(0)V_{e-ph}$. The Coulomb repulsion $N(0)V_C$ is called μ, so that $N(0)V = \lambda - \mu^*$, where μ^* is a "renormalized" Coulomb repulsion, reduced in value from μ to $\mu/[1 + \mu \ln(\omega_P/\omega_D)]$. This suppression of the Coulomb repulsion is a result of the fact that the electron-phonon attraction is retarded in time by an amount $\Delta t \approx 1/\omega_D$, whereas the repulsive screened Coulomb interaction is retarded by a much smaller time, $\Delta t \approx 1/\omega_P$, where ω_P is the electronic plasma frequency. Therefore, μ^* has the upper bound $1/\ln(\omega_P/\omega_D)$, which for conventional metals should be ≤ 0.2. Values of λ are known to range from ≤ 0.10 to ≤ 2.0. Also, The parameter μ^* is assigned a value in the range $0.10-0.15$, consistent with tunneling and with theoretical guesses. Calculations of μ or μ^* are computationally demanding and are not yet under theoretical control. Calculations of λ are slightly less demanding, are under somewhat better theoretical control, and have been attempted for many years. Prior to 1990, calculations of λ generally required knowing the phonon frequencies and eigenvectors as input information, and approximating the form of the electron-ion potential. McMillan [13] and Hopfield [21] pointed out that one could define a simpler quantity, $\eta = N(0)\langle I^2 \rangle$ with $\langle \omega^2 \rangle (2/\lambda) \int_0^\infty \mathrm{d}\Omega\ \Omega \alpha^2 F(\Omega)$. The advantage of this is that η and $\langle I^2 \rangle$ are purely "electronic" quantities, requiring no input information about phonon frequencies or eigenvectors. Gaspari and Gyorffy [22] then invented a simplified algorithm for calculating λ, and many authors have used it. These calculations generally require a "rigid ion approximation" or some similar guess for the perturbing potential felt by electrons when an atom has moved. Given η, one can guess a value for $\langle \omega^2 \rangle$ (for example, from θ_D). In the weak coupling limit of the electron-phonon interaction, the fundamental equations of the BCS theory should be derived from the Eliashberg equations. This conversion is possible upon some approximation of the phonon frequency $|\omega| \geq \omega_D$ with ω_D denoting the Debye frequency [23]. Morel and Anderson [24] have given the relation of the transition temperature $\lambda - \mu^* = \lambda - \mu/[1 + \mu \ln(E_F/\omega_l)]$, which is nearly equal to the factor 6 for monovalent, bivalent and tetravalent metals, where $E_F = k_F^2$ is the Fermi energy and ω is the phonon frequency of the metallic substances. The effect of phonon frequency is much smaller in comparison with the Fermi energy. Hence, the overall effect of the Coulomb pseudopotential is reduced by the large logarithmic term. Therefore, Rajput and Gupta [25] introduced the new term $20\theta_D$ in place of the phonon frequency ω_l from the Butler's [20] relation, for the sake of simplicity and ignoring the lattice vibrational effect, which generated consistent results of the Coulomb pseudopotential. The parameter μ^* represents the effective interelectronic Coulomb repulsion at the Fermi surface [23]. Hence, in the present case, we have adopted relation of the Coulomb pseudopotential given by Rajput

and Gupta [25]. Therefore, the Coulomb pseudopotential μ^* is given by [6 – 11, 25]

$$\mu^* = \frac{\dfrac{m_b}{\pi k_F}\displaystyle\int_0^1 \frac{\mathrm{d}X}{\epsilon(X)}}{1 + \dfrac{m_b}{\pi k_F}\ln\left(\dfrac{E_F}{20\,\theta_D}\right)\displaystyle\int_0^1 \frac{\mathrm{d}X}{\epsilon(X)}}\,. \tag{4}$$

As is evident from Eq. (4), which was originally derived by Bogoliubov et al. [23], the Coulomb repulsion parameter μ^* is essentially weakened owing to a large logarithmic term in the denominator. Here, $\epsilon(X)$ is the modified Hartree dielectric function, which is written as [15]

$$\epsilon(X) = 1 + \big(\epsilon_H(X) - 1\big)\big(1 - f(X)\big)\,. \tag{5}$$

$\epsilon_H(X)$ is the static Hartree dielectric function and $f(X)$ the local field correction function. In the present investigation, the local field correction functions due to H [15], T [16], IU [17], F [18] and S [19] are incorporated to see the impact of exchange and correlation effects.

The Hartree screening function [15] is purely static, and it does not include the exchange and correlation effects. The expression of it is,

$$f(q) = 0\,. \tag{6}$$

Taylor (T) [16] 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) [16],

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

The Ichimaru-Utsumi (IU) local field correction function [17] 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

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

On the basis of Ichimaru-Utsumi (IU) local field correction function [17], Farid et al. (F) [18] have given a local field correction function of the form

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

Based on Eqs. (8) and (9), Sarkar et al. (S) [19] proposed a simple form of the local field correction function, which is of the form

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

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 given in the respective papers of the local field correction functions [17–19].

After evaluating λ and μ^*, the transition temperature T_C and isotope effect exponent α are investigated using the McMillan's formula [6–13]

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

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

The expression for the effective interaction strength N_0V is studied using [6–12]

$$N_0V = \frac{\lambda - \mu^*}{1 + (10/11)\lambda}. \tag{13}$$

3. Results and discussion

The values of the input parameters for the ternary amorphous superconductors under investigation are assembled in Table 1. To determine the input parameters and various constants for PAA model [6–10], the following definitions for ternary metallic glasses $(A_xB_y)_{1-z}C_z$ $(x + y + z = 1)$ are adopted,

$$Z = (1-z)\big(x(Z_A) + y(Z_B)\big) + z(Z_C), \tag{14}$$

$$M = (1-z)\big(x(M_A) + y(M_B)\big) + z(M_C), \tag{15}$$

$$\Omega_0 = (1-z)\big(x(\Omega_{0A}) + y(\Omega_{0B})\big) + z(\Omega_{0C}), \tag{16}$$

$$\theta_D = (1-z)\big(x(\theta_{DA}) + y(\theta_{DB})\big) + z(\theta_{DC}), \tag{17}$$

where x, y and z are the concentration factors of the A, B and C pure metallic components ternary metallic glasses. The input parameters such as Z, Ω_0, M and θ_D of the pure metallic components are taken from the literature [11].

In the present work, we used input parameters computed from the PAA model using available data of pure metallic elements. This PAA model is found successful

TABLE 1. Input parameters and other constants of ternary amorphous superconductors.

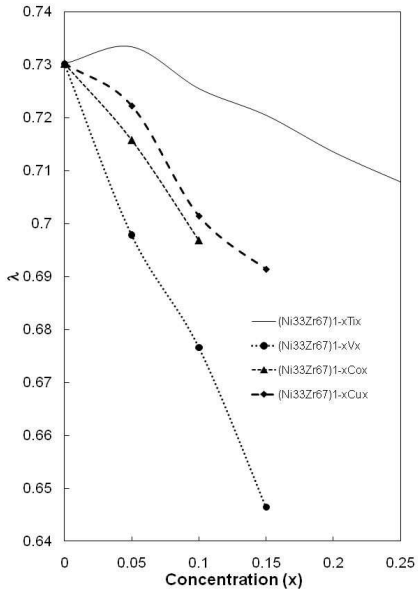
Superconductor	Z	r_C (au)	Ω_0 (au)^3	M (amu)	θ_D (K)
$(Ni_{33}\ Zr_{67})_1Ti_0$	3.34	1.4584	129.73	80.49	343.47
$(Ni_{33}Zr_{67})_{0.95}Ti_{0.05}$	3.37	1.4450	129.19	78.86	347.30
$(Ni_{33}Zr_{67})_{0.90}Ti_{0.10}$	3.41	1.4244	128.62	77.23	351.12
$(Ni_{33}Zr_{67})_{0.85}Ti_{0.15}$	3.44	1.4087	128.05	75.60	354.95
$(Ni_{33}Zr_{67})_{0.80}Ti_{0.20}$	3.47	1.3920	127.48	73.97	358.78
$(Ni_{33}Zr_{67})_{0.75}Ti_{0.25}$	3.51	1.3728	126.92	72.34	362.60
$(Ni_{33}Zr_{67})_1V_0$	3.34	1.4584	129.76	80.49	343.47
$(Ni_{33}Zr_{67})_{0.95}V_{0.05}$	3.42	1.3988	127.95	79.01	345.30
$(Ni_{33}Zr_{67})_{0.90}V_{0.10}$	3.51	1.3457	126.14	77.54	347.12
$(Ni_{33}Zr_{67})_{0.85}V_{0.15}$	3.59	1.2918	124.33	76.06	348.95
$(Ni_{33}Zr_{67})_1Co_0$	3.34	1.4584	129.76	80.49	343.47
$(Ni_{33}Zr_{67})_{0.95}Co_{0.05}$	3.27	1.4572	126.09	79.41	348.55
$(Ni_{33}Zr_{67})_{0.90}Co_{0.10}$	3.21	1.4626	124.21	78.33	353.62
$(Ni_{33}Zr_{67})_1Cu_0$	3.34	1.4584	129.76	80.49	343.47
$(Ni_{33}Zr_{67})_{0.95}Cu_{0.05}$	3.22	1.4756	127.26	79.64	343.45
$(Ni_{33}Zr_{67})_{0.90}Cu_{0.10}$	3.11	1.4852	124.75	78.80	343.42
$(Ni_{33}Zr_{67})_{0.85}Cu_{0.15}$	2.99	1.5060	122.25	77.95	343.40

only when experimental data were not available for metallic compounds. When the experimental data on the volume Ω_0 and the Debye temperature θ_D are available in the literature for metallic compounds, then one can reduce the fitting parameters of the ternary systems. Also, in the present work, the model potential parameter r_C is fitted with the experimental T_C of the ternary amorphous alloys for most of the local field correction functions. A common r_C is used for most of the local field correction functions in the present computation of the superconducting state parameters (SSP).

The presently calculated results for the superconducting state parameters (SSP) are tabulated in Tables 2 – 5 with other theoretical [11] and experimental [4] findings. Also, the graphical analyses of the superconducting state parameters (SSP) of $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors computed from Sarkar et al. (S) [19] local field correction function are also plotted in Figures 1 – 5 where these parameters are plotted against the concentration x of the third element (M) for the four different series of ternary amorphous alloys.

TABLE 2. Superconducting state parameters of $(Ni_{33}\ Zr_{67})_{1-x}Ti_x$ *ternary superconductors.*

x	SSP	Present results					Others	Exptl.
		H	T	IU	F	S	[11]	[4]
0.00	λ	0.4796	0.6909	0.7160	0.7302	0.5671	0.553	-
	μ^*	0.1443	0.1575	0.1593	0.1597	0.1519	0.14	-
	T_C (K)	1.2638	5.5337	6.1223	6.5066	2.6805	2.6734	2.68
	α	0.2598	0.3579	0.3628	0.3671	0.3080	0.341	-
	N_0V	0.2348	0.3291	0.3387	0.3445	0.2753	0.275	-
0.05	λ	0.4831	0.6943	0.7192	0.7334	0.5703	0.558	-
	μ^*	0.1441	0.1573	0.1592	0.1595	0.1517	0.142	-
	T_C (K)	1.3025	5.6034	6.1892	6.5754	2.7302	2.7438	2.73
	α	0.2620	0.3583	0.3631	0.3674	0.3091	0.338	-
	N_0V	0.2355	0.3292	0.3386	0.3443	0.2757	0.276	-
0.10	λ	0.4804	0.6875	0.7116	0.7255	0.5659	0.558	-
	μ^*	0.1439	0.1571	0.1589	0.1592	0.1514	0.143	-
	T_C (K)	1.2796	5.4912	6.0578	6.4382	2.6727	2.6948	2.67
	α	0.2600	0.3563	0.3610	0.3653	0.3069	0.332	-
	N_0V	0.2342	0.3264	0.3356	0.3413	0.2737	0.275	-
0.15	λ	0.4791	0.6833	0.7067	0.7205	0.5633	0.558	-
	μ^*	0.1438	0.1569	0.1587	0.1590	0.1512	0.145	-
	T_C (K)	1.2754	5.4420	5.9968	6.3739	2.6517	2.6552	2.65
	α	0.2591	0.3550	0.3597	0.3640	0.3057	0.327	-
	N_0V	0.2336	0.3247	0.3337	0.3393	0.2725	0.274	-
0.20	λ	0.4766	0.6773	0.7001	0.7135	0.5595	0.557	-
	μ^*	0.1436	0.1567	0.1585	0.1588	0.1510	0.146	-
	T_C (K)	1.2530	5.3415	5.8805	6.2520	2.6010	2.6137	2.60
	α	0.2569	0.3530	0.3576	0.3619	0.3035	0.322	-
	N_0V	0.2323	0.3222	0.3310	0.3365	0.2707	0.273	-
0.25	λ	0.4754	0.6726	0.6947	0.7079	0.5569	0.557	-
	μ^*	0.1434	0.1564	0.1582	0.1585	0.1508	0.147	-
	T_C (K)	1.2521	5.2811	5.8045	6.1706	2.5821	2.5902	2.58
	α	0.2565	0.3517	0.3562	0.3605	0.3025	0.317	-
	N_0V	0.2318	0.3203	0.3288	0.3343	0.2696	0.272	-



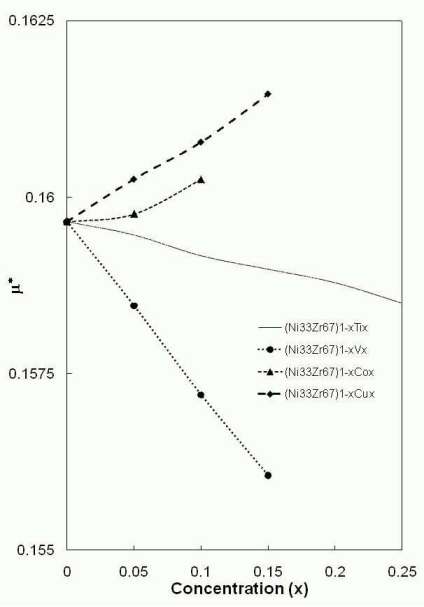


Fig. 1. (left). Variation of electron-phonon coupling strength λ with M*-concentration x.*

Fig. 2. Variation of Coulomb pseudopotential μ^* with M*-concentration x.*

The calculated values of the electron-phonon coupling strength λ for the $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors, using five different types of the local field correction functions with EMC model potential, are shown in Tables 2 – 5 with other theoretical data [11]. The graphical nature of λ is also displayed in Fig. 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 λ is 17.15% – 52.25%, 16.53% – 52.25%, 18.17% – 52.45% and 18.25% – 54.14% for $(Ni_{33}Zr_{67})_{1-x}Ti_x$, $(Ni_{33}Zr_{67})_{1-x}V_x$, $(Ni_{33}Zr_{67})_{1-x}Co_x$ and $(Ni_{33}Zr_{67})_{1-x}Cu_x$ ternary amorphous superconductors, respectively. It is also observed from the Tables 2 – 5 that λ is decreasing from the values of $0.7302 \rightarrow 0.4754$, $0.7302 \rightarrow 0.4459$, $0.7302 \rightarrow 0.4571$ and $0.7302 \rightarrow 0.4485$ as the concentration x of Ti is increased from $0.0 \rightarrow 0.25$, those of V is increased from $0.0 \rightarrow 0.15$, those of Co is increased from $0.0 \rightarrow 0.15$ and those of Cu is increased from $0.0 \rightarrow 0.15$, respectively. The decrease of λ with concentration x of Ti, V, Co and Cu 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 Ti, V, Co and Cu with increasing concentration (z). This may also be attributed to the increase role of ionic vibrations in the Ti-rich region. Presently computed λ from S-local field correction function is found in an excellent agreement with available theoretical data [11].

TABLE 3. Superconducting state parameters of $(Ni_{33}\ Zr_{67})_{\ 1-x}V_x$ *ternary superconductors.*

		Present results					Others	Exptl.
x	SSP	H	T	IU	F	S	[11]	[4]
	λ	0.4796	0.6909	0.7160	0.7302	0.5671	0.553	-
	μ^*	0.1443	0.1575	0.1593	0.1597	0.1519	0.14	-
0.00	T_C (K)	1.2638	5.5337	6.1223	6.5066	2.6805	2.6734	2.68
	α	0.2598	0.3579	0.3628	0.3671	0.3080	0.341	-
	N_0V	0.2348	0.3291	0.3387	0.3445	0.2753	0.275	-
	λ	0.4652	0.6622	0.6846	0.6978	0.5471	0.545	-
	μ^*	0.1433	0.1564	0.1582	0.1585	0.1508	0.146	-
0.50	T_C (K)	1.0417	4.7526	5.2526	5.5980	2.2523	2.2505	2.25
	α	0.2437	0.3472	0.3521	0.3567	0.2945	0.311	-
	N_0V	0.2262	0.3158	0.3245	0.3300	0.2647	0.266	-
	λ	0.4580	0.6439	0.6643	0.6766	0.5358	0.538	-
	μ^*	0.1424	0.1551	0.1569	0.1572	0.1496	0.151	-
0.10	T_C (K)	0.9686	4.3611	4.8023	5.1187	2.0804	1.9498	2.08
	α	0.2395	0.3420	0.3466	0.3513	0.2899	0.285	-
	N_0V	0.2228	0.3083	0.3164	0.3216	0.2597	0.260	-
	λ	0.4449	0.6172	0.6353	0.6464	0.5185	0.534	-
	μ^*	0.1415	0.1540	0.1558	0.1561	0.1485	0.154	-
0.15	T_C (K)	0.8196	3.7519	4.1234	4.3972	1.7911	1.7836	1.79
	α	0.2257	0.3311	0.3356	0.3404	0.2784	0.266	-
	N_0V	0.2161	0.2967	0.3040	0.3089	0.2515	0.256	-

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 Tables 2 – 5 with other theoretical data [11]. It is observed from the Tables 2 – 5 that for $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors, μ^* lies between 0.14 and 0.16, which is in accordance with McMillan [13], who suggested $\mu^* \approx 0.13$ for transition metals. The graphs of μ^* versus concentration (x) for S-local field correction functions are plotted in Figure 2, which shows the weak dependence of μ^* on the local field correction functions. 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 superconductors is observed in the range of 5.12% – 10.66%, 4.97% – 10.66%, 5.26% – 10.70% and 5.26% – 10.83% for $(Ni_{33}Zr_{67})_{1-x}Ti_x$, $(Ni_{33}Zr_{67})_{1-x}V_x$, $(Ni_{33}Zr_{67})_{1-x}Co_x$ and $(Ni_{33}Zr_{67})_{1-x}Cu_x$ ternary amorphous superconductors, respectively. The present results are found in good agreement with available theoretical data [11].

TABLE 4. Superconducting state parameters of $(Ni_{33}\ Zr_{67})_{\ 1-x}Co_x$ *ternary superconductors.*

x	SSP	Present results					Others [11]	Exptl. [4]
		H	T	IU	F	S		
0.00	λ	0.4796	0.6909	0.7160	0.7302	0.5671	0.553	-
	μ^*	0.1443	0.1575	0.1593	0.1597	0.1519	0.14	-
	T_C (K)	1.2638	5.5337	6.1223	6.5066	2.6805	2.6734	2.68
	α	0.2598	0.3579	0.3628	0.3671	0.3080	0.341	-
	N_0V	0.2348	0.3291	0.3387	0.3445	0.2753	0.275	-
0.05	λ	0.4701	0.6772	0.7018	0.7158	0.5556	0.541	-
	μ^*	0.1444	0.1576	0.1594	0.1598	0.1520	0.141	-
	T_C (K)	1.0969	5.1297	5.6997	6.0729	2.4024	2.4148	2.40
	α	0.2443	0.3503	0.3557	0.3603	0.2965	0.330	-
	N_0V	0.2282	0.3216	0.3311	0.3368	0.2682	0.268	-
0.10	λ	0.4571	0.6591	0.6832	0.6968	0.5404	0.527	-
	μ^*	0.1448	0.1581	0.1599	0.1603	0.1524	0.142	-
	T_C (K)	0.9147	4.6773	5.2272	5.5874	2.1004	2.1103	2.10
	α	0.2231	0.3405	0.3464	0.3514	0.2812	0.316	-
	N_0V	0.2206	0.3133	0.3228	0.3285	0.2602	0.260	-

Tables 2 – 5 contain calculated values of the transition temperature T_C for $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors computed from the various forms of the local field correction functions along with the theoretical [11] and experimental [4] findings. The present results obtained from the S-local field correction functions are found in good agreement with available theoretical [11] and experimental [4] data. The calculated results of the transition temperature T_C for $(Ni_{33}Zr_{67})_{1-x}Ti_x$, $(Ni_{33}Zr_{67})_{1-x}V_x$, $(Ni_{33}Zr_{67})_{1-x}Co_x$ and $(Ni_{33}Zr_{67})_{1-x}Cu_x$ ternary amorphous superconductors deviate in the range of 0.01% – 128.44%, 0.02% – 148.80%, 0.02% – 166.07% and 0.01% – 178.16% from the experimental findings [4], respectively. The variation of the computed values of the transition temperature T_C for $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors with the atomic concentration x, using S-local field correction functions with EMC potential are shown in Fig. 3. 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 $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors under investigation, as the relevant curves for S-screening almost overlap the theoretical curves. It is also seen from the graphs, T_C decreases considerably with increasing M-concentration x. Variation of

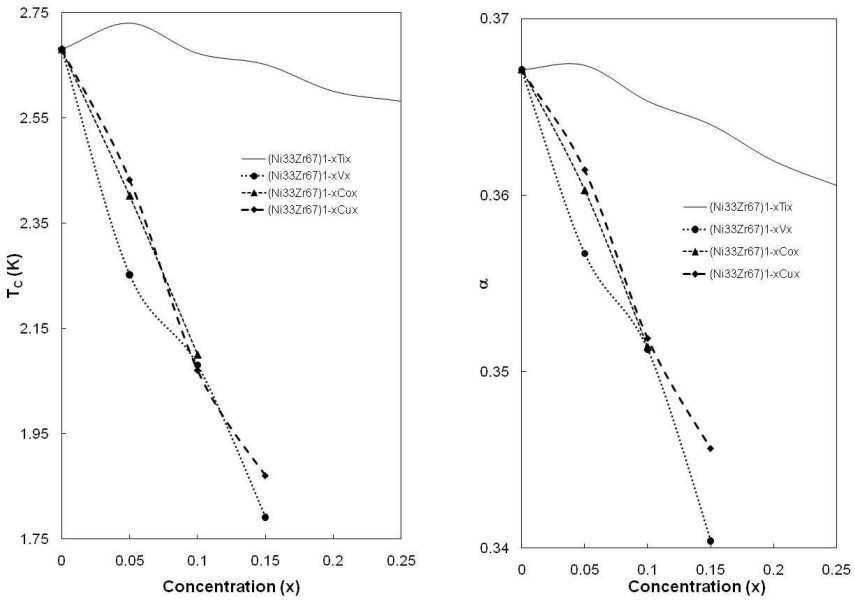


Fig. 3 (left). Variation of transition temperature T_C with with M*-concentration x.*

Fig. 4. Variation of isotope effect exponent α with M*-concentration x.*

the transition temperature T_C with the concentration x of the third element (M) can be expressed by following quadratic formulae

$$T_C(K) = -2.214x^2 + 0.033x + 2.698, \quad \text{for} \quad (Ni_{33}Zr_{67})_{1-x}Ti_x, \tag{18}$$

$$T_C(K) = 14x^2 - 7.78x + 2.661, \quad \text{for} \quad (Ni_{33}Zr_{67})_{1-x}V_x, \tag{19}$$

$$T_C(K) = -4,765x^2 - 5.324x + 2.680, \quad \text{for} \quad (Ni_{33}Zr_{67})_{1-x}Co_x, \tag{20}$$

$$T_C(K) = 5x^2 - 6.33x + 2.693, \quad \text{for} \quad (Ni_{33}Zr_{67})_{1-x}Cu_x. \tag{21}$$

The graph of the fitted T_C equation is displayed in Fig. 3, which indicates that T_C decreases considerably with increasing Ti, V, Co and Cu content with a slope dT_C/dx=0.033, 7.78, 5.324 and 6.33. A wide extrapolation predicts T_C =2.698K, 2.661K, 2.680K and 2.693K for the hypothetical case of pure amorphous $Ni_{33}Zr_{67}$ alloy. These quadratic formulae for T_C, Eqs. (18 – 21), obtained in the present study, closely resemble the quadratic T_C equations suggested by Sharma et al. [11] on the basis of experimental data for the ternary systems as follows,

$$T_C(K) = -3.1393x^2 + 0.3014x + 2.6961, \quad \text{for} \quad (Ni_{33}Zr_{67})_{1-x}Ti_x, \tag{22}$$

$$T_C(K) = 25.6700x^2 - 9.7907x + 2.6740, \quad \text{for} \quad (Ni_{33}Zr_{67})_{1-x}V_x, \tag{23}$$

$$T_C(K) = -9.1800x^2 - 4.713x + 2.6734, \quad \text{for} \quad (Ni_{33}Zr_{67})_{1-x}Co_x, \tag{24}$$

$$T_C(K) = 1.7190x^2 - 5.7677x + 2.6830, \quad \text{for} \quad (Ni_{33}Zr_{67})_{1-x}Cu_x. \tag{25}$$

From the overall comparisons of the presently computed results with those of Sharma et al. [11], it is noted that, the present results are found to be in good agreement with experimental data [4]. Therefore, the results obtained from Sarkar et al. (S) [15] with EMC model potential [14] produced consistent results for the superconductivity of ternary amorphous superconductors. It also observed that the transition temperature T_C decreases as V, Co or Cu is added to binary amorphous alloy $Ni_{33}Zr_{67}$. 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

TABLE 5. Superconducting state parameters of $(Ni_{33}\ Zr_{67})_{\ 1-x}Cu_x$ *ternary superconductors.*

		Present results					Others	Exptl.
x	SSP	H	T	IU	F	S	[11]	[4]
	λ	0.4796	0.6909	0.7160	0.7302	0.5671	0.553	-
	μ^*	0.1443	0.1575	0.1593	0.1597	0.1519	0.14	-
0.00	T_C (K)	1.2638	5.5337	6.1223	6.5066	2.6805	2.6734	2.68
	α	0.2598	0.3579	0.3628	0.3671	0.3080	0.341	-
	N_0V	0.2348	0.3291	0.3387	0.3445	0.2753	0.275	-
	λ	0.4721	0.6828	0.7081	0.7223	0.5596	0.543	-
	μ^*	0.1447	0.1581	0.1599	0.1603	0.1524	0.141	-
0.05	T_C (K)	1.1004	5.1778	5.7582	6.1337	2.4326	2.4411	2.43
	α	0.2448	0.3514	0.3569	0.3614	0.2977	0.332	-
	N_0V	0.2291	0.3237	0.3335	0.3392	0.2699	0.270	-
	λ	0.4573	0.6629	0.6876	0.7014	0.5430	0.526	-
	μ^*	0.1452	0.1586	0.1605	0.1608	0.1529	0.141	-
0.10	T_C (K)	0.8826	4.6117	5.1624	5.5191	2.0707	2.0787	2.07
	α	0.2210	0.3408	0.3469	0.3519	0.2812	0.317	-
	N_0V	0.2205	0.3146	0.3244	0.3301	0.2612	0.261	-
	λ	0.4485	0.6528	0.6776	0.6913	0.5339	0.517	-
	μ^*	0.1457	0.1593	0.1611	0.1615	0.1536	0.142	-
0.15	T_C (K)	0.7591	4.3096	4.8535	5.2015	1.8701	1.8759	1.87
	α	0.2030	0.3336	0.3403	0.3456	0.2694	0.307	-
	N_0V	0.2151	0.3097	0.3196	0.3254	0.2561	0.255	-

element (M). Since T_C is related to the modifications of density of states (DOS) at E_F, $N(E_F)$, a decrease in T_C can be related to the modifications of DOS at $N(E_F)$ [11]. The difference is noticed when the third element (M) is added to the binary amorphous alloy $Ni_{33}Zr_{67}$ (Fig. 3). In this case, T_C rises initially and then decreases with the concentration x of the third element (M), showing a peak at about $x = 0.05$. This indicates that on addition of the third element (M), 3d states grow near E_F and hence contribute substantially to the Fermi level, $N(E_F)$, favouring superconducting behaviour in this case [11].

The presently computed values for the T_C are found in the range which is suitable for further exploring the applications of the superconductors for usage like lossless transmission lines 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 7 K.

The values of the isotope effect exponent α for $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors are tabulated in Tables 2 – 5. Figure 4 depicts the variation of α when the M-concentration x decreases. The computed values of α show a weak dependence on the dielectric screening function. Since the experimental value of α has not been reported in the literature so far, the present data for α 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 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 values of the effective interaction strength N_0V are listed in Tables 2 – 5 and depicted in Fig. 5 for different local field correction functions. It is observed

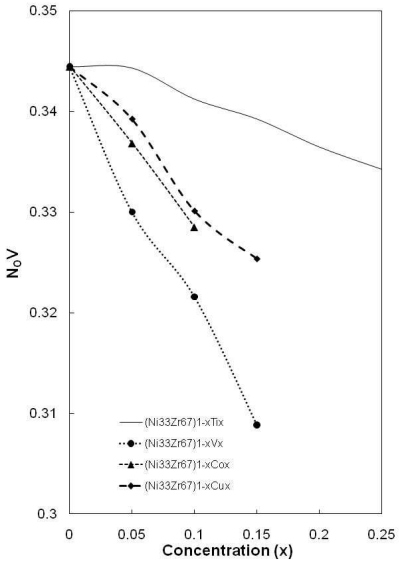


Fig. 5. Variation of effective interaction strength N_0V with M-*concentration x.*

that the magnitude of N_0V shows that the $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors under investigation lie in the range of weak to intermediate superconductors.

From the overall study, it is seen that from the present data of the superconducting properties of ternary amorphous superconductors that addition of V, Co and Cu as third element (M) to the binary amorphous alloy $Ni_{33}Zr_{67}$ causes the parameters λ, α and N_0V to decrease, whereas the Coulomb pseudopotential (μ^*) increases for Ti, Co and Cu based superconductors while those for V based superconductors, the Coulomb pseudopotential (μ^*) decreases with concentration of M, showing that the presence of third element (M) causes a suppression of the superconductivity in the alloy. A decrease in λ, α and N_0V suggests weak coupling in these superconductors, the coupling being weakest for Co. This is in conformity with the fact that $(Ni_{33}Zr_{67})_{1-x}Co_x$ ternary amorphous superconductors do not remain superconducting for higher values of the concentration x of the third element (M). This may be due to change in influential electron band structure from 4d to 3d as suggested by Varma and Dynes [26]. It is also observed that superconductivity persists only for small values of x (i.e. $x \leq 0.25$) which is because the third elements (M) considered here are all 3d transition metals which have smaller band width and stronger localized character than Zr, thus they cause a narrowing of bands in ternary system [11]. These narrow bands have magnetic instabilities which prevent superconductivity as suggested by Allen and Cohen [27]. The present results for the transition temperature T_C show an excellent agreement with the experimental [4] and theoretical [11] findings.

According to Matthias rules [28, 29], the ternary amorphous superconductors having $Z > 2$ do exhibit superconducting nature. Hence, $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors are exhibiting superconducting nature in the present case. When we go from $Z = 3.21$ to $Z = 3.34$, the electron-phonon coupling strength λ changes with the lattice spacing a. Similar trends are also observed in the values of T_C for all ternary amorphous superconductors. Hence, a strong dependency of the superconducting state parameters (SSP) of the ternary amorphous superconductors on the valence Z is found.

The main difference of the local field correction functions are playing an important role in the production of the superconducting state parameters (SSP) of $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors. The Hartree (H) dielectric function [15] is purely static and it does not include the exchange and correlation effects. Taylor (T) [16] 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 [17] 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, and it also satisfies the self consistency condition in the compressibility sum rule and short range correlations. On the basis of the Ichimaru-Utsumi (IU) local field correction function [17], Farid et al. (F) [18] and Sarkar et al. (S) [19] have given a local field correction function. Hence, Ichimaru-Utsumi (IU) [17] and Farid et al. (F) [18] functions have the same characteristic nature. Also, the super-

conducting state parameters (SSP) computed from Sarkar et al. (S) [19] local field correction are found in qualitative agreement with the available theoretical data [11].

The effect of the local field correction functions is playing an important role in the computation of λ and μ^*, which make drastic variation on T_C, α and N_0V. The local field correction functions due to IU, F and S can generate consistent results regarding the superconducting state parameters (SSP) of $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors as those obtained from the more commonly employed Hartree (H) and Taylor (T) functions. The computed results for α and N_0V are not showing any abnormal values for the $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu) ternary amorphous superconductors.

Lastly, we would like to emphasize the importance of using 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

We conclude that T_C, α and N_0V decrease as V, Co and Cu are added as the third element (M) to the binary amorphous superconductor $Ni_{33}Zr_{67}$, but when Ti is added, T_C increases initially and then decreases, and a peak is observed at about $x = 0.05$. The values of λ and T_C show an appreciable dependence on the local field correction function, whereas for μ^*, α and N_0V, a weak dependence is observed. The magnitude of λ, α and N_0V values shows that the ternary amorphous alloys are weak to intermediate superconductors. A good agreement between the presently computed results for T_C values from S-local field correction function and respective theoretical and experimental values proves the validity of this approach to ternary amorphous superconductors. Quadratic T_C equations have been proposed, which provide successfully the T_C values of the ternary amorphous alloys under consideration. In the absence of experimental data for α and N_0V, 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 present results confirm 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.

References

[1] U. Mizutani, C. Mishima and T. Goto, J. Phys. Cond. Matter **1** (1989) 1831.

[2] R. Zehringer, P. Oelhafen, H.-J. Guntherodt, Y. Yamada and U. Mizutani, Mater. Sci. Eng. **99** (1988) 317.

[3] U. Mizutani, U. Mizutani and C. Mishima, Solid State Commun. **62** (1987) 641.

[4] Y. Yamada, Y. Itoh and U. Mizutani, Mater. Sci. Eng. **99** (1988) 289.

[5] A. V. Narlikar and S. N. Ekbote, *Superconductivity and Superconducting Materials*, South Asian Publishers, New Delhi, Madras (1983).

[6] Aditya M. Vora, Armenian J. Phys. **2** (2009) 213.

[7] Aditya M. Vora, J. Condensed Matter **10** (2008) 15.

[8] Aditya M. Vora, Sci. Technol. Adv. Mater. **9** (2008) 025017.

[9] Aditya M. Vora, Physica C **468** (2008) 937, 2292.

[10] Aditya M. Vora, Chin. Phys. Lett. **27** (2010) 026102-1.

[11] S. Sharma, H. Khan and K. S. Sharma, Czech. J. Phys. **55** (2005) 1005.

[12] P. Chatterjee, Can. J. Phys. **58** (1980) 1383.

[13] W. L. McMillan, Phys. Rev. **167** (1968) 331.

[14] N. W. Ashcroft, Phys. Lett. **23** (1966) 48.

[15] W. A. Harrison, *Elementary Electronic Structure*, World Scientific, Singapore, (1999).

[16] R. Taylor, J. Phys. F: Met. Phys. **8** (1978) 1699.

[17] S. Ichimaru and K. Utsumi, Phys. Rev. B **24** (1981) 7386.

[18] B. Farid, V. Heine, G. Engel and I. J. Robertson, Phys. Rev. B **48** (1993) 11602.

[19] A. Sarkar, D. Sen, H. Haldar and D. Roy, Mod. Phys. Lett. B **12** (1998) 639.

[20] W. H. Butler, Phys. Rev. B **15** (1977) 5267.

[21] J. J. Hopfield, Phys. Rev. **186** (1969) 443.

[22] G. D. Gaspari and B. L. Gyorff, Phys. Rev. Lett. **28** (1972) 801.

[23] see N. P. Kovalenko, Yu. P. Krasny and U. Krey, *Physics of Amorphous Metals*, Wiley-VCH, Berlin (2001).

[24] P. Moral and P. W. Anderson, Phys. Rev. **125** (1962) 1263.

[25] J. S. Rajput and A. K. Gupta, Phys. Rev. **181** (1969) 743.

[26] C. M. Varma and R. C. Dynes, in: *Superconductivity in d- and f-Band Metals*, ed. D. H. Douglass, Plenum Press, New York (1976) p. 507.

[27] P. B. Allen and M. L. Cohen, Phys. Rev. **187** (1969) 525.

[28] B. T. Matthias, *Progress in Low Temperature Physics*, ed. C. J. Gorter, North Holland, Amsterdam (1957), Vol. 2.

[29] B. T. Matthias, Physica **69** (1973) 54.

PARAMETRI SUPRAVODLJIVOG STANJA TROJNIH AMORFNIH LEGURA $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu)

Dobro poznat Ashcroftov model potencijala s praznom jezgrom (EMC) smo primijenili u istraživanju parametara supravodljivog stanja (SPP), i to jakosti vezanja elektron-fonon λ, Coulombovog pseudopotencijala μ^*, prijelazne temperature T_C, eksponenta izotopnog učinka α i efektivne jakosti međudjelovanja N_0 trojnih amorfnih supravodiča, $(Ni_{33}Zr_{67})_{1-x}M_x$ (M = Ti, V, Co, Cu). Primijenili smo pet različitih funkcija za popravku lokalnog polja, koje su predložili Hartree (H), Taylor (T), Ichimaru-Utsumi (IU), Farid i sur. (F) i Sarkar i sur. (S), radi proučavanja utjecaja zasjenjenja na ta svojstva. Dobivene vrijednosti s popravkom lokalnog polja prema Sarkaru i sur. su u odličnom skladu s poznatim teorijskim podacima. Predlaže se kvadratna jednadžba za T_C koja uspješno daje T_C vrijednosti za navedene trojne amorfne legure. Ishodi ovih računa su također u skladu s ranije objavljenim podacima, što potvrđuje supravodljivu fazu u tim supravodičima.