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Theoretical study of superconducting state parameters of binary metallic glasses by a pseudopotential method

Aditya M. Vora *

Humanities and Social Science Department, STBS College of Diploma Engineering, Opp. Spinning Mill, Varachha Road, Surat 395 006, Gujarat, India

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ABSTRACT

The theoretical investigations 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 binary 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 λ and T_C are quite sensitive to the selection of the local field correction functions in comparisons with μ^*, α and N_0V. The T_C obtained from H-local field correction function is found in qualitative agreement with available experimental data and show linear nature with the concentration (C). A linear T_C equation is proposed by fitting the present outcomes for H-local field correction function, which is in conformity with other results for the 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.

1. Introduction

During the last few years, superconducting bulk metallic glasses superconductors based on various simple as well as transition metals have been obtained and studied by many researchers. Studying the superconducting state parameters (SSP) of binary superconductors may be of great significance in deciding their applications [1–18]. Though the pseudopotential theory is found to be very successful in studying various properties of the bulk metallic glasses superconductors, there are very few scattered attempts to study the SSPs of bulk superconductors based on model potential [3–12]. Very recently, we have studied recently the SSP of some bulk superconductors theoretically using model potential formalism [3,4]. Wang et al. [14–16] have been reported experimental SSPs for some BMG superconductor. Also, Li and Bai [17] have studied superconductivity in a representative Zr-based bulk metallic glass. The theoretical investigation of the SSPs of bulk metallic glasses superconductors has been reported in the literature very rarely. In the present work, we have used the screening functions of Hartree (H) [19], Taylor (T) [20], Ichimaru–Utsumi (IU) [21], Farid et al. (F) [22] and Sarkar et al. (S) [23]. Also, binary bulk metallic glasses superconductors may be quite suitable for industrial applications. Hence, in this Letter, we study the SSP viz. λ, μ^*, T_C, α and N_0V of seven $Cu_{100-C}Sn_C$ (C = 20, 39, 50, 60, 75, 84 and 90 at.%) viz. $Cu_{80}Sn_{20}$, $Cu_{61}Sn_{39}$, $Cu_{50}Sn_{50}$, $Cu_{40}Sn_{60}$, $Cu_{25}Sn_{75}$, $Cu_{16}Sn_{84}$ and $Cu_{10}Sn_{90}$ binary metallic glasses superconductors theoretically for the first time on the basis of Ashcroft's empty core (ECM) model potential [24]. Also, 'Cu' being a good conductor and exhibits conditional superconducting nature, while 'Sn' being a metallic element and also exhibits superconducting nature in normal condition, this class of glasses may be quite suitable for industrial applications. In the present work, the pseudo-alloy-atom (PAA) model was used to explain electron–ion interaction for alloying systems [3,4].

2. Computational methodology

The mathematical expressions used for the present computation of the SSP viz. λ, μ^*, T_C, α and N_0V for binary metallic glasses superconductors are as follows [1–17]:

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

$$\mu^* = \frac{\frac{m_b}{\pi k_F}\int_0^1 \frac{dX}{\varepsilon(X)}}{1+\frac{m_b}{\pi k_F}\ln\left(\frac{E_F}{10\theta_D}\right)\int_0^1 \frac{dX}{\varepsilon(X)}}, \tag{2}$$

* Permanent address: Parmeshwari 165, Vijaynagar Area, Hospital Road, Bhuj–Kutch, 370 001, Gujarat, India. Tel.: +91 2832 256424.
E-mail address: voraam@yahoo.com

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$$T_C = \frac{\theta_D}{1.45}\exp\left[\frac{-1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right], \quad (3)$$

$$\alpha = \frac{1}{2}\left[1-\left(\mu^*\ln\frac{\theta_D}{1.45T_C}\right)^2\frac{1+0.62\lambda}{1.04(1+\lambda)}\right], \quad (4)$$

$$N_0V = \frac{\lambda-\mu^*}{1+10\lambda/11}, \quad (5)$$

where m_b is the band mass, M, the ionic mass, Ω_0, the atomic volume, k_F, the Fermi wave vector, $W(X)$, the screened pseudopotential, E_F, the Fermi energy, $\varepsilon(X)$, the modified Hartree dielectric function [4] and $\langle\omega^2\rangle$ is the averaged square phonon frequency, respectively. The $\langle\omega^2\rangle$ is calculated using the relation given by Butler [25], $\langle\omega^2\rangle = 0.69\theta_D$, where θ_D is the Debye temperature.

The well known screened Ashcroft's empty core (EMC) model potential [24] used in the present computations of the SSP of binary metallic glasses is of the form,

$$W(X) = \frac{-\pi Z}{\Omega_0 X^2 k_F^2 \varepsilon(X)}\cos(2k_F X r_C), \quad (6)$$

here r_C is the parameter of the model potential of binary metallic glasses. The Ashcroft's empty core (EMC) model potential is a simple one-parameter model potential [24], which has been successfully found for various metallic complexes [3–12]. 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 [3–12]. Therefore, in the present work we use the Ashcroft's empty core (EMC) model potential with Hartree (H) [19], Taylor (T) [20], Ichimaru–Utsumi (IU) [21], Farid et al. (F) [22] and Sarkar et al. (S) [23] 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 available experimental data [18] of T_C in the literature for the particular metallic glass. After fitting the model potential parameter r_C, same r_C is then used in the computation of the SSP of binary metallic glasses. We have not fitted r_C from the first-principles calculations.

In the present investigation, the local field correction functions due to H [19], T [20], IU [21], F [22] and S [23] are incorporated to see the impact of exchange and correlation effects. The details of all the local field correction functions are narrated below.

The Hartree screening function [19] is purely static, and it does not include the exchange and correlation effects. The expression of it is,

$$f(q) = 0. \quad (7)$$

Taylor (T) [20] 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) [20],

$$f(q) = \frac{q^2}{4k_F^2}\left[1+\frac{0.1534}{\pi k_F^2}\right]. \quad (8)$$

The Ichimaru–Utsumi (IU) local field correction function [21] 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,

$$f(q) = A_{IU}Q^4 + B_{IU}Q^2 + C_{IU} + \left[A_{IU}Q^4 + \left(B_{IU}+\frac{8A_{IU}}{3}\right)Q^2 - C_{IU}\right]\left\{\frac{4-Q^2}{4Q}\ln\left|\frac{2+Q}{2-Q}\right|\right\}. \quad (9)$$

On the basis of Ichimaru–Utsumi (IU) local field correction function [21], Farid et al. (F) [22] have given a local field correction function of the form,

$$f(q) = A_FQ^4 + B_FQ^2 + C_F + \left[A_FQ^4 + D_FQ^2 - C_F\right]\left\{\frac{4-Q^2}{4Q}\ln\left|\frac{2+Q}{2-Q}\right|\right\}. \quad (10)$$

Based on Eqs. (9) and (10), Sarkar et al. (S) [23] have proposed a simple form of local field correction function, which is of the form,

$$f(q) = A_S\{1-(1+B_SQ^4)\exp(-C_SQ^2)\}, \quad (11)$$

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

Table 1
Input parameters and other constants.

Metallic glass	Z	r_C (au)	Ω_0 (au)^3	M (amu)	θ_D (K)
$Cu_{80}Sn_{20}$	1.60	0.3931	100.08	74.58	313.40
$Cu_{61}Sn_{39}$	2.17	0.6723	119.41	85.05	285.28
$Cu_{50}Sn_{50}$	2.50	0.7278	130.61	91.12	269.00
$Cu_{40}Sn_{60}$	2.80	0.7517	140.79	96.63	254.20
$Cu_{25}Sn_{75}$	3.25	0.8083	156.06	104.91	232.00
$Cu_{16}Sn_{84}$	3.52	0.8563	165.22	109.87	218.68
$Cu_{10}Sn_{90}$	3.70	0.8647	171.32	113.18	209.80

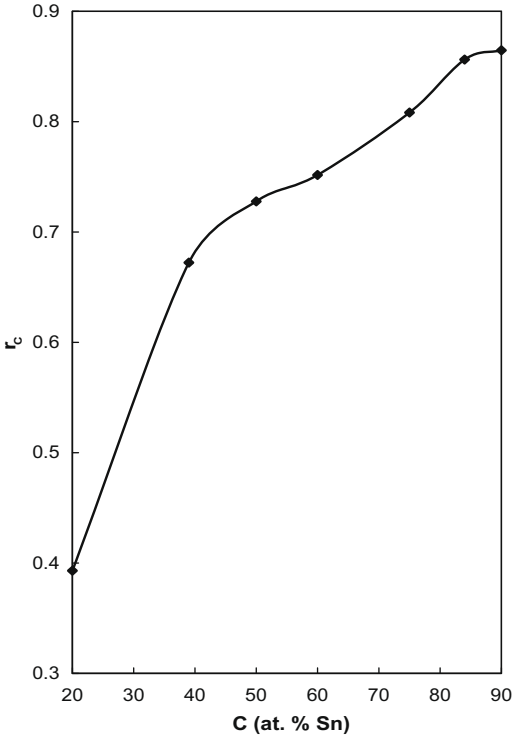

Fig. 1. Variation of the model potential parameter r_C with Sn-concentration (C) (in at.%).