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Superconducting state parameters of binary alloys

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ABSTRACT

The theoretical investigation of the superconducting state parameters (SSP) viz. electron–phonon coupling strength λ, Coulomb pseudopotential μ^*, transition temperature T_C, isotope effect exponent α and effective interaction strength N_OV of large numbers of binary alloys have been made extensively in the present work using a model potential formalism for the first time with pseudo-atom-alloy (PAA) model. A considerable influence of various exchange and correlation functions on λ and μ^* is found from the present study. The present results of the SSP are found in qualitative agreement with the available experimental data wherever exist.

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 and 18 K. Even some heavily doped semiconductors have also been found to be superconductors. The pseudopotential theory has been used successfully in explaining the superconducting state parameters (SSP) for metallic complexes by many workers [1–14]. 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 metallic complexes using single parametric model potential formalism. The study of the SSP of the binary 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 binary alloys involves the assumption of pseudoions with average properties, which are assumed to replace three types of ions in the binary systems, and a gas of free electrons is assumed to permeate through them. The electron–pseudoion is accounted for by the pseudopotential and the electron–electron interaction is involved through a dielectric screening function. For successful prediction of the superconducting properties of the alloying systems, the proper selection of the pseudopotential and screening function is very essential [3–12].

A well known empty core (EMC) model potential of Ashcroft [15] is applied here in the study of the SSP viz. electron–phonon coupling strength λ, Coulomb pseudopotential μ^*, transition temperature T_C, isotope effect exponent α and effective interaction strength N_OV of transition metals based binary alloys. To see the impact of various exchange and correlation functions on the aforesaid properties, we have used five different types of local field correction functions proposed by Hartree (H) [16], Taylor (T) [17], Ichimaru–Utsumi (IU) [18], Farid et al. (F) [19] and Sarkar et al. (S) [20]. We have incorporated for the first time the more advanced and newly developed local field correction functions i.e. IU, F and S in the investigation of the SSP of transition metals based binary alloys. In the present work, we have reported SSP of transition metals based binary alloys using pseudopotential method with five different types of local field correction functions.

In the present work, the pseudo-alloy-atom (PAA) model was used to explain electron–ion interaction for binaries. It is well known that the pseudo-alloy-atom (PAA) model is a more meaningful approach to explain such kind of interactions in binary systems [3–11]. 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 [3–11]. The complete miscibility in the alloy systems is considered as a rare case. Therefore, in such binary systems the atomic matrix elements in the pure states are affected by the

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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 [3–11]. Looking to the advantage of the PAA model, we propose a use of PAA model to investigate the SSP of transition metals based binaries.

To describe electron–ion interactions in the binary systems, the Ashcroft's empty core (EMC) single parametric local model potential [15] is employed in the present investigation. The form factor $W(q)$ of the EMC model potential in wave number space is (in au) [15]

$$W(q) = \frac{-8\pi Z}{\Omega_O q^2 \varepsilon(q)} \cos(qr_C). \tag{1}$$

Here Z, Ω_O, $\varepsilon(q)$ and r_C are the valence, atomic volume, Hartree dielectric function and parameter of the model potential of transition metals based binary alloys, respectively. Our study is differentiated with previous work in such a way that, in the most of the previous work, the model potential parameter is fitted with experimental data of the transition temperature T_C. But, in the present work, the model potential parameter r_C is determined using the first zero of the form factor.

2. Method of computation

In the present investigation for binary mixtures, the electron–phonon coupling strength λ is computed using the relation [3–12]

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

Here m_b is the band mass, M the ionic mass, Ω_O the atomic volume, k_F the Fermi wave vector and $W(q)$ the screened pseudopotential. The effective averaged square phonon frequency $\langle\omega^2\rangle$ is calculated using the relation given by Butler [21], $\langle\omega^2\rangle^{1/2} = 0.69\theta_D$, where θ_D the Debye temperature of the transition metals based binary alloys.

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

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

where Z and $W(X)$ are the valence and the screened EMC pseudopotential [14] of the transition metals based binary alloys, respectively.

The Coulomb pseudopotential μ^* is given by [3–12]

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

where E_F is the Fermi energy, m_b the band mass of the electron and $\varepsilon(X)$ the modified Hartree dielectric function, which is written as [16]

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

$\varepsilon_H(X)$ is the static Hartree dielectric function [16] 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 details of all the local field corrections are below.

The H-screening function [16] is purely static, and it does not include the exchange and correlation effects. The expression of it is,

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

Taylor (T) [17] 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) [17],

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

The Ichimaru–Utsumi (IU)-local field correction function [18] is a fitting formula for the dielectric screening function of the degenerate electron liquids at metallic and lower densities, which accurately reproduces the Monte-Carlo results as well as it also, satisfies the self consistency condition in the compressibility sum rule and short range correlations. The fitting formula is

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

On the basis of Ichimaru–Utsumi (IU)-local field correction function [18], Farid et al. (F) [19] have given a local field correction function of the form

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

Based on Eqs. (8) and (9), Sarkar et al. (S) [20] have proposed a simple form of local field correction function, which is of the form

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

where $Q = 2X$. 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 [18–20].

After evaluating λ and μ^*, the transition temperature T_C and isotope effect exponent α are investigated from the McMillan's formula [3–14]

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

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

The expression for the effective interaction strength $N_O V$ is studied using [3–12]

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

3. Results and discussion

The constants and parameters used in the present investigation are tabulated in Table 1. To determine the input parameters and various constants for PAA model [3–11], the following definitions for transition metals based binary alloys $A_{1-x}B_x$ are adopted,

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

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

$$\Omega_O = (1-x)(\Omega_O A) + x(\Omega_O B), \tag{16}$$

$$r_C = (1-x)(r_{CA}) + x(r_{CB}), \tag{17}$$