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Superconducting state parameters of metallic glass $Mg_{70}Zn_{30}$ using linearized screened pseudopotential

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Abstract. A linearized form for the screened form factors of electron-phonon interaction in the metallic glass $Mg_{70}Zn_{30}$ is applied for the first time to predict the superconducting state parameters viz. electron-phonon coupling strength (λ), Coulomb pseudopotential (μ^*), transition temperature (T_c), isotope effect exponent (α) and the interaction strength ($N_0 V$). Computed results agree with the experimental data available in the literature.

Keywords. Superconductivity; metallic glass; superconducting state parameters; pseudopotential.

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1. Introduction

The basic problem of determining the superconducting transition temperature T_c of a superconductor has two separate aspects; firstly, understanding the material properties (electron-phonon coupling strength, λ), the Coulomb pseudopotential (μ^*), and the phonon spectrum, which is usually over simplified by some frequency (ω), and secondly calculating $T_c\{\lambda, \mu^*, \omega\}$. This paper deals with both the aspects of glassy materials. These materials have interested scientists, engineers and technologists because of their widespread applications in material science and engineering. Extensive work has been done on vibrational dynamics [1, 2], elastic [3] and transport properties of metallic glasses. However, the superconductivity in these materials has, to our knowledge, not been much explored [4–6] and this prompted us to study the superconductivity in the metallic glasses.

With this aim, we apply BCS–Eliashberg McMillan model [7–9] to these materials for computation of superconducting properties of metallic glass $Mg_{70}Zn_{30}$. For achieving this goal, we have constructed the form factors for this metallic glass by using a quadratic form of screened potential, called linearized screened pseudopotential by Sharma *et al* [10], as it provides almost linear form for $V_s(q)-q$ curve in the limit $0<q<2k_F$. Parameters of this pseudopotential are determined by graph fitting method to realistic pseudopotential form factors of the relevant constituent metal as obtained from HA potential [11] and modify these parameters as suggested by Saxena *et al* [12]. The form factors of glass obtained by this potential are then used to calculate superconducting state properties, namely electron-phonon coupling strength (λ), Coulomb pseudopotential (μ^*), transition temperature (T_c), isotope effect coefficient (α) and the interaction strength ($N_0 V$).

2. Theory

The linearized screened pseudopotential by Sharma *et al* [10] has the following quadratic form,

$$V_s(q) = \frac{\langle k+q|w|k\rangle}{\varepsilon_q} = A_1 + B_1 q + C_1 q^2 \tag{1}$$

where A_1, B_1 and C_1 are the potential parameters and q is the momentum transfer. If we define $x = q/2k_F$, where k_F is the Fermi momentum, then potential form reduces to

$$V_s(x) = A + Bx + Cx^2 \tag{2}$$

where A, B and C are the new potential parameters.

We modify this potential (2) by incorporating the concept of mean effective density dependent interatomic potential in glass forming alloy of the type $\alpha_{\varsigma_\alpha}\beta_{\varsigma_\beta}$ [12]

$$V_{\text{eff}}(x) = \varsigma^2{}_\alpha V_{\alpha\alpha}(x) + 2\varsigma_\alpha \varsigma_\beta V_{\alpha\beta}(x) + \varsigma^2{}_\beta V_{\beta\beta}(x). \tag{3}$$

Here, $V_{\alpha\alpha}(x)$ is the pair potential for the α-α component, $V_{\alpha\beta}(x)$ for α-β component and $V_{\beta\beta}(x)$ for the β-β component in the $\alpha_{\varsigma_\alpha}\beta_{\varsigma_\beta}$ metallic glass alloy, having concentrations ς_α of α-type and ς_β of β-type. Now pair potentials using (2) are

$$V_{\alpha\alpha} = A_\alpha + B_\alpha x + C_\alpha x^2 \tag{4}$$

$$V_{\beta\beta} = A_\beta + B_\beta x + C_\beta x^2 \tag{5}$$

$$V_{\alpha\beta} = A_{\alpha\beta} + B_{\alpha\beta} x + C_{\alpha\beta} x^2. \tag{6}$$

Substituting (4), (5) and (6) into (3), new form of linearized screened potential obtained is

$$\begin{aligned} V_s(x) = {} & (\varsigma^2{}_\alpha A_\alpha + 2\varsigma_\alpha C_\beta A_{\alpha\beta} + \varsigma^2{}_\beta A_\beta) \\ & + (\varsigma^2{}_\alpha B_\alpha + 2\varsigma_\alpha C_\beta B_{\alpha\beta} + \varsigma^2{}_\beta B_\beta)x \\ & + (\varsigma^2{}_\alpha C_\alpha + 2\varsigma_\alpha C_\beta C_{\alpha\beta} + \varsigma^2{}_\beta C_\beta)x^2. \end{aligned} \tag{7}$$

The parameters of $V_{\alpha\alpha}$ i.e. A_α, B_α, C_α and the parameters of $V_{\beta\beta}$ i.e. A_β, B_β, C_β are determined by the graph fitting method to the form factors of the HA potential [11] for the constituents of the metallic glass $Mg_{70}Zn_{30}$. Defining again new potential parameters A', B' and C', (7) finally takes the form

$$V_s(x) = A' + B'x + C'x^2, \tag{8}$$

where

$$A' = \varsigma^2{}_\alpha A_\alpha + 2\varsigma_\alpha C_\beta A_{\alpha\beta} + \varsigma^2{}_\beta A_\beta,$$

$$B' = \varsigma^2{}_\alpha B_\alpha + 2\varsigma_\alpha C_\beta B_{\alpha\beta} + \varsigma^2{}_\beta B_\beta,$$

$$C' = \varsigma^2{}_\alpha C_\alpha + 2\varsigma_\alpha C_\beta C_{\alpha\beta} + \varsigma^2{}_\beta C_\beta.$$

We termed the relation (8) as modified linearized potential. This modified linearized potential (8) has been tested by applying it for the evaluation of superconducting state parameters of metallic glass $Mg_{70}Zn_{30}$. The electron-phonon coupling strength for the alloy $\alpha_{\varsigma_\alpha}\beta_{\varsigma_\beta}$ may be written as follows by extending the relevant formula for metals [13]

$$\lambda = \frac{12m^*z^*}{M\langle\omega^2\rangle}\int_0^1 \mathrm{d}x|V_s(x)|^2x^3, \tag{9}$$

where $M = \varsigma_\alpha M_\alpha + \varsigma_\beta M_\beta$ is the ionic mass, $m^* = \varsigma_\alpha m_\alpha^* + \varsigma_\beta m_\beta^*$ is the effective mass. In the effective mass relation, m_α^* and m_β^* are the effective masses of Mg and Zn respectively, which are taken as $m_\alpha^* = 1{\cdot}33$ and $m_\beta^* = 0{\cdot}86$ from [14].

$V_s(x)$ is the pseudopotential used, defined by (8), and $\langle\omega^2\rangle$ is the average square phonon frequency of the glassy system under consideration defined as given by Butler [15]

$$\langle\omega^2\rangle^{1/2} = 0{\cdot}69\Theta_D \tag{10}$$

where Θ_D is the Debye temperature for the glass, which is obtained using the GrimVall formula [16]

$$\frac{1}{(\Theta_D)^2} = \frac{\varsigma_\alpha}{(\Theta_{D\alpha})^2} + \frac{\varsigma_\beta}{(\Theta_{D\beta})^2}. \tag{11}$$

Here $\Theta_{D\alpha}$ and $\Theta_{D\beta}$ are the Debye temperatures for Mg and Zn respectively, which are taken as $\Theta_{D\alpha} = 342$ K and $\Theta_{D\beta} = 235$ K from [17]. The effective balance Z^* used in (9) for glass is computed by [18]

$$z^* = (2 - m_E)z. \tag{12}$$

Here z is the mean balance of the glassy system and m_E is the component of effective mass. The values for m_E are 0·92 and 0·89 for Mg and Zn respectively [14].

Electron-phonon coupling strength formula (9), after substituting potential (8) and simplified takes the form

$$\lambda = \frac{12m^*z^*}{M\langle\omega^2\rangle}\left[\frac{A'^2}{4} + \frac{B'^2}{6} + \frac{C'^2}{8} + \frac{2}{5}A'B' + \frac{1}{3}A'C' + \frac{2}{7}B'C'\right]. \tag{13}$$

Other parameter Coulomb pseudopotential (μ^*) is given by Rajput and Gupta [19]

$$\mu^* = \frac{m^*}{\pi k_F}\int_0^1 \frac{\mathrm{d}x}{x\varepsilon(x)} \Bigg/ \left[1 + \frac{m^*}{\pi k_F}\ln\left(\frac{k_F^2}{20\Theta_D}\right)\int_0^1 \frac{\mathrm{d}x}{x\varepsilon(x)}\right]. \tag{14}$$

Here $\varepsilon(x)$ is the dielectric screening function, which is taken in the Hartree form [20] for simplicity. The relevant expression for the transition temperature (T_c) and isotope effect exponent α are respectively given [20] by

$$T_c = \frac{\Theta_D}{1{\cdot}45}\exp\left[\frac{-1{\cdot}04(1+\lambda)}{\lambda - \mu^*(1+0{\cdot}62\lambda)}\right] \tag{15}$$

and

$$\alpha = \frac{1}{2}\left[\ln - \left(\mu^*\ln\frac{\Theta_D}{1{\cdot}45T_c}\right)^2\frac{1+0{\cdot}62\lambda}{1{\cdot}04(1+\lambda)}\right]. \tag{16}$$

The effective interaction strength $N_0 V$, given by Rajput and Gupta [19], is

$$N_0 V = \frac{\lambda - \mu^*}{1 + (10/11)\lambda}. \tag{17}$$

3. Results and discussion

The form factors of $V_{\alpha\alpha}$ and $V_{\beta\beta}$ i.e. pair-potential for Mg-component and Zn-component, have been compared with that of the HA potential in figures 1 and 2. The new form factors show an excellent agreement with that of the HA potential. The values of parameters A', B' and C' as computed through (8) are given in table 1.

In the calculation of superconducting state parameters, the input parameters used are listed in table 2. The superconducting state parameters for the present work as well as others [5, 6, 21] are shown in table 3. The evaluated value of the electron-phonon coupling strength (λ) is 0·48, which shows that there should be a weak coupling between electrons and phonons. The Coulomb pseudopotential (μ^*) is found to be of the same order as suggested by Allèn and Dynes [13], which strengthens the present theory for this new type of material. The T_c value 1·21 K shows the best agreement with the experimental data $T_c = 0·7$ K due to Calka *et al* and with $T_c = 1·4$ K as reported in [6]. The present result is also in good agreement with the other theoretical result $T_c = 0·369$ K [21] for this metallic glass. In [21], the superconducting state parameters of this metallic glass have been calculated by applying Ashcroft's empty core model potential which is different from the pseudopotential used in the present work. The positive value $N_0 V$, in table 3 reveals the superconducting character of the metallic glass $Mg_{70}Zn_{30}$.

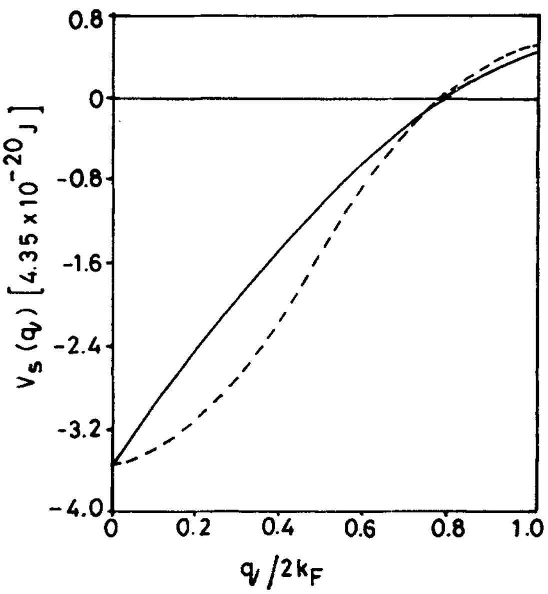

Figure 1. Comparison of present work form factors with HA for Mg: —— modified linearized potential, -.- HA.

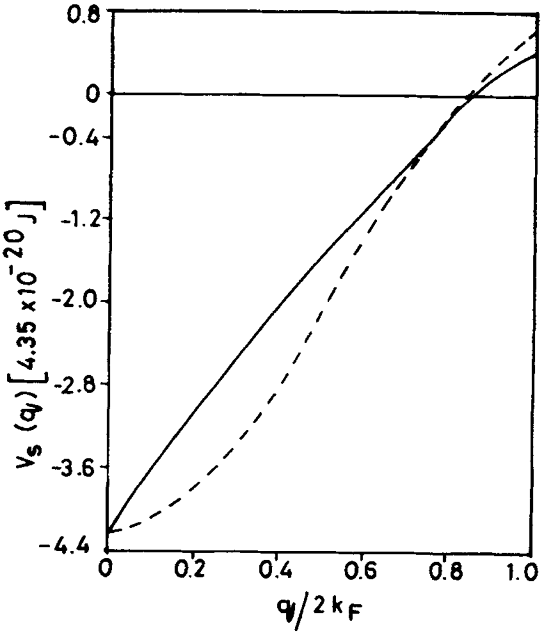

Figure 2. Comparison of present work form factors with HA for Zn: —— modified linearized potential, –·– HA.

Table 1. Values of parameters A', B', C' computed through (8).

A'	B'	C'
−0·2748	0·4542	−0·1424

Table 2. Input parameters used in the calculation.

Parameters	m^*	z^*	M 10^{-28} kg	Θ_D (K)	k_F (10^{10} m^{-1})
Values	1·189	2·178	844·400	295·950	1·390

Table 3. Superconducting state parameters of the metallic glass $Mg_{70}Zn_{30}$.

	λ	μ^*	T_c(K)	α	$N_0 V$
Present work	0·48	0·14	1·21	+0·232	+0·238
[5]	–	–	0·70	–	–
[6]	–	–	1·40	–	–
[21]	0·39	0·13	0·369	+0·185	+0·130

Finally, we may conclude that overall satisfactory reproduction of all the superconducting state parameters confirms the validity of the proposed very simple pseudopotential i.e. the quadratic form of potential called linearized screened pseudopotential by its proposers [10]. Because of its simple form and since screening of the bare ion potential is not required in this method, this potential is being applied for the other metallic glasses also in our group and the results will be reported shortly. The fitting of the pseudopotential to the form factors of standard HA potential will be more realistic if we add more terms i.e. beyond quadratic in (1). But addition of more terms makes handling of the potential more complex in the calculation of superconducting state parameters. But since the potential parameters are fitted to the realistic form factors given by HA potential [11], the variation in the results is expected to be subtle. However, the investigation of changes on this account may certainly be of theoretical interest. We therefore propose to carry out this investigation in future.

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