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Superconducting parameters of metals and alloys : HFP technique

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Abstract : The superconducting parameters of metals and alloys have been studied within the framework of BCS theory *via* McMillan [1] technique for different metals and alloys using Harrisons First Principles (HFP) pseudopotential. This technique is being used for the first time for this investigation although it is more rigorous and based on sound theoretical background. In the present paper we have studied the electron phonon coupling strength λ, Coulomb pseudopotential μ^*, superconducting transition temperature T_C of MgAl and ZnAl binary alloys. The results are compared with available experimental and theoretical data giving a reasonable agreement and providing an insight into the systems under investigation.

Keywords : Superconductivity, pseudopotential, alloys

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1. Introduction

In the present era the study of Superconductivity (SC) of metals and alloys occupies the centre stage in the field of condensed matter physics. The theoretical work in this field got impetus since the proposition of BCS theory which was later developed to suite within the framework of pseudopotentials by McMillan [1], Allen and Cohen [2] and Eliashberg [3]. The theory was extended to binary alloys by Allen and Dynes [4]. Scattered attempts have been made to apply this technique using model potentials or other techniques [5–10].

A study of the existing literature reveals that one of the more rigorous and theoretically sound technique *viz.* Harrison's first principle (HFP) pseudopotential [11] has not been used for the purpose although it has been successfully used in the past few decades to explain the atomic, electronic and other properties of metals and alloys [12–15]. This has encouraged us to apply this technique to study the superconducting transition parameters of binary alloys MgAl and ZnAl.

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2. Formalism

The parameters under investigation are the electron-phonon coupling strength (EPCS) λ, the Coulomb coupling strength μ^* and the SC transition temperature T_C represented by

$$\lambda = \frac{m^* \Omega_o}{4\pi^2 k_F M k_B^2 \theta_D^2} \int_0^{2k_f} q^3 |w(k,q)|^2 dq , \tag{1}$$

$$\mu^* = \frac{\mu}{1+\mu \ln(E_F / k_B \theta_D)} . \tag{2}$$

where

$$\mu = \frac{1}{\pi k_F} \int_0^{2k_F} \frac{dq}{q\varepsilon^*(q)} , \tag{3}$$

$$T_C = \frac{\theta_D}{1.45} \exp\left[-\left(\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right) \right] . \tag{4}$$

In these equations, k_B is the Boltzmann's constant, m^* is the effective electronic mass, M the atomic mass, Z the valence, k_F the Fermi wave vector, θ_D the Debye temperature, q the phonon wave vector, $w(k,q)$ the screened form factor, $\varepsilon^*(q)$ the modified Hartree dielectric function using Vashista-Singwi (V-S) form of exchange correlation [16] and E_F the Fermi energy.

The input parameters (X) of alloys are evaluated through

$$X_{AB} = (1 - c)X_A + cX_B, \tag{5}$$

where A and B are constituent metals, c is the concentration of B and X represents the atomic volume Ω_o, valence Z, atomic mass M, Fermi wave vector k_F of the species. The Debye temperature of the alloy is given by

$$\frac{1}{(\theta_D)^2_{AB}} = \frac{1-c}{(\theta_D)^2_A} + \frac{c}{(\theta_D)^2_B} . \tag{6}$$

The electron-phonon coupling strength λ involves the screened form factor given by

$$w(k,q) = \left(v_q^{a,b} + v_q^c + v_q^d\right) / \varepsilon^*(q) + [1 - G(q)] v_q^l / \varepsilon^*(q) + W^R , \tag{7}$$

where $v_q^{a,b}$, v_q^c, v_q^d and v_q^l are the valence charge and core electron potential, conduction band-core exchange potential, conduction electron potential and screening potential respectively and W^R is the repulsive potential. $G(q)$ is the exchange correlation function which is given by

$$G(\eta) = A\left[1 - e^{-B\eta^2}\right] \quad \text{where} \quad \eta = q/k_F \tag{8}$$

in the V-S form of exchange-correlation [17]. $\varepsilon^*(\eta)$ is the modified Hartree dielectric function given by

$$\varepsilon^*(\eta) = [1 - G(\eta)][\varepsilon_H(\eta) - 1] + 1, \tag{9}$$

where

$$\varepsilon_H(\eta) = 1 + \frac{2}{\pi k_F \eta^2}\left[1 + \frac{4-\eta^2}{4\eta} ln\left|\frac{2+\eta}{2-\eta}\right|\right] \tag{10}$$

is the Hartree dielectric function. The parameter $\varepsilon^*(\eta)$ is also involved in the expression for the Coulomb coupling μ^*.

3. Computation

The computation of the form factor $w(k,q)$ and the modified Hartree dielectric function $\varepsilon^*(q)$ is carried on through eqs. (7) and (8), respectively. The core energy eigenvalues ε_{nl} needed for the computation of $w(k,q)$ is taken from Herman-Skillman program [17] and the input parameters are presented in Table 1. From these computed $w(k,q)$ of constituent metals the form factor of the alloys and other constants are obtained through eq. (5) and the Debye temperature $(\theta_D)_{AB}$ is obtained through eq. (6). After these computations we proceed to compute the superconducting parameters through eqs. (1) to (4). The results thus obtained have been presented in Table 1 for comparison with experimental observations.

Table 1. SC parameters of binary alloys *AB*.

Alloy (*AB*)		SC parameters		Present		Expt.
MgAl	0.3	m_b	1.0000	1.2780	0.9180	
		λ	0.2777	0.3550	0.2549	
		μ^*	0.0773	0.0773	0.0773	
		T_C	0.2300	1.2900	0.1000	0.84
MgAl	0.5	m_b	1.0000	1.4650	1.0200	
		λ	0.3022	0.4427	0.3082	
		μ^*	0.0767	0.0767	0.0767	
		T_C	0.4613	3.6400	0.5316	0.84
ZnAl	0.3	m_b	1.0000	1.0200	0.9360	
		λ	0.3480	0.3549	0.3257	
		μ^*	0.0753	0.0753	0.0753	
		T_C	0.9702	1.1400	0.6900	0.5–0.84
ZnAl	0.5	m_b	1.0000	1.2500	0.9800	
		λ	0.3531	0.4414	0.3460	
		μ^*	0.0752	0.0752	0.0752	
		T_C	1.1131	3.1600	0.9900	0.5–0.84

4. Result and observation

The computed SC parameters λ, μ^* and T_C, alongwith the band mass m_b of the alloys MgAl and ZnAl treated as effective mass m^* have been presented in Table 1 for two different concentration c = 0.3 and c = 0.5 (equiatomic composition). Considering the free electron behavior of the constituent metals band mass m_b = 1 has been taken initially for the above alloys. Two other band masses have also been evaluated for the binary alloy, as provided in this table. Other theoretical data of λ and μ^* or T_C is not available for comparison. Hence, only the experimental value of T_C has been given in the table.

An inspection of Table 1 brings out the fact that for MgAl with c = 0.3 and m_b = 1.278 we get λ = 0.355 and T_C = 1.29 against the experimental value 0.84 K. With c = 0.5 and m_b = 1.02 we get λ = 0.3082 and T_C = 0.53. These are in qualitative agreement with experiment. For ZnAl with c = 0.3 and m_b = 0.936 we get λ = 0.3257 and T_C = 0.69 which lies within the experimental range 0.5–0.84 K. However, with c = 0.5 and m_b = 0.980 we get λ = 0.346 and T_C = 0.99 which is slightly higher than the experimental range.

5. Conclusion

Harrison's first principle (HFP) pseudopotential technique has been used for the first time to study the superconducting parameters of binary alloys MgAl and ZnAl with reasonable success. The present investigation shows that the transitin temperature T_C is quite sensitive to the electron-phonon coupling strength λ. The Coulomb pseudopotential μ^* is in general of the order of 0.1 as for pure metals. The accuracy of λ and T_C mainly depends upon the correctness of the form factor which, in turn, hinges upon the input parameters such as core energy eigenvalues, $X\alpha$-exchange parameter, *opw* parameter and the form of exchange-correlation function.

References

[1] W L McMillan *Phys. Rev.* **167** 331 (1968)
[2] P B Allen and M L Cohen *Phys. Rev.* **187** 525 (1969)
[3] G M Eliashberg *Soviet Phys. JETP* **11** 696 (1960); **12** 1000 (1961)
[4] P B Allen and R C Dynes *Phys. Rev.* **B12** 905 (1975)
[5] H Khan, V Singh and K S Sharma *Indian J. Pure Appl. Phys.* **31** 628 (1993)
[6] V Singh, H Khan and K S Sharma *Indian J. Pure Appl. Phys.* **32** 915 (1994)
[7] P P Singh *Bull. Mater Sci.* **26** 131 (2003)
[8] D M Gaitonde, P Modak, R S Rao and B K Godwal *Bull. Mater Sci.* **26** 137 (2003)
[9] S Sharma, Haniph Khan and K S Sharma *Indian J. Pure Appl. Phys.* **41** 301 (2003)
[10] A M Vora, M H Patel, P N Gajjar and A R Jani *Pramana* **58** 849 (2002)
[11] R S Day, F Sun and P H Cutler *Phys. Rev.* **A19** 328 (1979)
[12] J Hafner *Phys. Stat. Sol.* **(b)56** 579 (1973); **57** 101 (1973); **57** 497 (1973)

[13] J A Morlarty *Phys. Rev.* **B16** 2537 (1977)

[14] M M Khan and S M Rafique *Phys. Stat. Sol.* **(b)139** K131 (1987)

[15] K K Mukerjee, S M Rafique, M M Khan and S Bagchi *Phys. Stat. Sol.* **(b)147** K51 (1988)

[16] P Vashishta and K S Singwi *Phys. Rev.* **B6** 875 (1972)

[17] F Herman and J Skillman *Atomic Structure Calculation* (Englewood Cliff, N.J. : Prentice Hall) (1963)