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Impact of eigenvalues on the electron-phonon coupling strength of aluminium and its binary alloys

B. K. Kanth[1], S. K. Chakrabarti[2*], I. S. Jha[2], B. P. Singh[3]

[1]Department of Chemistry, M. M. A. M. Campus, Tribhuvan University, Biratnagar, Nepal
[2]Department of Physics, M. M. A. M. Campus, Tribhuvan University, Biratnagar, Nepal
[3]Department of Physics, T. M. Bhagalpur University, Bhagalpur, Bihar, India
*E-mail: skc_2007@yahoo.com

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Abstract

Aluminium is a third group element according to the periodic table. Chemically it is a reactive metal often forming complexes within its binary alloys. In the present work we have dealt with the impact of eigenvalues on the superconducting state parameter viz. the electron-phonon coupling strength of this metal. We have also dealt with the same for two binary alloys of it viz. aluminium-magnesium and aluminium-zinc. For this purpose we have computed the non-local screened form factor for each of them. Initially the orthogonalised plane wave parameter has been taken as unity. Thereafter Vashishta-Singwi form of exchange and correlation is employed. The core energy eigenvalues of Herman-Skillman have been used. Our results are quite satisfactory for the metal as well as its present alloys. Our computation reveals that the superconducting state parameter can be reasonably reproduced by Harrison's first principle pseudopotential technique along with McMillan's formalism provided a proper choice of the core energy eigenvalues is made.

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Keywords: Superconducting state parameter; orthogonalised plane wave parameter; eigenvalue; form factor.

1. Introduction

The electron-phonon coupling strength gives us the superconducting state parameter. The basis of a general quantum theory of superconductivity was given in the year 1957 by Bardeen, Cooper and Schrieffer [1]. After a decade McMillan developed this BCS theory by the concept of pseudopotential [2]. Few years later the theory was developed further by Allen and Dynes for application on binary alloys [3]. In the present theoretical work we have used Harrison's first principle (HFP) pseudopotential technique to study the impact of eigenvalues on the electron-phonon coupling strength of the trivalent metal aluminium and its binary alloys i.e. aluminium-magnesium and aluminium-zinc [4].

In Section 2 the necessary formula for computation is furnished. The results of our computation have been discussed in Section 3 which is followed by a brief conclusion in Section 4.

2. Formulation

The electron-phonon coupling strength is given by

$$\lambda = \frac{12mZ}{M < \omega^2 >} \int_0^2 \eta^3 \left| w(k, q) \right|^2 d\eta,$$

where M is the atomic mass, Z the valency, m the mass of electron, $<\omega^2>$ the average phonon frequency, $w(k, q)$ the non-local screened form factor and

$$\eta = \frac{q}{k_F}.$$

3. Results and Discussion

3.1 Metal Aluminium

We have computed the form factors of aluminium using the core energy eigenvalues of Herman-Skillman and considering the orthogonalised plane wave parameter to be unity [5]. Due to small core in case of aluminium the Xα-exchange parameter has been taken as $\alpha=\alpha_{vt}$ satisfying virial theorem. Then the Vashishta-Singwi form of exchange and correlation has been used [6]. The nature of the form factors is furnished in Figure–1.

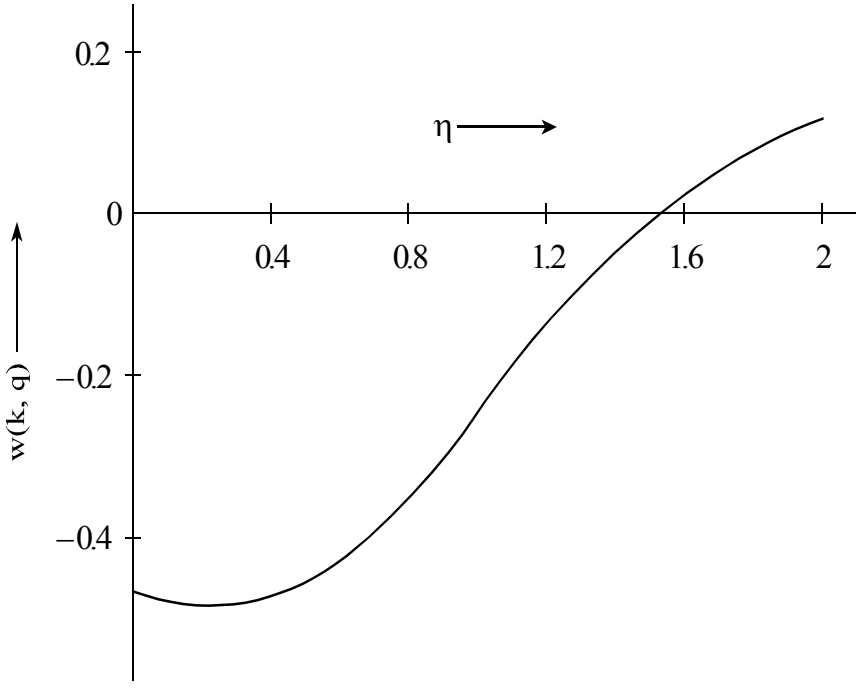

Fig. 1 : Form factors of aluminium.

The computed value of λ is given in the table below. Our result is quite satisfactory. The impact of eigenvalues on the electron-phonon coupling strength of aluminium can be realized from this table.

Table: Electron-Phonon Coupling Strength

Matter		Computed λ		λ desired	λ due to others	
Nature	**Name**	**Value**	**EV of**		**Value**	**Researcher**
Metal	Al	0.43	HS*	0.43	0.43	RG**
Alloy	Al-Mg	0.40	HS-HS	0.37	0.42	YRK***
Alloy	Al-Zn	0.36	HS-HS	0.35	0.37	Allen-Dynes

*HS≡Herman-Skillman **RG≡Rajput-Gupta [7]
***YRK≡Yadav-Rafique-Kumar [8]

3.2 Alloys of Aluminium

In case of the alloy aluminium-magnesium the Herman-Skillman eigenvalues have been considered for aluminium [9]. For magnesium also we have taken the eigenvalues of Herman-Skillman. The nature of the form factors is shown in Figure–2.

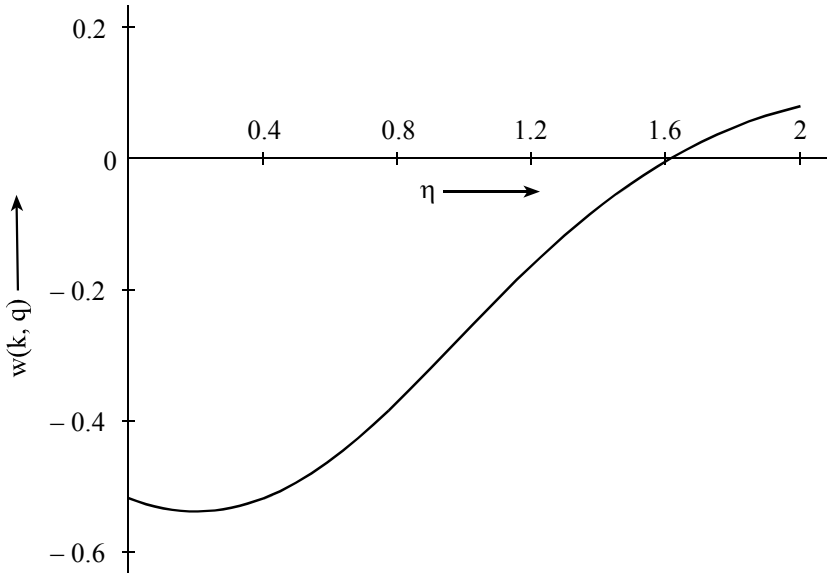

Fig. 2 : Form factors of aluminium-magnesium alloy.

The nature of the form factors of aluminium-zinc alloy is depicted in Figure–3. Herman-Skillman eigenvalues have been used for aluminium. For zinc also the eigenvalues of Herman-Skillman have been considered to have better result.

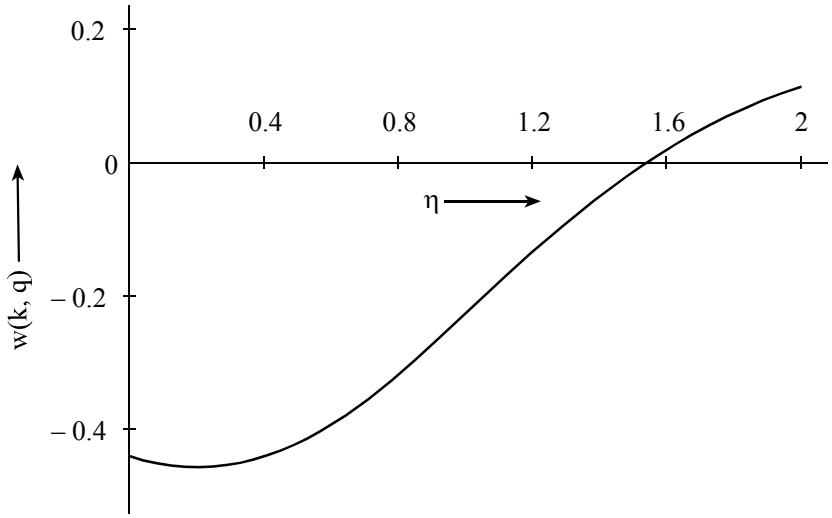

Fig. 3 : Form factors of aluminium-zinc alloy.

The computed values of the electron-phonon coupling strength of the present alloys are furnished in the said table along with the respective values provided by previous researchers. The desired value of λ for Al-Mg alloy is 0.37 and our computed value is 0.40. For Al-Zn alloy our computed value of λ is 0.36 whereas the desired value is 0.35.

4. Summary and Conclusion

HFP pseudopotential technique based on BCS theory and McMillan's formalism has been used to compute the electron-phonon coupling strength (λ) of aluminium. Besides this the values of λ have been computed for two binary alloys of it—Al-Mg and Al-Zn. Our results are quite satisfactory as compared to the values obtained by previous researchers.

Our computation reveals that the superconducting state parameter is reasonably reproducible by HFP pseudopotential technique if the core energy eigenvalues can be chosen properly.

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