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

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Abstract. Magnesium is a highly reactive alkaline earth metal. In the present work we have dealt with the impact of eigenvalues on the superconducting state parameter viz. the electron-phonon coupling strength (λ) of this metal. Side by side two binary alloys of it viz. magnesium-aluminium and magnesium-indium have also been considered for the same. In this course the form factors for all of them have been computed. For the purpose of this initially the orthogonalised plane wave parameter has been taken as unity. Then the Vashishta-Singwi form of exchange and correlation is employed. Finally the results have been compared with the theoretical values derived by others. Our computation reveals that λ can be reasonably reproduced by the Harrison's first principle pseudopotential technique provided a proper choice of the core energy eigenvalue is made.

Keywords. Superconducting state parameter, Orthogonalised plane wave parameter, Eigenvalue, Form factor, Correlation.

1. Introduction

The electron-phonon coupling strength (λ) 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 in 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 bivalent metal magnesium and its binary alloys i.e. magnesium-aluminium and magnesium-indium [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 summary and conclusion in Section 4.

2. Basic formalism

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 magnesium*

We have computed the form factors of magnesium using the core energy eigenvalues of Clementi and considering the orthogonalised plane wave parameter to be unity [5]. Due to small core in case of magnesium 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.

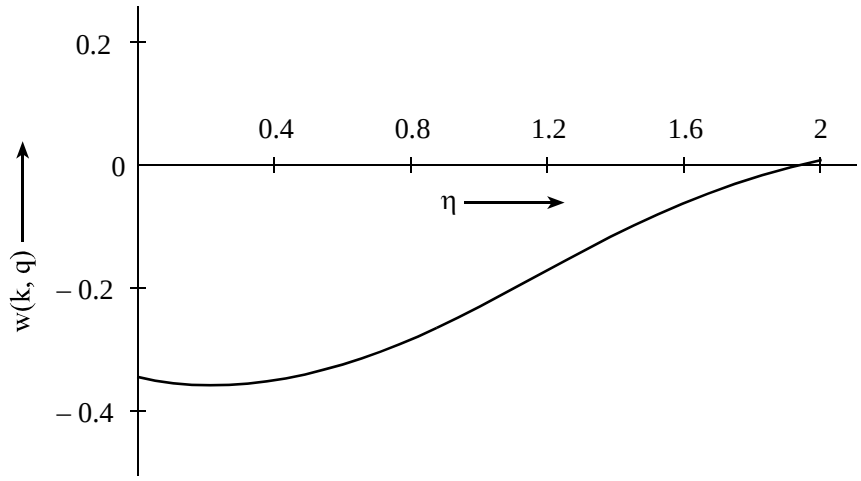

Fig. 1. Form factors of magnesium

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 magnesium can be realised from this table.

Table. Electron-phonon coupling strength

Matter		**Computed λ**		**λ due to others**	
Nature	**Name**	**Value**	**EV of**	**Value**	**Researcher**
Metal	Mg	0.39	Clementi	0.39	Janak [7]
Alloy	Mg-Al	0.41	HS-HS*	0.42	YRK**
Alloy	Mg-In	0.58	C-E***	0.29–0.73	McMillan

*HS≡Herman-Skillman **YRK≡Yadav-Rafique-Kumar [8]
***C-E≡Clementi-Experimental

3.2 *Alloys of magnesium*

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

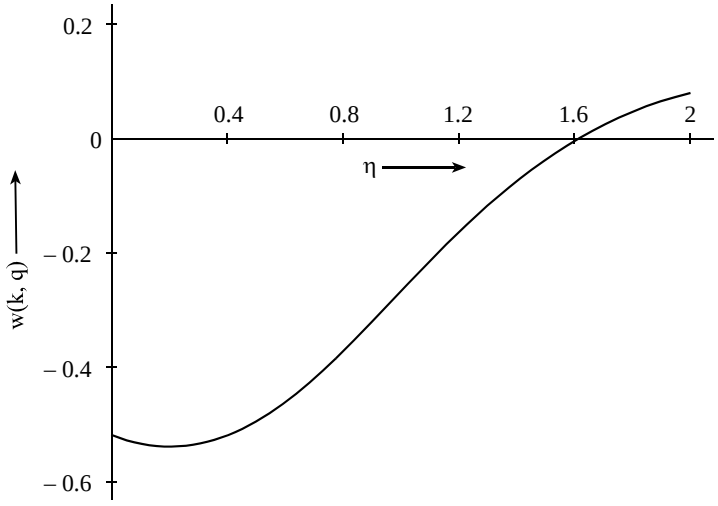

Fig. 2: Form factors of magnesium-aluminium alloy

The nature of the form factors of magnesium-indium alloy is depicted in Figure 3. Clementi eigenvalues are not available for indium [10]. So, for indium the experimental energy values have been taken. For magnesium the eigenvalues of Clementi have been considered to have better result.

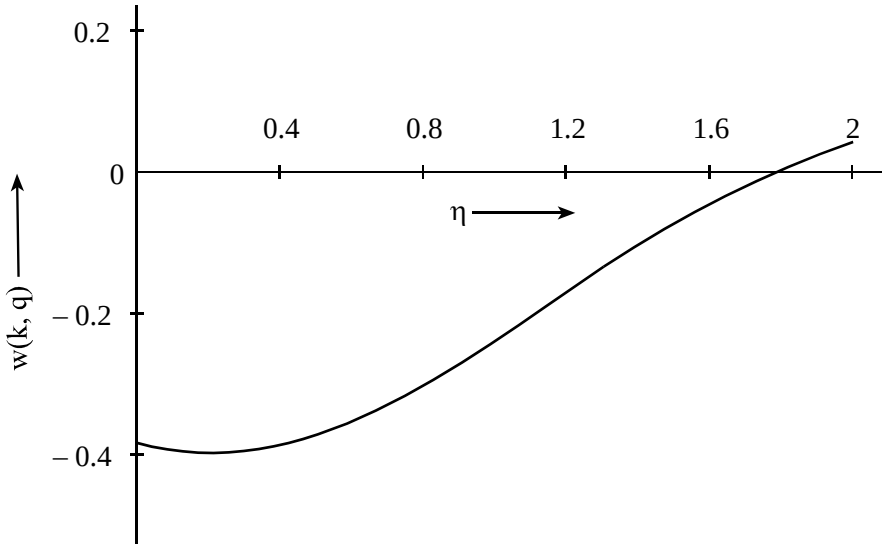

Fig. 3: Form factors of magnesium-indium alloy

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 Mg-Al alloy is 0.37 and our computed value is 0.41. For Mg-In alloy our computed value of λ is 0.58 whereas the desired value is 0.64.

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 magnesium. Besides this the values of λ have been computed for two binary alloys of it—Mg-Al and Mg-In. 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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