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IMPACT OF EIGENVALUES ON THE ELECTRON-PHONON COUPLING STRENGTH OF INDIUM AND ITS BINARY ALLOYS

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ABSTRACT

Indium is a trivalent metal. Though chemically not so reactive, it often forms complexes within its binary alloys. In this theoretical work we have studied the impact of eigenvalues on the electron-phonon coupling strength of indium. We have also dealt with the same for two binary alloys of it viz. indium-magnesium and indium-zinc. First of all we have computed the non-local screened form factor for each of them. For this purpose initially the orthogonalised plane wave parameter is considered as unity. Thereafter Vashishta-Singwi form of exchange and correlation are employed. For indium the Clementi eigenvalues being not available, the experimental energy values have been taken besides the Herman-Skillman core energy eigenvalues. Our results are quite satisfactory for the metal. For the alloys our results lie within the range of values as obtained by other researchers. 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.

Key words: Superconducting state parameter, Orthogonalised plane wave parameter, Core energy eigenvalue, Non-local screened form factor, Harrison's first principle pseudopotential.

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]. In the present work we have used Harrison's first principle pseudopotential technique to study the impact of eigenvalues on the electron-phonon coupling strength of the trivalent metal indium and its binary alloys i.e. indium-magnesium and indium-zinc [3].

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.

MATERIALS AND METHOD

BASIC FORMALISM

The electron-phonon coupling strength is given by

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

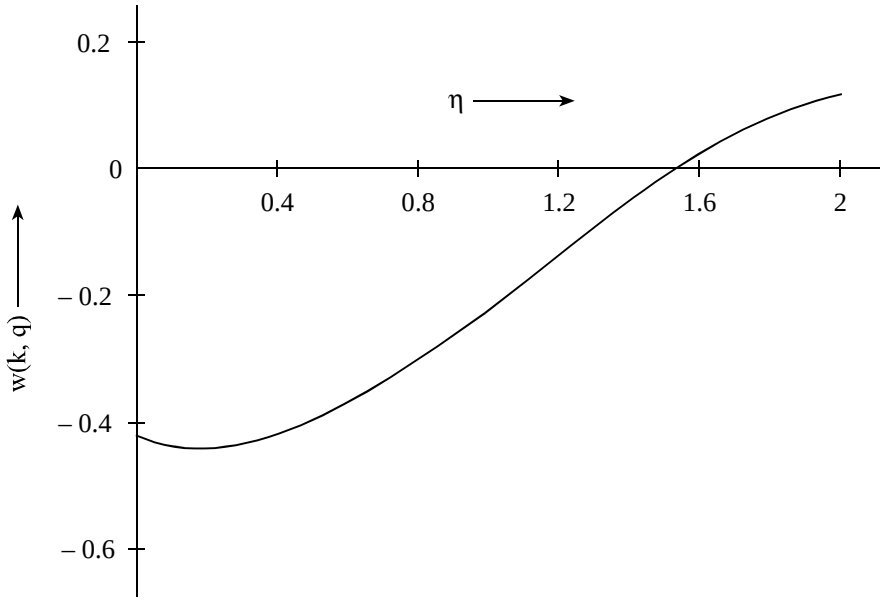
where M is the atomic mass, Z the valency, 'm' the mass of electron, <□^{2}> the average phonon frequency, w(k, q) the non-local screened form factor and

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

RESULT AND DISCUSSION

Metal Indium

We have computed the form factors of indium using the core energy eigenvalues of Herman-Skillman and considering the orthogonalised plane wave parameter to be unity [4]. The X□-exchange parameter has been taken as □=2/3 and Vashishta-Singwi form of exchange and correlation have been used [5]. Clementi eigenvalues are not available for indium [6]. The nature of the form factors is furnished in Figure–1.



Figure–1: Form factors of indium

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 indium can be realised from this table.

TABLE

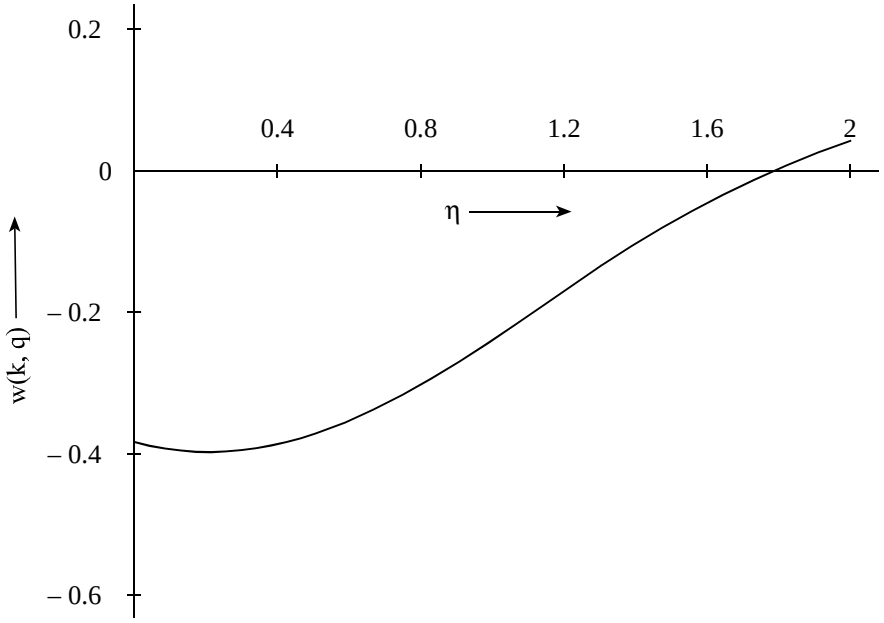
Electron-Phonon Coupling Strength

Matter		Computed λ		λ due to others	
Nature	**Name**	**Value**	**EV of**	**Value**	**Researcher**
Metal	In	0.91	HS*	0.29	AC**
Alloy	In-Mg	0.58	E-C***	0.29–0.73	McMillan
Alloy	In-Zn	0.88	HS-HS	0.26–0.94	AC

*HS≡Herman-Skillman **AC≡Allen-Cohen [7] ***E-C≡Experimental-Clementi

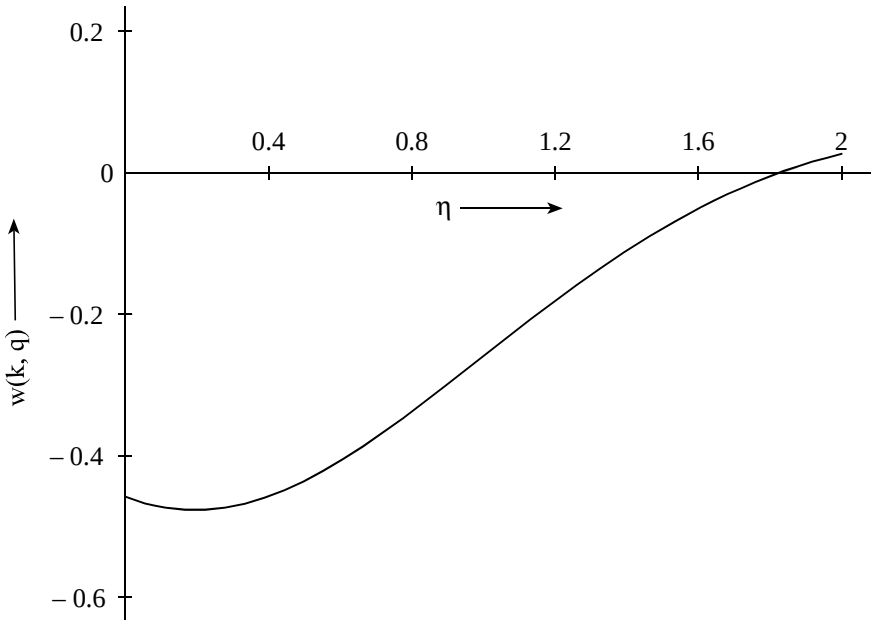
Alloys of Indium

The nature of the form factors of indium-magnesium alloy is shown in Figure–2. For indium the experimental energy values and for magnesium the eigenvalues of Clementi have been considered to have better result.



Figure–2: Form factors of indium-magnesium alloy

In case of the alloy indium-zinc the Herman-Skillman eigenvalues have been considered for indium. For zinc also we have taken the eigenvalues of Herman-Skillman. The nature of the form factors is depicted in Figure–3.



Figure–3: Form factors of indium-zinc alloy

The computed values of the electron-phonon coupling strength of the present alloys are furnished in the above table along with the respective values provided by previous researchers. For In-Mg alloy our computed value of λ is 0.58 whereas the desired value is 0.64. The desired value of λ for In-Zn alloy is 0.57 but our computed value is 0.88.

CONCLUSION

HFP pseudopotential technique based on BCS theory and McMillan's formalism has been used to compute the electron-phonon coupling strength (λ) of indium. Side by side the values of λ have been computed for two binary alloys of it—In-Mg and In-Zn. For indium and its alloy In-Mg the eigenvalues produce satisfactory result. But for In-Zn alloy the eigenvalues could not give satisfactory result. However, for these alloys our results lie within the range of values as obtained by previous researchers.

Our computation reveals that the superconducting state parameter is reasonably reproducible by Harrison's first principle pseudopotential technique if the core energy eigenvalues can be chosen properly.

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