A MATHEMATICAL STUDY OF THE IMPACT OF EIGENVALUES ON THE ELECTRON-PHONON COUPLING STRENGTH OF ZINC AND ITS BINARY ALLOYS

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Abstract: *In this paper we have made a mathematical study of the impact of eigenvalues on the electron-phonon coupling strength of the bivalent metal zinc and its binary alloys Zn-Al and Zn-In.*

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 in binary alloys[3]. In the present work we have dealt with the impact of eigenvalues on the superconducting state parameter viz. the electron-phonon coupling strength (□) of the bivalent metal zinc. Side by side two binary alloys of it viz. zinc-aluminium and zinc-indium have also been considered for the same. For this purpose we have used Harrison's first principle (HFP) pseudopotential technique[4]. Initially the orthogonalised plane wave parameter has been taken as unity. Then the Vashishta-Singwi form of exchange and correlation is employed[5]. Finally the results have been compared with the theoretical values derived by others.

In the next section the necessary formula for computation is furnished. It is followed by the section in which the results of our computation have been discussed. The last section comprises of a brief summary as well as conclusion.

Basic Formalism

The electron-phonon coupling strength is given by

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

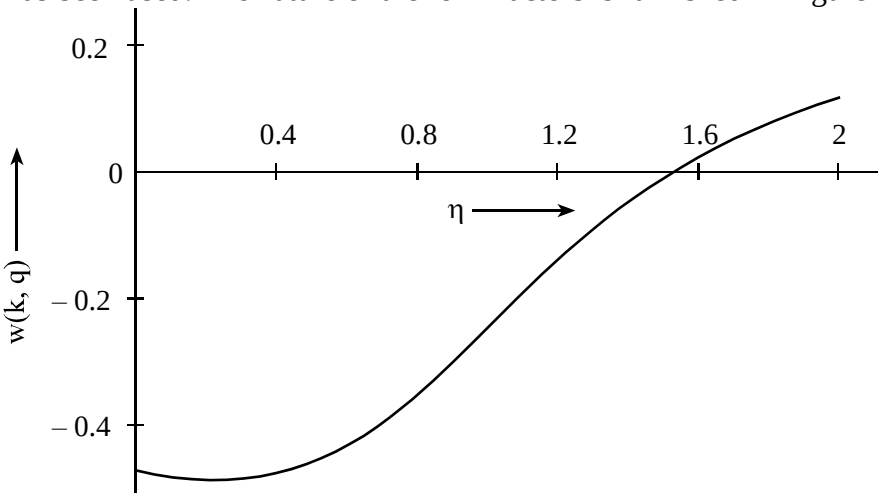
where M is the atomic mass, Z the valency, m the mass of electron, <□^{2}> the average phonon frequency, $w(k, q)$ the non-local screened form factor and

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

Results and Discussion

Metal Zinc

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



Figure–1: Form factors of zinc

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

TABLE

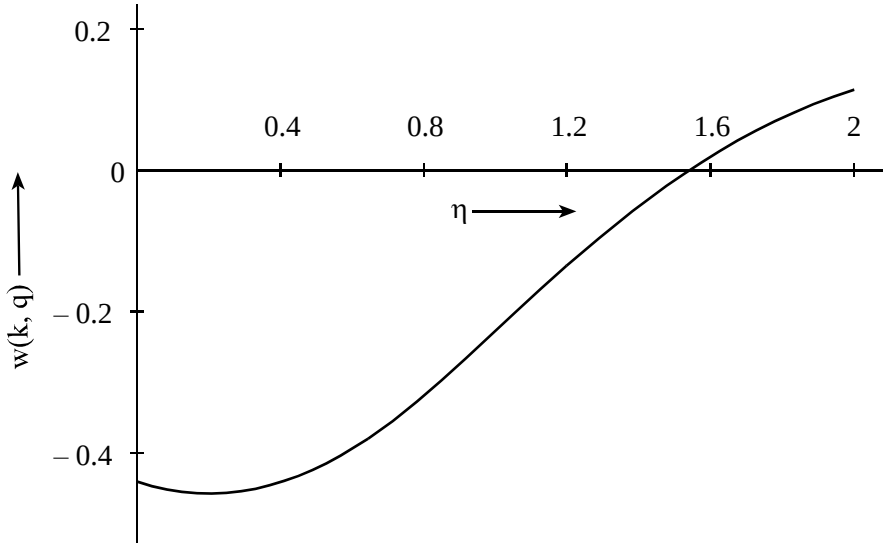
Electron-Phonon Coupling Strength

Matter		Computed □		□ due to others	
Nature	**Name**	**Value**	**EV of**	**Value**	**Researcher**
Metal	Zn	0.17	HS	0.17	RG*
Alloy	Zn-Al	0.36	HS-HS	0.37	YRK**
Alloy	Zn-In	0.87	HS-HS	0.26–0.94	AC***

*RG≡Rajput-Gupta[7] **YRK≡Yadav-Rafique-Kumar[8]
***AC≡Allen-Cohen[9]

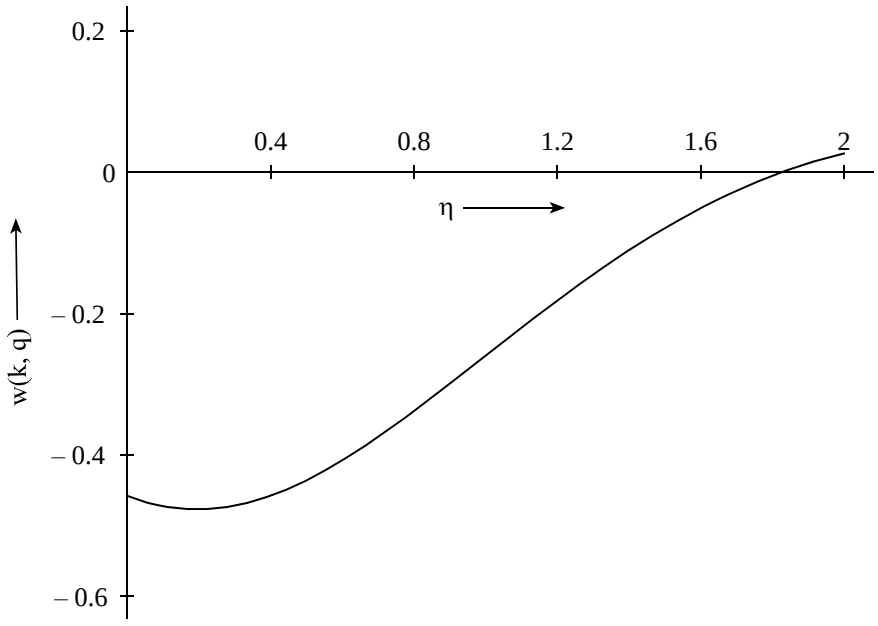
Alloys of Zinc

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



Figure–2: Form factors of zinc-aluminium alloy

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



Figure–3: Form factors of zinc-indium 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 found out by previous researchers. The desired value of for Zn-Al alloy is 0.35 and our computed value is 0.36. For Zn-In alloy our computed value of is 0.87 whereas the desired value is 0.57.

Summary and Conclusion

HFP pseudopotential technique based on BCS theory and McMillan's formalism has been used to compute the electron-phonon coupling strength () of zinc. Besides this the values of have been computed for two binary alloys of it i.e. Zn-Al and Zn-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.

References

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