Impact of Eigenvalues on the Superconducting State Parameter for Some Trivalent Metals and their Binary Alloys

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Abstract

In this mathematical work we have considered the trivalent metals aluminium and indium. Aluminium is a reactive metal, generally forming complexes within its alloys. Indium is chemically not so reactive. However, within its alloys also it often forms complexes. Here we have studied the impact of eigenvalues on the superconducting state parameter for not only these metals but also some binary alloys of them. In case of aluminium we have considered the binary alloys aluminium-magnesium and aluminium-zinc. For indium too two binary alloys of it have been studied for the same: indium-magnesium and indium-zinc. Our results are quite satisfactory for the metal aluminium as well as its present alloys. For the metal indium also our result is very satisfactory. For its alloys our results lie within the range of values 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.

Keywords: Superconducting state parameter; Orthogonalised plane wave parameter; Eigenvalue, form factor; Correlation.

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\textsuperscript{1}. After a decade McMillan developed this BCS theory by the concept of pseudopotential\textsuperscript{2}. Few years later the theory was developed further by Allen and Dynes for application on binary alloys\textsuperscript{3}. In the present mathematical 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 metals aluminium and indium and the binary alloys Al-Mg and Al-Zn of the former and In-Mg and In-Zn of the later\textsuperscript{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. Basic Formalism

The superconducting state parameter is given by

\[
\lambda = \frac{12mZ}{M} \frac{1}{\langle \omega^2 \rangle} \int_0^2 \eta^3 |w(k, q)|^2 \, d\eta,
\]

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

\[
\eta = \frac{q}{k_F}.
\]
3. Results and Discussion

First of all we have computed the non-local screened form factors for each of these metals and alloys. For this purpose initially the orthogonalised plane wave parameter has been considered as unity. Thereafter Vashishta-Singwi form of exchange and correlation are employed³.

3.1 Aluminium and its Alloys

3.1.1 Metal Aluminium

In case of metal aluminium the core energy eigenvalues of Herman-Skillman have been used⁶. Due to small core of aluminium the Xα-exchange parameter has been taken as α=αc, satisfying virial theorem⁷. The nature of the form factors is shown in Figure–1.

![Figure–1: Form factors of aluminium](image)

The computed value of the superconducting state parameter is furnished in Table–1. Our result is in very good agreement with the desired value. The impact of eigenvalues on λ for aluminium can be realised from this table.

<table>
<thead>
<tr>
<th>Matter</th>
<th>Computed λ</th>
<th>λ desired</th>
<th>λ due to others</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metal</td>
<td>Al</td>
<td>0.43</td>
<td>0.43</td>
</tr>
<tr>
<td>Alloy</td>
<td>Al-Mg</td>
<td>0.40</td>
<td>HS-HS</td>
</tr>
<tr>
<td>Alloy</td>
<td>Al-Zn</td>
<td>0.36</td>
<td>HS-HS</td>
</tr>
</tbody>
</table>

³HS=Herman-Skillman ³³RG=Rajput-Gupta ³³³YRK=Yadav-Rafique-Kumar

3.1.2 Alloys of Aluminium

3.1.2.1 Aluminium-Magnesium Alloy

For both the constituent species of this alloy the Herman-Skillman eigenvalues have been considered to have better result. The nature of the form factors is depicted in Figure–2.
3.1.2.2 Aluminium-Zinc Alloy

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

3.2 Indium and its Alloys

3.2.1 Metal Indium

For indium the Clementi eigenvalues are not available\[^{10}\]. So, the experimental energy values have been taken into account. Indium having larger core the $X\alpha$-exchange parameter has been taken as\[^{11}\] $\alpha=2/3$. The nature of the form factors is furnished in Figure–4.
The computed value of $\lambda$ is put in Table–2. Our result is quite satisfactory. The impact of eigenvalues on the superconducting state parameter for indium can be realised from this table.

Table–2 Superconducting State Parameter

<table>
<thead>
<tr>
<th>Nature</th>
<th>Name</th>
<th>Computed $\lambda$</th>
<th>$\lambda$ desired</th>
<th>$\lambda$ due to others</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metal</td>
<td>In</td>
<td>0.91</td>
<td>HS</td>
<td>0.89</td>
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<tr>
<td>Alloy</td>
<td>In-Mg</td>
<td>0.58</td>
<td>E-C$^{**}$</td>
<td>0.64</td>
</tr>
<tr>
<td>Alloy</td>
<td>In-Zn</td>
<td>0.88</td>
<td>HS-HS</td>
<td>0.57</td>
</tr>
</tbody>
</table>

$^*$JK=Jain-Kachhava$^{12}$  
$^{**}$E-C=Experimental-Clementi  
$^{***}$AC=Allen-Cohen$^{13}$

3.2.2 Alloys of Indium

3.2.2.1 Indium-Magnesium Alloy

In case of In-Mg alloy the eigenvalues of Clementi have been considered for magnesium while the experimental energy values for indium. The nature of the form factors of this alloy is shown in Figure–5.
### 3.2.2.2 Indium-Zinc Alloy

In case of the alloy In-Zn the Herman-Skillman eigenvalues are used for both the ingredients. The nature of the form factors is depicted in Figure–6.

#### Figure–6: Form factors of indium-zinc alloy

The computed values of the superconducting state parameter of these two alloys of indium are furnished in Table–2 along with the respective values provided by previous researchers. For In-Mg alloy our computed value of $\lambda$ is 0.58 whereas the desired value is 0.64. The desired value of $\lambda$ for In-Zn alloy is 0.57 but our computed value is 0.88.

### 4. Summary and Conclusion

HFP pseudopotential technique based on BCS theory and McMillan's formalism has been used to compute the superconducting state parameter ($\lambda$) for aluminium. Besides this the values of $\lambda$ 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.

For indium and its alloy In-Mg the eigenvalues produce satisfactory results. But for In-Zn alloy the eigenvalues could not give satisfactory result. However, for these alloys our results lie within the range of 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