THERMO-ELECTRONIC PROPERTIES OF BINARY LIQUID AMALGAMS AT DIFFERENT CONCENTRATION

Dr. Sebilal Sebak
P.G. Department of Physics, B. N. M. U., Madhepura.
**Dr. Ranjan Prasad**
P.G. Department of Physics, B. N. M. U., Madhepura.
Dr. Umashanker Choudhary
Prof. & Head, Department of Physics, H.P.S. College, Nirmali.

ABSTRACT

The theoretical investigation of Thermo-Electronic transport properties in liquid metals and binary alloys requires the knowledge of Pseudopotential matrix element as well as the structure of the system. Since the advent of Ziman formula, this has been widely used to make such investigation based on model potential approach. The form factors have been computed for two self consistent sets of eigenvalues and eigenfunctions. The eigenfunctions affect the form factors through the energy independent terms and also through the energy dependent terms, whereas the eigenvalue comes into the play through the energy dependent terms only We have found that the eigenfunction do

not affect the form factors appreciably-the effect is within 4 to 5% The eigenvalues on the other hand affect the form factor prominently. We have observed that the major contributions to the form factor come from highest filled s-eigenvalue followed by P and d- eigenvalue. The impact of structure factor on the evaluation of the Thermo-Electronic transport properties has been computed for the complex forming alloys and observed that those are also showing anomalous behavior.
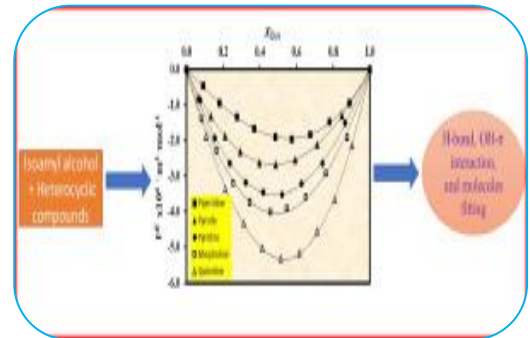
KEYWORDS: *Pseudopotential; Hard-Sphere diameter; Structure Factor.*

INTRODUCTION

In many cases it is convenient to position variable. With a view to take a simple approach. The energy operator can be substituted by a simple non-operator term V, that is.

$$W (q) = V(q) + V (k) \tag{1}$$

Which defines a local Pseudopotential. We assumed W (q) is made up of the sum of N individual ion contribution W (q). We also assume that

N ions are located at the points $R_1, R_2, R_3 \ldots\ldots R_N$; In a specific configuration. Thus the total potential energy of an electron may be expressed as.

$$W (q) = \Sigma_j W (r_i - R_j)$$

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Contribution of W is small. So it can be treated as a perturbation. The first order perturbation can be written in terms of the so called plane wave matrix elements of the Pseudopotential.

$$(k+q|W|k) = 1/\Omega \int e^{-i(k+q).r} \Sigma_j W(|r_i - R_j|) e^{ikr} d_3r$$

$$= 1/N\Sigma_i e^{iq.R} N/\Omega \int e^{-i(k+q).(ri-Rj).}$$

$$W(|r_i - R_j| e^{ik.(ri-Rj)} d^3r \tag{2}$$

Here (k +q (W|k) is the plane wave matrix elements where the wave function (k) is plane waves exp (ik.r)

Or, $(k + q|W|k) = S(q)(k + q|W|k)$

Where $S(q) = 1/N \Sigma_i e^{-iqR} \tag{3}$

S(q) is called structure factor which depends only on ion position R_j and

$$(k+q|W|k) = \Omega \int e^{-i(k+q).r} W(q) e^{ik.r} d^3r$$

Is called form factor. It depends upon the individual ion potential and is independent of the ion position where $\Omega = \Omega / N$. Ashcroft and Langreth (1967) developed formalism in the hard sphere model system to calculate theoretically the three partial structure factors. The formalism is based on the solution of well-known Percus-Yevick equation. The volume of the alloy is determined in ideal sense (i.e. assuming no volume change on alloying) using the relation

$$\Omega_{alloy}^{Ideal} (1-C) \Omega_1 + C \Omega_2$$

Here Ω_1 . Ω_2 are the atomic volume of the component species of the alloys and C is concentration of the second component.

Hard sphere diameter:

The basic input data to determine six partial structure factors. (S_{11}, S_{22}, S_{33}, S_{12}, S_{13}, S_{23}) are hard sphere diameters and packing fraction.

Inter ionic pair potential:

The hard sphere diameters have been determined using the relation

$$V_{ij}(\sigma_i) - V_{man} + \frac{2}{3} K_B T$$

Where $\frac{2}{3} K_B T$ is the main kinetic energy and V_{min} is the first minimum.

in the inter ionic pair potential which can be obtained [Mishra *et al*. (1993)] as

$$V_{ij} = \frac{Z_i Z_j}{R} \left[1 - \frac{2}{\pi} \int_0^\infty {}^N F_{ij}(q) \frac{\sin qR}{q} dq \right] \tag{3.31}$$

Where Z_i and Z_j are the Valencies of the constituent elements of the alloy, q is the phonon wave vector. $F_{ij}(q)$ are normalized wave number characteristics.

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$$\text{given by } \Gamma_{ij}(q) = -\left(\frac{q^2\Omega}{2\pi Z_i Z_j}\right) F_{ij}(q) \tag{3.32}$$

Here
$$\Omega = \Omega_{ideal} + \Delta\Omega$$

With
$$\Omega_{ideal} = C_1\Omega_2 + C_2\Omega_2 \tag{3.33}$$

Ω_1 and Ω_2 are the atomic volume of the constituent elements of the alloy at required temperature and Ω accounts the contraction or expansion on alloying. C_1 and C_2 are the concentrations of the component metals of the alloy.

In the local approximation $F_{ij}(q)$ is expressed as

$$F_{ij} = \left(\frac{q^2\Omega}{8\pi}\right)\left[W_i(q)W_j(q)\frac{\in *(q)-1}{\in *(q)}\frac{1}{1\backslash -G(q)}\right] \tag{3.32}$$

$E^*(q)$ is the modified Hartree dielectric function given by

$$E^*(q) = 1 + (\in(q)-1)(1-G(q))$$

FABER-ZIMAN FORMULA:
It was shown by Faber and Ziman (1965) that the diffraction model for liquid metals proposed by Ziman (1961) could easily be extended for binary alloys. For the sake of better representation. We express the resistivity of binary alloys as consisting of three distinct contributions. i.e.

$$R = R_{\alpha.\alpha} + R_{\beta.\beta} + R_{\alpha.\beta}$$

where the first two terms on right hand side arise due to same particle correlation and the third term ($R_{\alpha.\beta}$) is due to the cross term scattering. α and β represent here the constituent species of the binary alloys. The different contributions are given by

$$R_{\alpha.\alpha} = [\frac{3\pi}{h|e|^2}][\frac{\Omega}{NV_F^2}]\,4\int_0^1 C_1 W_1 S_{11}[\frac{q}{2K_F}]^3\, d[\frac{q}{K_F}]$$

$$R_{\beta.\beta} = [\frac{3\pi}{h|e|^2}][\frac{\Omega}{NV_F^2}]\,4\int_0^1 C_2 W_2 S_{22}[\frac{q}{2K_F}]^3\, d[\frac{q}{K_F}]$$

And

$$R_{\alpha.\beta} = [\frac{3\pi}{h|e|^2}][\frac{\Omega}{NV_F^2}]\,4\int_0^1 2(C_1 C_2)\frac{1}{2}W_1 W_2 S_{12}[\frac{q}{2K_F}]^3\, d[\frac{q}{K_F}]$$

In a composite form R can be expressed as

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$$R = [\frac{3\pi}{h\,|e|^2}][\frac{\Omega}{NV_F^2}]\frac{<\sum_{\alpha,\beta}}{}(C_1C_2)^{\frac{1}{2}}S_{ij}(q)W_\alpha(q)S_\beta(q)>$$

Where $<\quad>$ stands for

$$<\quad> = 4\,[\int_0^1 C_1 S_{11}(q)\,W_1^2(q) + C_2 S_{22}(q)\,W_2^2(q)$$

$$+\,2\,(C_1C_2)^{\frac{1}{2}}S_{12}(q)W_1(q)W_2(q)$$

here $W_1(q)$ and $W_2(Q)$ are the form factors of species 1 and 2 constituting the alloys; C_1, C_2 are the concentrations and $S_{11}(q)$ $S_{22}(q)$ and $S_{12}(q)$ are the partial structure factors of the alloy.

Table
Hard sphere diameter of Hg and Pb and Hg-In alloys

SYSTEM	CONCEN. CZN	VOLUME	K_F	σ_1	σ_2	ELECTRICAL RESISTIVITY		
						Present	Expt.	Previous Theo. Value
Hg-Zn	0.00	164.89	0.6996		5.530	112.26	117.03	130.00
	0.50	138.52	0.7603	6.115	5.568	63.33	4015	094.00
	1.00	121.03	0.8099	6.150		41.65	31.23	091.13
Hg-Pb	0.00	184.89	0.6998		5.463	112.29	117.03	101.02
	0.50	191.02	0.7747	5.160	5.450	079.81	87.52	106.54
	1.00	216.93	0.8173	5.253		60.65	91.21	096.23
*Mott (1966) Ashcroft and Langreth								

CONCLUSION:

It has been shown that the Eigen functions do not affect the form factor appreciably on the other hand the Eigen value affect the form factor appreciably .By theoretical observations it has been found that the major contribution to the form factor comes from highest filled s-Eigen value followed by p and d –Eigen values. This trend has been confirmed by finding anomalies when we have evaluated the thermo electronic transport properties for complex alloys in this study

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