ANOMALOUS BEHAVIOR OF ELECTRONIC TRANSPORT PROPERTIES IN Cu-Sn LIQUID BINARY ALLOY

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Abstract–The Harrison's First Principle technique in conjunction with the hard sphere technique of Ashcroft and Langreth has been used for the study of electrical resistivity, Knight shift, Fermi energy and density of states of Cu-Sn alloy. The alloy show the behavior of "rigid hard-sphere" model found for the first time in this alloy. Also, the Knight shift varies as a linear function of concentration supporting Kaeck's assumption. The partial structure factors and hence resistivity shows anomalous behavior at a particular composition representing a dynatron type characteristic thereby producing a negative-resistance phenomenon in this alloy and hence making this material an important candidate for various industrial and commercial applications.

Keywords: Cu-Sn liquid alloy, electrical conductivity, Knight shift, electronic density of states, NMR

1. Introduction

Metals are free to dissolve in one another in their liquid state and the number of different alloy systems whose physical properties have now been studied as a function of composition in the liquid state is very considerable. To extend this study to liquid alloys is trivial from a formal point of view. However, it becomes necessary to distinguish between the pseudo-potentials of different species of ion which are present, and for a given system these are liable to vary with concentration.

The liquid Cu-Sn alloy is a matter of investigation since past few decades [1-9]. There are various anomalies found in past during the study of partial structure factors (PSF) of this monopolyvalent alloy. Enderby et al. [10] have measured the PSF of Cu-Sn with the aid of neutron experiment and isotropic replacement. They reported that the peaks in $S_{\text{Cu-Cu}}(k)$ and $S_{\text{Sn-Sn}}(k)$ are in almost the same place for the alloy as they are for pure Cu and pure Sn, respectively, while the peak in $S_{\text{Cu-Sn}}(k)$ does not lie half midway between them and is virtually coincident with the peak in $S_{\text{Cu-Sn}}$, which is quite inconsistent with the rigid sphere model. Orton and Williams [11] found that at $C_{\text{Sn}} = 0.45$ and 0.60, the main peak gets split usually into two sub-peaks.

The well-known electrical conduction theory by Ziman (1961, 1967) [12, 13] for liquid metals and its extended form by Faber-Ziman (1965) [14] for liquid metal binary alloys using pseudopotential concept have been found very successful in predicting the electrical resistivity of several liquid metals and alloys. The presence of conduction electrons and their interaction with the background of positive ions is treated through the Harrison's First principle (HFP) pseudopotential technique which is a branch of orthogonalized plane wave (OPW) formalism first proposed by Herring (1940) [15] and later developed by Philips and Kleinmann (1959) [16] and others. In the present paper, we theoretically deal with the structure, electrical resistivity, Knight shift, Fermi energy and electronic density of states of Cu-Sn liquid binary alloy. The structure factor S(k) needed for the present computation has been obtained through the hard sphere model via Percus-Yevik (PY) approximation along the lines of Ashcroft and Langreth [17] and Enderby and North [18].

The form factor w(k,q) of the constituent metals has been derived through the well-known Harrison's First Principle (HFP) pseudopotential technique. From these two ingredients the properties under investigation have been computed. In the HFP pseudopotential technique, the various interacting potentials are arrived through fundamental considerations employing quantum mechanical and statistical mechanical approaches along with Poisson's equation. Although the technique was much rigorous than the model potential technique and also free from arbitrariness in choosing a model or its parameter, it lagged behind due to some cumbersome calculations involved. However, this was employed by King and Cutler [19] and Hafner [20] along with their co-workers. The HFP technique has been claimed to be superior to the model potential techniques as no arbitrary adjustable parameter is introduced and no arbitrary model is proposed. Further it has input requirements and is based on sound theoretical background (Harrison, 1966 [21]).

In spite of various favorable points regarding HFP technique the workers found that there are several considerations to be kept in mind while choosing the input parameters, the most significant among them was the energetic problem. In computation of the form factor the important input parameters are the eigenfunctions and eigenvalues of the core electrons represented by $P_{nl}(r)$ and ε_{nl} , n and l being the quantum numbers of the core states. The basic characteristics of the pseudopotential technique which distinguishes it from the band structure calculations is the use of the first-order perturbation theory and the factorization of crystal matrix elements into form factor w(k,q) and static structure factor S(k). Both these ingredients are involved in all the physical properties studied in this project.

Usually, the researchers in this field obtained these input parameters from Herman-Skillman (HS) [22] or generated with some improvement in his program while some authors preferred to use the experimental eigenvalues. Clementi [23] also published his atomic structure calculations in which he provided the eigenfunctions and eigenvalues of elements of one-third of the periodic table.

In the present work, the HFP pseudopotential technique has been applied for the computation of form factor of liquid binary alloys. The hard sphere diameters at various concentrations are taken from the work of Veazy et al. [24] for the use in the determination of their PSF. Then, in order to determine the physical aspects and explanation of the concentration dependence of the observed electrical resistivity and Knight shift in the liquid binary alloys, other physical properties like the Fermi energy and density of states (DOS) of the alloy are calculated and considered for the study.

2. Formalism

2.1. Form Factor

The potential-dependent term is called the form factor (*FF*) $w(\mathbf{k}, \mathbf{q}) = \langle \mathbf{k} + \mathbf{q} | w | \mathbf{k} \rangle$. It is the Fourier transform of the crystal potential in the reciprocal lattice. The non-local screened form factor may be expressed as

$$w(\mathbf{k},\mathbf{q}) = \left\{\frac{v_q^{a,b} + v_q^c + v_q^d}{\varepsilon^*(q)}\right\} + \left[\frac{1 - G(q)}{\varepsilon^*(q)}\right] v_q^f + W^R,\tag{1}$$

where $v_q^{a,b}$, v_q^c , v_q^d , v_q^f , W^R , $\varepsilon^*(q)$ and G(q) are the valence charge and core electron potential, conduction band-core exchange potential, conduction electron potential, screening potential, repulsive potential, the dielectric screening function and the exchange-correlation function, respectively.

2.2. Structure Factor

The scattering of radiation (e.g., low-energy neutrons or X-rays) from a system containing N identical scattering centers can be conveniently described in terms of the so-called scattering law. This quantity measures the probability that energy $\hbar \omega$ will be transferred to the neutron if momentum $\hbar q$ is imparted to the system. Attempts have been made to evaluate PSF which characterize the short-range order (SRO) i.e. short-range atomic arrangements in a binary liquid alloy. Knowledge of the PSF is also essential if we interpret the anomalies observed in the system. The computation of partial structure factors through the formalism given by Ashcroft and Langreth [17] requires the hard sphere diameters σ_1 , σ_2 of the first and second components of the alloy and packing density η which is related to σ_1 and σ_2 as given by

$$\eta = \frac{\pi}{6\Omega} \sum_{i=1}^{2} C_i \sigma_i^3.$$
⁽²⁾

In the present work σ_1 and σ_2 are taken from the work of Veazy et al. [24].

The three partial structure factors for a binary liquid mixture can be expressed in terms of the Fourier transform of direct correlation functions and are computed on the lines of Ashcroft and Langreth [17] and Enderby and North [18]:

$$S_{\alpha\alpha}(k) = \left[1 - n_{\beta} c_{\beta\beta}(q)\right] / D_d(q), \qquad (3)$$

$$S_{\beta\beta}(k) = \left[1 - n_{\alpha} c_{\alpha\alpha}(q)\right] / D_d(q), \qquad (4)$$

$$S_{\alpha\beta}(k) = \left(n_{\alpha}n_{\beta}\right)^{1/2} \frac{c_{\alpha\beta}(q)}{D_{d}(q)},\tag{5}$$

with

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$$D_d(q) = [1 - n_\alpha c_{\alpha\alpha}(q)] [1 - n_\beta c_{\beta\beta}(q)] - n_\alpha n_\beta c_{\alpha\beta}^2$$
(6)

 $S_{\alpha\alpha}$, $S_{\beta\beta}$ and $S_{\alpha\beta}$ are called the Ashcroft–Langreth partial structure factors.

2.3. Electrical Resistivity

For the computation of resistivity of liquid metals, Ziman gave the diffraction model formula (Ziman, 1961 [12]), which has been quite successful especially when applied to simple metals. The derivation of the Ziman formula relies on the use of the relaxation time approximation for the Boltzmann equation and the use of pseudopotential for the interaction between an electron and an ion.

It was shown by Faber and Ziman (1965) [14] that the diffraction model formula for liquid metals proposed by Ziman (1961) [12] 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.,

$$R = R_{\alpha\alpha} + R_{\beta\beta} + R_{\alpha\beta},\tag{7}$$

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

$$R_{\alpha\alpha} = \left(3\pi / \hbar |e|^{2}\right) \left(\Omega / N v_{F}^{2}\right) 4 \int_{0}^{1} c_{1} |w_{1}(k,\eta)|^{2} S_{11}(k) \eta^{3} d\eta,$$
(8)

$$R_{\beta\beta} = \left(3\pi / \hbar |e|^{2}\right) \left(\Omega / N v_{F}^{2}\right) 4 \int_{0}^{1} c_{2} |w_{2}(k,\eta)|^{2} S_{22}(k) \eta^{3} d\eta,$$
(9)

$$R_{\alpha\beta} = \left(3\pi/\hbar|e|^{2}\right) \left(\Omega/Nv_{F}^{2}\right) 4 \int_{0}^{1} 2(c_{1}c_{2})^{1/2} |w_{1}(k,\eta)| |w_{2}(k,\eta)| S_{12}(k)\eta^{3}d\eta.$$
(10)

In a composite form *R* can be expressed as

$$R = \left(3\pi / \hbar |e|^2\right) \left(\Omega / N v_F^2\right) \left\langle \sum_{\alpha,\beta} (c_1 c_2)^{1/2} S_{ij}(k) w_\alpha(k,\eta) w_\beta(k,\eta) \eta^3 \right\rangle,$$
(11)

where $\langle \rangle$ stands for

$$\left\langle \right\rangle = 4 \left[\int_{0}^{1} c_{1} S_{11}(k) \left| w_{1}(k,\eta) \right|^{2} + c_{2} S_{22}(k) \left| w_{2}(k,\eta) \right|^{2} + 2(c_{1}c_{2})^{1/2} S_{12}(k) \left| w_{1}(k,\eta) \right| \left| w_{2}(k,\eta) \right| \right] \eta^{3} d\eta \qquad (12)$$

where $w_1(k,\eta)$ and $w_2(k,\eta)$ are the form factors of species 1 and 2 constituting the alloys; c_1 , c_2 are the concentrations and $S_{11}(k)$, $S_{22}(k)$ and $S_{12}(k)$ are the partial structure factors of the alloy and $\eta = q/2k_F$.

2.4. Knight shift

The frequency of nuclear magnetic resonance (NMR) associated with a metallic state is generally higher than the corresponding frequency for non-metallic state, such a shift of the NMR frequency is known as the Knight Shift. This arises due to the hyperfine contact interaction between the nucleus and the surrounding conduction electrons. The Knight shift (K%) is defined as a ratio of the frequency shift to the frequency at which the NMR is observed for the metallic state. The hyperfine interaction between conduction electrons and nuclear moment in metal provides a rich array of properties that can be studied through nuclear magnetic technique (Mahanti et al., (1970) [25]), Knight (1956) [26] and Slater (1951) [27]]. Although the experimental techniques of the measurement of Knight shift have been developed much earlier, its theoretical development had been in a state of infancy and has been developed much later. The previous theoretical works (Ziman 1961 [12], Bradley et al. 1962 [28], Ziman 1964 [29], Muto et al. 1962 [30], Mishra and Roth 1969 [31], Mishra et al. 1990 [32], Tripathi et al. 1989 [33]), on the magnetic properties of metal substantiate the view that like electrical resistivity, the nearly free electron approximation is also valid for the theoretical treatment of various magnetic properties viz., Knight shift, magnetic susceptibility, Hall coefficient, etc. We shall now present its concise theory within the framework of pseudopotential technique. The Knight [Pake (1955) [34]] may be written as

$$K = \left(\frac{8\pi}{3}\right) \chi_P P_F \Omega.$$
(13)

Here χ_P is the spin paramagnetic susceptibility of conduction electrons per unit volume, Ω is the volume of the crystal and P_F the average electron density at the site of the nucleus from the conduction electrons with an energy E_F . Assuming the form factor w(k,q) and structure factor S(k) to be spherically symmetric, we get

$$\frac{K_1}{K_0} = \frac{P_F^{\ 1}}{P_F^{\ 0}} = -\frac{3Z}{4E_F k_F^2} \int_0^\alpha S(k) w(k,q) q \ln \left| \frac{q+2k_F}{q-2k_F} \right| dq,$$
(14)

where P_F^{0} and P_F^{1} are the zero-order and first-order terms, K_0 and K_1 are the zero-order and first-order terms, E_F is the Fermi energy, k_F is the Fermi wave vector and the other symbols have their usual significance. For the alloys the integrand of Eq. (14) is replaced by

$$I_{K} = \int_{0}^{\infty} \left[C_{1}S_{11}(k)w_{11}(k,q) + C_{2}S_{22}(k)w_{22}(k,q) + 2(C_{1}C_{2})^{1/2}w_{11}(k,q)w_{22}(k,q)S_{12}(k) \right] q \ln \left| \frac{q+2k_{F}}{q-2k_{F}} \right| dq \quad (15)$$

Also Z, E_F and k_F are those of the alloys evaluated through $X = c_1 X_1 + c_2 X_2$ where c_1 and c_2 are the concentrations of the constituents X, X_1 , X_2 are the input parameters of the alloy viz., Z, E_F , k_F , Ω_0 etc.

The Knight shift of liquid binary alloys mostly varies in the form of a nearly linear function of the solute concentration [35, 36]. The Knight shift variation with concentration appears attributable largely to change in Pauli spin susceptibility χ_P , atomic volume Ω . This is consistent with Kaeck's assumption that the factor P_F remains constant, equal to that for the pure metal, over the entire concentration range in that alloy. For polyvalent alloys many attempts have been made to explain the NMR data from the point of view of phase shift methods [37, 38]. Such calculations are very sensitive to the structure factors and the pseudopotential or partial wave phase shifts employed.

2.5. Fermi energy and Density of states

The electronic structure of solids and liquids can be precisely described through an accurate knowledge of its electronic states. There are a number of theoretical methods of determining different aspects of electronic structure of liquid metals among which the density of states and the Fermi energy have significant bearing. The calculations of Fermi energy E_F and the density of states $N(E_F)$ for simple liquid metals have been reported by Schneider and Stoll (1967) [39], Ashcroft (1968) [40], Shaw and Smith (1969) [41], Srivastava and Sharma (1969) [42], Jena and Halder (1971, 1972) [43, 44], Stoll et al. (1971) [45], Halder (1973) [46], Ichikewa (1973) [47], Dixit and Nigam (1973) [48], Srivastava (1974, 1975) [49, 50] and Kumar and Hemkar (1977) [51]. While the study of density of states have been made by Watabe and Tanaka (1964) [52], Ballentine (1966) [53], Chan and Ballentine (1971, 1972) [54, 55], Itami and Shimoji (1972) [56], Ballentine and Chan (1973) [57] and Kuroha and Suziki (1974) [58] using various pseudopotentials and the Green function theory. It does not appear that the Harrison's first principle pseudopotential has been used for the study of these properties except for Thakur (1980) [59] for alkali metals. We, therefore, present our work on the Fermi energy and density of states of multivalent liquid metals on the basis of the first principle pseudopotential approach of Harrison. In the framework of conventional perturbation theory, the energy of liquid metal is expressed as (Harrison, 1966 [21])

$$E(K) = \frac{\hbar^2 K^2}{2m} + \langle k | w | k \rangle + \frac{2m}{\hbar^2} \sum_{q}^{k} \frac{S(k) |N \langle k+q | w | k \rangle|^2}{|k|^2 - |(k+q)|^2}.$$
 (16)

Here S(k) is the liquid structure factor and is non-zero for a liquid, $\langle k | w | k \rangle$ are the matrix elements for the crystal potential (*W*), $|N \langle k + q | w | k \rangle|$ are the unscreened form factor, *m* is the electron mass and $\hbar = h/2\pi$, where *h* is the Planck's constant.

At the melting point, the above expression reduces to (Schneider and Stoll, 1967 [39])

$$E(K) = \frac{\hbar^2 K^2}{2m} + \frac{2m}{\hbar^2} \sum_{q} \left(\frac{S(k) w^2(q)}{\left|k\right|^2 - \left|(k+q)\right|^2} - \frac{S(k) w^2(q)}{q^2} \right),\tag{17}$$

where w(k,q) = w(q). Replacing Σ by $\frac{\Omega_0}{8\pi^3} \int d^3 q$ and putting $k = k_F$, we obtain for the energy at the Fermi level,

$$E(k_F) = \frac{\hbar^2 k_F^2}{2m} + \Delta(k_F) - \Delta(0),$$
(18)

where

$$\Delta(k_F) = -\frac{m\Omega_0}{4\pi^2 \hbar^2 k_F^2} \int_0^\infty q S(k) w^2(q) \ln \left| \frac{2k_F + q}{2k_F - q} \right| dq$$
(19)

and

$$\Delta(0) = -\frac{m\Omega_0}{4\pi^2 \hbar^2} \int_0^\infty S(k) w^2(q) dq.$$
 (20)

For the alloy the integrand of Eq. (24) is replaced by

$$I_{E} = \int_{0}^{\infty} \left[c_{1}S_{11}(k) |w_{11}(k,q)|^{2} + c_{2}S_{22}(k) |w_{22}(k,q)|^{2} + 2(c_{1}c_{2})^{1/2} w_{11}(k,q) w_{22}(k,q) S_{12}(k) \right] q \ln \left| \frac{q + 2k_{F}}{q - 2k_{F}} \right| dq \qquad (21)$$

and the integrand of Eq. (20) is replaced by

$$I'_{E} = \int_{0}^{\infty} \left[c_{1}S_{11}(k) \left| w_{11}(k,q) \right|^{2} + c_{2}S_{22}(k) \left| w_{22}(k,q) \right|^{2} + 2(c_{1}c_{2})^{1/2} w_{11}(k,q) w_{22}(k,q) S_{12}(k) \right] dq.$$
(22)

Here Ω_0 is the atomic volume related to the Fermi wave vector k_F and valence Z by the relation.

$$\Omega_0 = 3\pi^2 Z / k_F^3. \tag{23}$$

It has been assumed that S(k) and w(q) are isotropic.

The expression for the density of states of liquid metal is given as

$$N(E_{F}) = \frac{k_{F}^{3}\Omega_{0}}{\pi^{2}} \left[\left| \frac{\partial E(k)}{\partial k} \right|_{k=k_{F}} \right]^{-1} =$$

$$= \frac{k_{F}^{2}\Omega_{0}}{\pi^{2}} \left[\frac{\hbar^{2}k_{F}}{m} + \frac{m\Omega_{0}}{4\pi^{2}\hbar^{2}k_{F}^{2}} \int_{0}^{\infty} qS(k)w^{2}(q)\ln \left| \frac{2k_{F}+q}{2k_{F}-q} \right| dq + \frac{m\Omega_{0}}{\pi^{2}\hbar^{2}k_{F}} \int_{0}^{\infty} \frac{S(k)w^{2}(q)q^{2}dq}{(4k_{F}^{2}-q^{2})} \right]^{-1}.$$
(24)

The first integrand of Eq. (24) is the same as I_E and the second integrand for alloy becomes

$$I_{N} = \int_{0}^{\infty} \left[c_{1}S_{11}(k) |w_{11}(k,q)|^{2} + c_{2}S_{22}(k) |w_{22}(k,q)|^{2} + 2(c_{1}c_{2})^{1/2} w_{11}(k,q) w_{22}(k,q) S_{12}(k) \right] \frac{q^{2}}{\left(4k_{F}^{2} - q^{2}\right)} dq.$$
(25)

3. Results and Discussion

3.1. Structure

The partial structure factors have been computed using hard sphere diameters through the expression given by Ashcroft and Langreth, 1967 [17].



Fig. 1. (Continued)



Fig. 1. Partial structure factors of Cu-Sn at equiatomic composition.

The partial structure factors of Cu-Sn at T = 1400 K have been computed. The structure factors at various compositions are graphically represented in Fig. 1. The characteristic nature of the partial structure factors are reproduced except for $C_{\text{Cu}} = 0.4$. At equiatomic composition, the principal peaks of $S_{11}(k)$ and $S_{22}(k)$ lie near $k/k_F = 1.147$ and 1.5, respectively. The position of the first principal peak of the partial structure factors and the crossover point q_0 of the form factor decides the range of $\eta = q/k_F$ which is most contributing to the resistivity integrands for the alloy. The main peak in $S_{12}(k)$ lies between of them as contrary to other results reported earlier. This signifies that at 1400 K the alloy shows the behavior expected in the "random hard-sphere" model.

The system shows anomalous behavior at $C_{\text{Cu}} = 0.4$. There are certain high positive up to 22.5 and negative peaks up to 18 found at this particular composition. It is also found that after $C_{\text{Cu}} = 0.7$, $S_{\text{Cu-Cu}}$ starts dominating and get right shifted to $S_{\text{Sn-Sn}}$ throughout the whole concentration range.

3.2. Electrical Resistivity

For the study of the electrical resistivity of the liquid alloys we need the PSF at the melting temperature for different concentrations. Although the experimental knowledge on partial structure factors is limited to a few systems only at the certain composition, we undertake a theoretical approach based on Percus–Yevik (PY) approximation on the lines of Ashcroft and Langreth (1967) [17] and Enderby and North (1968) [18] and presented their natures for the entire composition range in Fig. 1 for the alloy.

The form factors required for this computation were computed from Eq. (1). But it was found that some form factors, which reproduced good electrical resistivity with the experimental structure factors in case of metals, did not perform well in alloys. However, slight change in the choice of input parameters e.g., β or exchange correlation function improved the agreement in case of Cu-Sn.

For, Cu and Sn the form factors are evaluated through eigenvalues of HS with $\alpha = 2/3$ and $\beta = 5/8$ using V-S exchange correlation gave satisfactory agreement in case of Cu-Sn.



Fig. 2. Concentration dependence of electrical resistivity of Cu-Sn.

After the computation of PSF and FF we have calculated the electrical resistivity of the alloy. Similar to the PSF, we found a negative peak of high magnitude at $C_{Cu} = 0.4$. It appears that the Cu atoms around a dissolved Sn atom are strongly bound to it. This alloy is representing a dynatron type characteristic producing a negative-resistance phenomenon. Hence this material can be used for switching, signal relaying, memory devices and other various controlling or data processing applications. Also these peaks may represent the tendency for compound formation at this composition also.

3.3. Physical Properties

The computed form factors, which have been found suitable for the evaluation of electrical resistivities of the alloys under investigation, have been further put to test through the computation of the Knight shift (*K*%), its concentration dependence and the Fermi energy (E_F) in eV alongwith the electronic density of states for the alloys under investigation. It is to be mentioned that the integrand of the Knight shift involves within itself the form factor w (*k*, *q*) linearly. Hence the computed Knight shift may be taken as a test for the accuracy of the form factor both with respect to magnitude and sign. As shown in Fig. 3, the Knight shift varies in the form of a linear function of the solute concentration.

Since such calculations are very sensitive to the structure factors and the pseudopotential employed so we can say that the anomaly as observed in PSF and electrical resistivity at $C_{Cu} = 0.4$

is not a deviation from the model or error in computational work but it signifies a unique feature that we have observed at this temperature and composition.

Other physical quantities like electrical resistivity, Fermi energy and density of states have their integrands involving the square of the form factor and thus they are only concerned with the magnitude of the form factor.



Fig. 3. Concentration dependence of Knight shift of Cu-Sn.

The study of computed results reveals that for Cu-Sn, $(K\%)_{th} = 0.497$ against $(K\%)_A = 0.26$, $(K\%)_B = 0.73$. The Fermi energy $(E_F)_{th} = 5.86$ and the electronic density of states being $N(E_F)_{th} = -4.065$. The K_0 values of the constituent metals is that evaluated through zero-order OPW method (Faber, 1972 [60]; Shimoji, 1977 [61]).

Such calculations are very sensitive to the structure factors and the pseudopotential form factor. Thus the results are not always in quantitative agreement with experiment (Shimoji, 1977 [61]).

Also it should be mentioned that the integrand of electrical resistivity involves the square of the form factors. This is also true for the integrands of Fermi energy and density of states. However, the integrand of the Knight shift involves the form factor linearly. Hence, the sign of the form factor is quite material in the computation of the Knight shift. Thus a form factor reproducing good electrical resistivity may not reproduce the Knight shift so nicely.

In spite of the above mentioned facts and the inherent approximations of the HFP technique, Ziman formalism, Knight formalism and Fermi energy formalisms a fairly reasonable agreement is obtained in the present work.

Conclusions

- 1. The Harrison's First Principle technique in conjunction with the hard sphere technique of Ashcroft and Langreth can be safely used for the study of transport property (viz., electrical resistivity) of Cu-Sn alloy.
- 2. The partial structure factors play a key role in binary alloys due to the randomness of various scattering centers A, B and AB where A and B are the species. The system shows the behavior of rigid hard sphere model.
- 3. The accuracy of resistivity values are sensitive to the accuracy of structure factor S(k) and form factor $\langle k+q|w|k \rangle$. The resistivity in Cu-Sn shows a negative peak of high magnitude at

 $C_{\text{Cu}} = 0.4$. It signifies that the Cu atoms around a dissolved Sn atom are strongly bound to it. Also, this alloys represent a dynatron type characteristic producing a negative-resistance phenomenon. Hence, it may become a useful candidate for various industrial and commercial applications.

- The sharp peaks in liquid alloys may also signify the formation of compounds or complexes. This is certainly suggestive for describing energetically favorable configuration of ions in liquid alloys.
- 5. The Knight shift of Cu-Sn alloy shows linear function with respect to solute concentration supporting Kaeck's assumption.

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REFERENCES

- 1. M.Li, Z.Du, C.Guo, C.Li, J. Alloys Comp., 477, 104 (2009).
- 2. P.C.Wallbrecht, R.Blachnik, K.C.Mills, Thermochimica Acta, 46, 167 (1981).
- 3. H.Oikawa, A.Hosoi, Scripta Metallurgica, 9, 823 (1975).
- 4. A.P.Miodownik, J. Less Common Metals, 114, 81 (1985).
- 5. H.Flandorfer, C.Luef, U.Saeed, J. Non-Cryst. Sol., 354, 2953 (2008).
- 6. S.-K.Seo, S.K.Kang, D-Y.Shih, H.M.Lee, Microelectronics Reliability, 49, 288 (2009).
- 7. V.T.Witusiewicz, F.Sommer, J. Alloys Comp., 312, 228 (2000).
- 8. L.C.Prasad, S.K.Chatterjee, R.K.Jha, J. Alloys Comp., 441, 43 (2007).
- 9. F.Sommer, R.N.Singh, V.Witusiewicz, J. Alloys Comp., 325, 118 (2001).
- 10. J.E.Enderby, D.M.North, P.A.Eglestaff, Phil Mag., 14, 961 (1966).
- 11. B.R.Orton, G.I.Williams, Fulmer Institute Report R, 129, 5 (1960).
- 12. J.M.Ziman, Phil. Mag., 6, 1013 (1961).
- 13. J.M.Ziman, Adv. Phys. 16, 551 (1967).

- 14. T.E.Faber, J.M.Ziman, Phil. Mag., 11, 153 (1965).
- 15. C.Herring, Phys. Rev., 57, 1169 (1940).
- 16. J.B.Phillips, L.Kleinman, Phys. Rev., 116, 287 (1959).
- 17. N.W.Ashcroft, D.C.Langreth, Phys. Rev., 155, 682 (1967).
- 18. J.E.Enderby, D.M.North, Phys. Chem. Liq., 1, 1 (1968).
- 19. W.F.King III, P.H.Cutler, J. Phys. F, 5, L187 (1975).
- 20. J.Hafner, Sol. Stat. Comm., 27, 263 (1978).
- 21. W.A.Harrison, Pseudopotential in the Theory of Metals, Benjamin Inc., New York, 1966.
- 22. F.Herman, J.Skillman, Atomic Structure Calculation, Prentice Hall, New Jersey, 1963.
- 23. E.Clementi, IBM. J. Res. Dev., 9, 2 (1965), (Tables of Atomic Functions).
- 24. S.D.Veazy, W.C.Roe, J. Mat. Sci., 7, 445 (1972).
- 25. S.D.Mahanti, T.P.Das, Magnetic Resonance, Plenum Press, New York, 1970.
- 26. W.D.Knight, in Solid State Phys., 2, p.93; F.Seitz, D.Turnbull, Ed., Acad. Press, New York, 1956.
- 27. J.C.Slater, Phys. Rev., 81, 385 (1951).
- 28. C.G.Bradley, T.E.Faber, E.G.Wilson, J.M.Ziman, Phil. Mag., 7, 865 (1962).
- 29. J.M.Ziman, Adv. Phys., 13, 89 (1964).
- 30. T.Muto, S.Kobayasi, M.Watabe, H.Kozima, J. Phys. Chem. Solids, 23, 1303 (1962).
- 31. P.K.Mishra, L.M.Roth, Phys. Rev., 177, 1089 (1969).
- 32. B.Mishra, L.K.Das, T.Sahu, G.S.Tripathi, P.K.Mishra, J. Phys. Cond. Matt., 2, 9891 (1990)
- 33. G.S.Tripathi, C.M.Mishra, P.Tripathi, P.K.Mishra, Phys. Rev. B, 39, 94 (1989).
- 34. G.E.Pake, Sol. St. Phys., 2; F.Seitz, D.Turnbull, Ed., Acad. Press, New York, 1956.
- 35. J.A.Kaeck, Phys. Rev., 175, 897 (1968).
- 36. S.B.Van der Molen, W.Van der Lugt, G.G.Draisma, W.Smit, Physica, 38, 275 (1968).
- 37. J.Heighway, E.F.W.Seymour, Phys. Condens. Mater., 13, 1 (1971).
- 38. C.J.Ford, J.Heighway, E.F.Seymour, J. Phys. F.:Met. Phys., 2, 373 (1972).
- 39. T.Schneider, E.Stoll, Adv. Phys., 16, 731 (1967).
- 40. N.W.Ashcroft, J. Phys. C, 2, 232 (1968).
- 41. R.W.Shaw, N.V.Smith, Phys. Rev., 178, 985 (1969).
- 42. S.K.Srivastava, P.K.Sharma, IJPAP, 7, 644 (1969).
- 43. P.Jena, N.C.Halder, Phys. Rev. Lett., 26, 1024 (1971).
- 44. P.Jena, N.C.Halder, Phys. Rev. B, 6, 2131 (1972).
- 45. E.Stoll, N.Szabo, T.Schneider, Phys. Condens. Mater., 12, 279 (1971).
- N.C.Halder, The Properties of Liquid Metal, S.Takeuchi, Ed., Taylor and Francis, London, 1973, p.337.
- 47. K.Ichikewa, Phil. Mag., 27, 177 (1973).
- 48. J.P.Dixit, S.K.Nigam, IJPAP, 11, 433 (1973).
- 49. S.K.Srivastava, J. Phys. Chem. Solid, 36, 993 (1974).
- 50. S.K.Srivastava, Phys. Stat. Sol. (b), 61, 731 (1975).
- 51. K.Kumar, M.P.Hemker, Phys. Stat. Sol. (b), 29, 82 (1977).
- 52. M.Watabe, M.Tanaka, Prog. Theor. Phys., 31, 525 (1964).
- 53. L.E.Ballentine, Can. J. Phys., 44, 1533 (1966).
- 54. T.Chan, L.E.Ballentine, Phys. Chem. Liq., 2, 165 (1971).
- 55. T.Chan, L.E.Ballentine, Can. J. Phys., 50, 813 (1972).
- 56. T.Itami, M.Shimoji, Phil. Mag., 25, 229 (1972).

- 57. **L.E.Ballentine, T.Chan,** The Properties of Liquid Metal, **S.Takeuchi, Ed.,** Taylor and Francis, London, 1973, p.197.
- 58. M.Kuroha, K.Suziki, Phys. Lett., 47A, 329, (1974).
- 59. J.Thakur, Phys. Stat. Sol. (b), 99, 771 (1980).
- 60. T.E.Faber, Introduction to the Theory of Liquid Metals, Cambridge University Press, 1972.
- 61. M.Shimoji, Liquid Metals, Acad. Press, London, 1977.