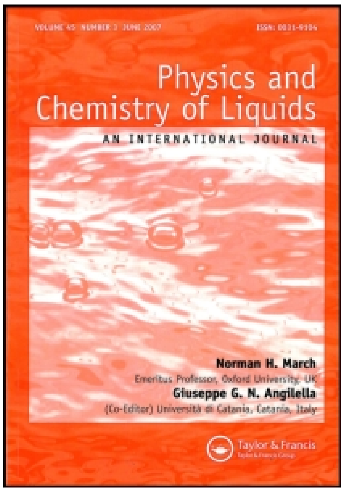

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Structure and Electrical Resistivity of Liquid Alkali Alloys

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STRUCTURE AND ELECTRICAL RESISTIVITY OF LIQUID ALKALI ALLOYS

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The evaluation of the electrical resistivity of binary liquid alloys requires the true knowledge of the partial structure factors as well as the form factors of the constituent species. In principle partial structure factors are measurable, but the practical difficulties are severe and it is not promising to use the measured data. We, therefore, consider a simple theoretical approach based on hard sphere reference system and the Percus–Yevick equation to compute the partial structure factor. The concentration dependence of the hard sphere parameters are obtained by minimising the Helmholtz free energy of the system following the Gibbs–Bogoliubov variational technique. We have used it to compute the concentration dependence of electrical resistivity of NaK, KRb and NaCs liquid alloys. Our study reveals the like particle correlation contributes positively to the absolute value of electrical resistivity while the unlike particle correlation makes a negative contribution.

KEY WORDS: Hard spheres, Percus–Yevick method.

1 INTRODUCTION

In past, the electrical resistance in liquid metals has been studied extensively by using the diffraction model formula proposed by Ziman[1]. Subsequently it was shown by Faber and Ziman[2] that the formula for pure liquid metals could easily be extended to binary liquid alloys. The two important ingredients of the formula are respectively the partial structure factors and the form factors. When one is calculating the transport properties of binary alloys, problems arise from the partial structure factors rather than the form factors. Experimental data on partial structure factors are scarce or have insufficient accuracy[3]. Due to this one usually assumes[4–5] that all the three partial structure factors are the same in a binary system. But recent developments reveal (for review see Vander Lugt and Geertsma[6]) that the three partial structure factors can not be the same.

Therefore, in the present work, we consider a theoretical model to calculate the partial structure factors. The most popular model is the solution of hard sphere potential of the Percus–Yevick equation[4,7]. The basic problem is to determine the hard sphere diameters of the constituent species of the binary system. This has been achieved by making use of the variational thermodynamics where hard sphere diameters are so chosen that ensure minimum Helmholtz free energy for the system. In this way we also ensure that the form factors and the structure factors occurring in the formula of electrical resistivity are mutually dependent. This point is usually ignored by different workers but its importance has recently been emphasized by Vander Lugt and Geertsma[6].

The form factors have been computed in a fully nonlocal way by using the optimised model potential of Shaw[8]. This has been preferred because it has successfully explained various atomic and electrical properties of pure liquid metals.

Application is made to liquid alkali alloys mainly NaK, NaCs and KRb. These systems were preferred as their densities as a function of concentration are experimentally available and also these are typical representations of simple systems where the sizes of the constituent atoms differ from a factor of 1 to 3; $\Omega\mathrm{Rb}/\Omega\mathrm{K} = 1.22$, $\Omega\mathrm{K}/\Omega\mathrm{Na} = 1.93$ and $\Omega\mathrm{Cs}/\Omega\mathrm{Na} = 2.99$. Out of these, NaCs binary molten alloy is of particular interest for both theoretical[9–12] and experimental workers[13–15] due to its larger size effect. The evaluation of partial structure factors is discussed in Section 2 and that of electrical resistivity is provided in Section 3. This follows summary and conclusion given in Section 4.

2 PARTIAL STRUCTURE FACTORS OF LIQUID ALKALI ALLOYS

Since the pioneer work by Ashcroft and Langreth[7] it has become possible to obtain the partial structure factors $S_{ij}(i, j = 1, 2)$ in terms of direct correlation function C_{ij} i.e.,

$$\begin{aligned} S_{11}(q) &= [1 - n_2 c_{22}(q)]/Q(q) \\ S_{22}(q) &= [1 - n_1 c_{11}(q)]/Q(q) \\ S_{12}(q) &= [(n_1 n_2)^{1/2} C_{12}(q)]/Q(q) \end{aligned} \tag{1}$$

with

$$Q(q) = 1 - n_1 C_{11}(q) - n_2 C_{22}(q) + n_1 n_2 C_{11}(q) C_{22}(q) - n_1 n_2 C_{12}^2(q) \tag{2}$$

n_1 and n_2 are number densities of species 1 and 2 respectively. $C_{ij}(q)$ are the Fourier transform of the direct correlation function $C_{ij}(r)$ i.e.,

$$C_{ij}(q) = \int C_{ij}(r) e^{iq\cdot r}\, dr^3 \tag{3}$$

The direct correlation function $C_{ij}(r)$ have been successfully obtained from the solution of hard sphere potentials of Percus–Yevick equation[16]. The most important input parameters are the hard sphere diameters σ_1 and σ_2. Usually these are obtained from the data of entropy. In order to avoid any such fitting we use here the variational method based on Gibbs–Bogoliubov inequality to determine the effective hard sphere diameter as a function of concentration by minimising the free energy of the system i.e.,

$$\left(\frac{\partial F}{\partial \sigma_i}\right)_{T,\Omega} = 0 \qquad i = 1, 2 \tag{4}$$

The details of variational method are available from the study of Umar *et al.*[17], Ashcroft and Stroud[18] and Singh[19]. The Helmholtz free energy F can be expressed as

$$F = F_{eg} + F_{fp} + F_{sp} + F_M + 3/2 K_B T - TS \tag{5}$$

F_{eg} is the contribution due to free electron gas, F_{fP} and F_{sp} are, respectively, first and second order perturbation energies due to electron–ion interaction. F_M represents the ion–ion contribution and 3/2 K_BT is the mean kinetic energy. S stands for the entropy of the mixture. The detailed expression for various energy contributions can be expressed (Ashcroft and Stroud[18]) as

$$F_{eg} = (0.3K_F^2) - (3/4\pi)K_F - 0.0474 - 0.0155 \ln K_F - 0.5(\pi K_B/K_F)T^2\bar{Z} \tag{6}$$

$$F_{fp} = \lim_{q\to 0} \bar{Z}n\left(\sum_i^{1,2} C_i W_i(q) + 4\pi\bar{Z}/q^2\right) \tag{7}$$

$$F_{sp} = \frac{1}{16\pi^3}\int_0^\infty q^4\, dq \sum_{i,j}^{1,2} W_i(q)W_j(q)(C_iC_j)^{1/2}S_{ij}(q)\left(\frac{1}{\varepsilon^*(q)} - 1\right) \tag{8}$$

$$F_M = \frac{1}{\pi}\sum_{i,j} Z_iZ_j(C_iC_j)^{1/2}\int_0^\infty (S_{ij}(q) - \delta_{ij})\, dq \tag{9}$$

where

$$K_F = (3\pi^2\bar{Z}n)^{1/3},\ \bar{Z}n = Z_1n_1 + Z_2n_2 \text{ and } \bar{Z} = C_1Z_1 + C_2Z_2;$$

Z_1 and Z_2 are valencies, n_1 and n_2 are number densities of the ion species and $n = n_1 + n_2$. W is the form factor which has been obtained in local approximation for optimised model potential of Shaw[8] i.e.,

$$W_i = -\frac{4\pi Z_i}{\Omega_i q^2}\operatorname{Cos} r_i^m - \frac{4\pi A_i}{\Omega_i q^3}(\operatorname{Sin} qr_i^m - qr_i^m \operatorname{Cos} qr_i^m) \tag{10}$$

where Ω is the volume of the species i. A_i and r_i^m are well depth and model radius which are obtained quantum mechanically by matching the wave function of the inner and outer region (Ese and Reissland[20]). $\varepsilon^*(q)$ is the modified Hartree dielectric function

$$\varepsilon^*(q) = 1 + \{1 - G(q)\}\ \{\varepsilon(q) - 1\} \tag{11}$$

$\varepsilon(q)$ is the usual Hartree dielectric function and $G(q)$ takes into account of the exchange and correlation effect of the conduction electrons. In this work we considered the Hubbard–Sham (Hubbard[21], Sham[22]) expression for $G(q)$

$$G(q) = 1/2\,\frac{q^2}{q^2 + \gamma K_F^2} \tag{12}$$

By making use of the interpolation scheme of Noziers and Pines[23] γ is given by (Hafner and Schmuck[24]).

$$\gamma = \frac{2K_F}{K_F + 0.153}$$

S in Eq. (5) stands for entropy whose detailed expression can be had from the work by Singh and Singh[25].

Now Eqs (4) and (5) have been utilised to obtain σ_i of NaK, NaCs, KRb as a function of concentration. These are tabulated in Table 1. It has been observed that on alloying the sizes of the hard spheres of the pure constituent elements readjust to attain an equilibrium value. The heavier elements contract while the lighter ones expand. This is more pronounced in NaCs than NaK and KRb. The ratio of the diameters of the two species, $\alpha(=\sigma_1/\sigma_2)$, remains almost constant throughout the concentration range. α is found to be around 0.86 for NaK, around 0.8 for NaCs and 0.96 for KRb. Singh and Bhatia[12] using Flory's model, also suggests that the sizes of Na and Cs atoms change on alloying and may depend on concentration.

The contraction and expansion of hard spheres can qualitatively be understood[26] by considering the redistribution of the electronic charges at the Fermi surface on alloying. The Fermi wave vector of Cs ($K_F^{Cs} = 0.329$ au) is smaller than Na($K_F^{Na} = 0.474$ au). When Cs and Na are mixed together, the flow of electrons takes place from Cs to Na as the latter has lower Fermi energy. This leads to expansion of Na atoms and the contraction of Cs atoms. Similar is the case with NaK and KRb. In KRb, the Fermi wave vector of the constituent elements are not very much different ($K_F^K = 0.381$ and $K_F^{Rb} = 0.356$) and thus the effect is least noticeable. The contraction and the expansion phenomena can also be understood from the electro negativity values. The hard spheres of more electronegative element expand. The difference in electronegativity values leads to an accumulation of the electronic charge around the electro negative atomic site giving rise to its effective diameter and on the other hand reducing the size of other constituent atoms.

Table 1 Hard sphere parameters of liquid alloy as a function of concentration.

Alloy	*T*	*Concentration*	σ_1 *(a.u)*	σ_2 *(a.u)*	$\alpha\left(=\frac{\sigma_1}{\sigma_2}\right)$	Ω *(a.u)*
NaK	373°K	$C_{Na=0}$	—	7.609	—	535.332
		0.105	6.639	7.577	0.876	506.971
		0.3	6.567	7.508	0.874	453.803
		0.501	6.488	7.426	0.873	400.802
		0.599	6.446	7.383	0.873	375.559
		0.8	6.357	7.285	0.872	325.796
		1.0	6.252	—	—	278.009
NaCs	373°K	$C_{Na=0}$	—	8.680	—	830.565
		0.3	6.770	8.512	0.795	638.325
		0.5023	6.635	8.380	0.792	522.248
		0.7014	6.499	8.240	0.789	419.041
		0.8	6.427	8.154	0.788	370.837
		0.9	6.344	8.062	0.787	323.394
		1.0	6.252	—	—	277.932
KRb	373°K	$C_{K=0}$	—	8.062	—	656.168
		0.202	7.725	8.036	0.961	631.114
		0.50	7.684	7.993	0.961	594.530
		0.684	7.657	7.968	0.961	572.475
		0.852	7.632	7.940	0.961	552.333
		1.0	7.609	—	—	535.332

The optimised values of hard spheres (see Table 1) are used to compute the partial structure factors S_{ij} of NaK, NaCs and KRb as a function of concentration.

It is often convenient to express the Ashcroft-Langreth partial structure factor (S_{ij}) in terms of Faber and Ziman[2] structure factor a_{ij} i.e.,

$$\begin{aligned} a_{11}(q) &= (S_{11}(q) - C_2)/C_1 \\ a_{22}(q) &= (S_{22}(q) - C_1)/C_2 \\ a_{12}(q) &= \frac{S_{12}(q)}{(C_1C_2)^{1/2}} + 1 \end{aligned} \tag{13}$$

a_{ij} are plotted in Figures 1 to 3 for different concentrations of NaK, NaCs and KRb liquid alloys.

The figures indicate that the cross term a_{12} always oscillates between a_{11} and a_{22} around the first principal maxima. In every alloy the position of the first maximum shifts towards lower q values with increasing contents of heavier elements in the alloy. For example the maximum of a_{12} occurs at $q \simeq 1(\mathrm{au})^{-1}$ for $\mathrm{Na_{0.9}Cs_{0.1}}$ which shifts to $q \simeq 0.85\ (\mathrm{au})^{-1}$ for $\mathrm{Na_{0.31}Cs_{0.69}}$. This is most visible in NaCs followed by NaK and KRb. Our results indicate that the three partial structure factors of the alloy depend considerably on concentration. The position of the first principal maxima, as well as its amplitude depend on concentration. The three partial structure factors differ among themselves considerably in NaCs but it is negligibly small in KRb. It appears that the difference of the three partial structure factors has some relevance to the size factor. For example the size factor in NaCs is maximum and minimum in KRb.

It may be mentioned here that the calculation of partial structure factor of binary liquid alloys has been carried out on the basis of hard sphere potential which in true sense is not a realistic potential. Weeks *et al.*[27] (WCA) have suggested that it can be improved by considering the contribution arising from the attractive part of the pair potential. Waseda[3] has noted that the structure factor due to WCA method is superior to hard sphere method in the larger q region however in the low q region, the WCA method is less suitable compared to the hard sphere results. For the computation of electrical resistivity the hard sphere results are thus more suitable and are widely used.

3 ELECTRICAL RESISTIVITY OF BINARY LIQUID ALLOY

The necessary formulation for electrical resistivity of binary liquid alloys was first carried out by Faber and Ziman[2]. For the sake of better representation, we express the resistivity of binary liquid alloys as consisting of three distinct contributions i.e.,

$$R = R_{11} + R_{22} + R_{12} \tag{14}$$

where the first two terms of the R.H.S arise due to the same particle correlation and the third term (R_{12}) is due to the cross term scattering. As usual 1 and 2 represent

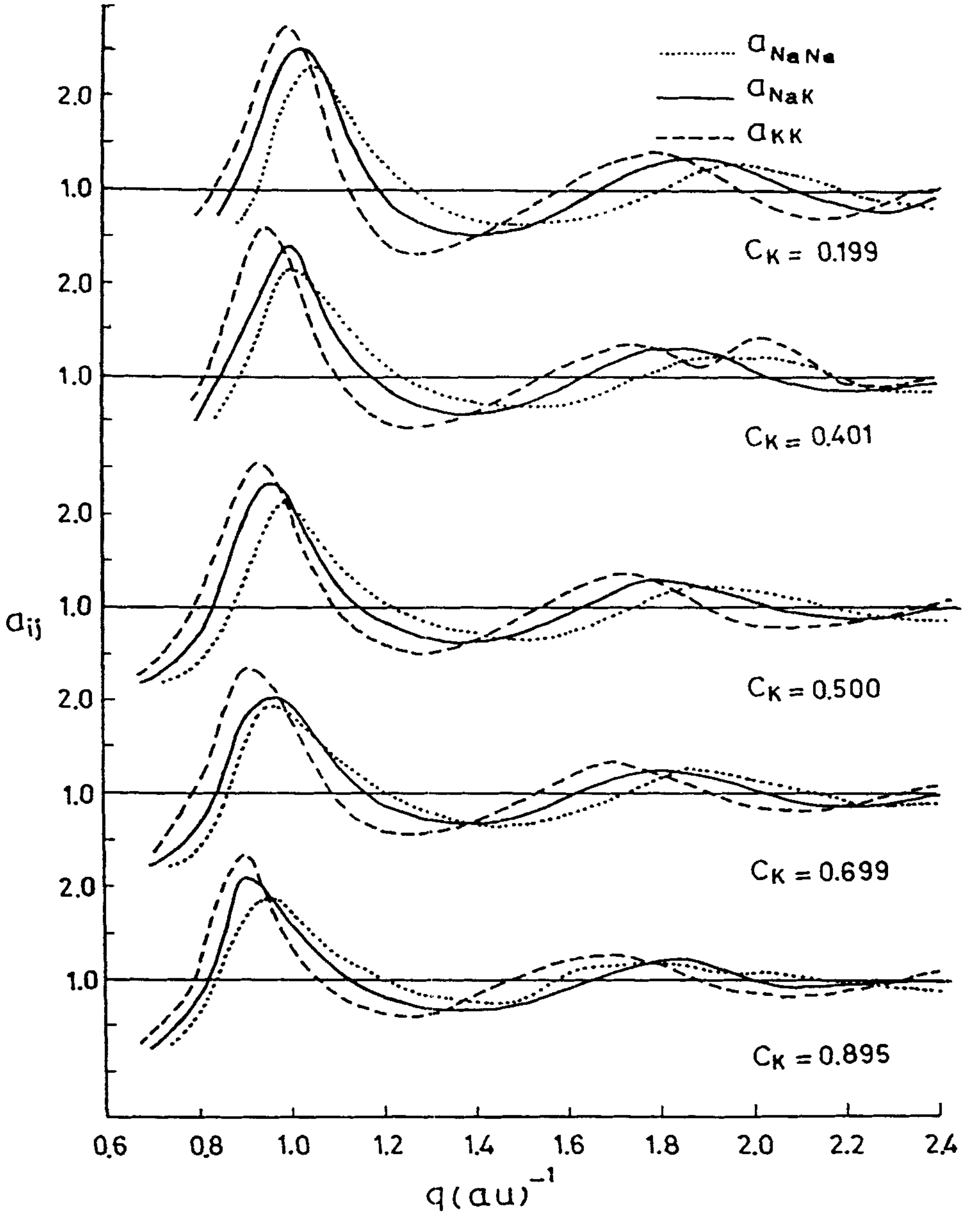

Figure 1 Partial structure factors for NaK liquid alloy at 373°K. ····· (a_{NaNa}), – – – – – – (a_{KK}) and ——— (a_{NaK}).

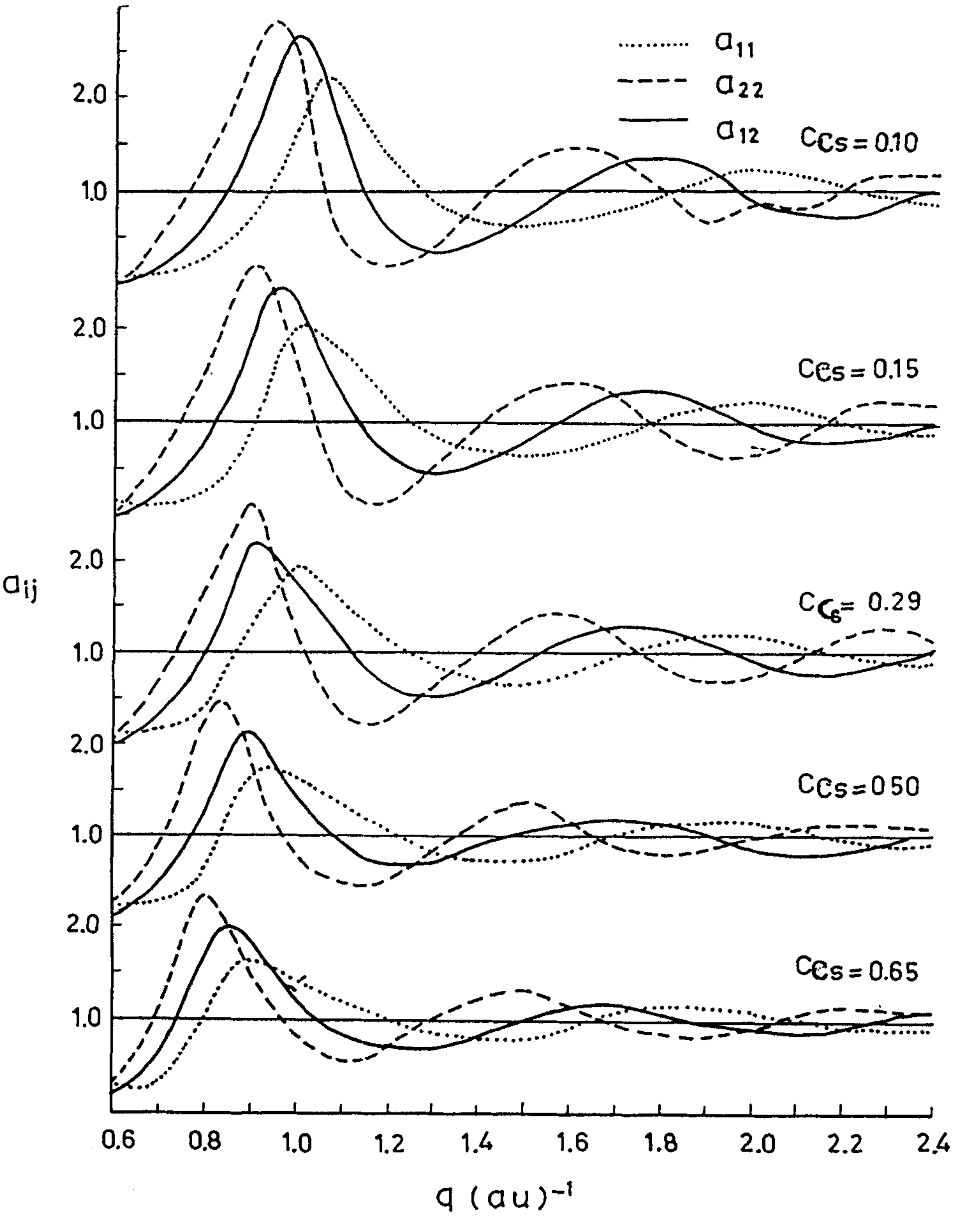

Figure 2 Partial structure factors for NaCs liquid alloy at 373°K. ······ (a_{NaNa}), ------ (a_{CsCs}) and ——— (a_{NaCs}).

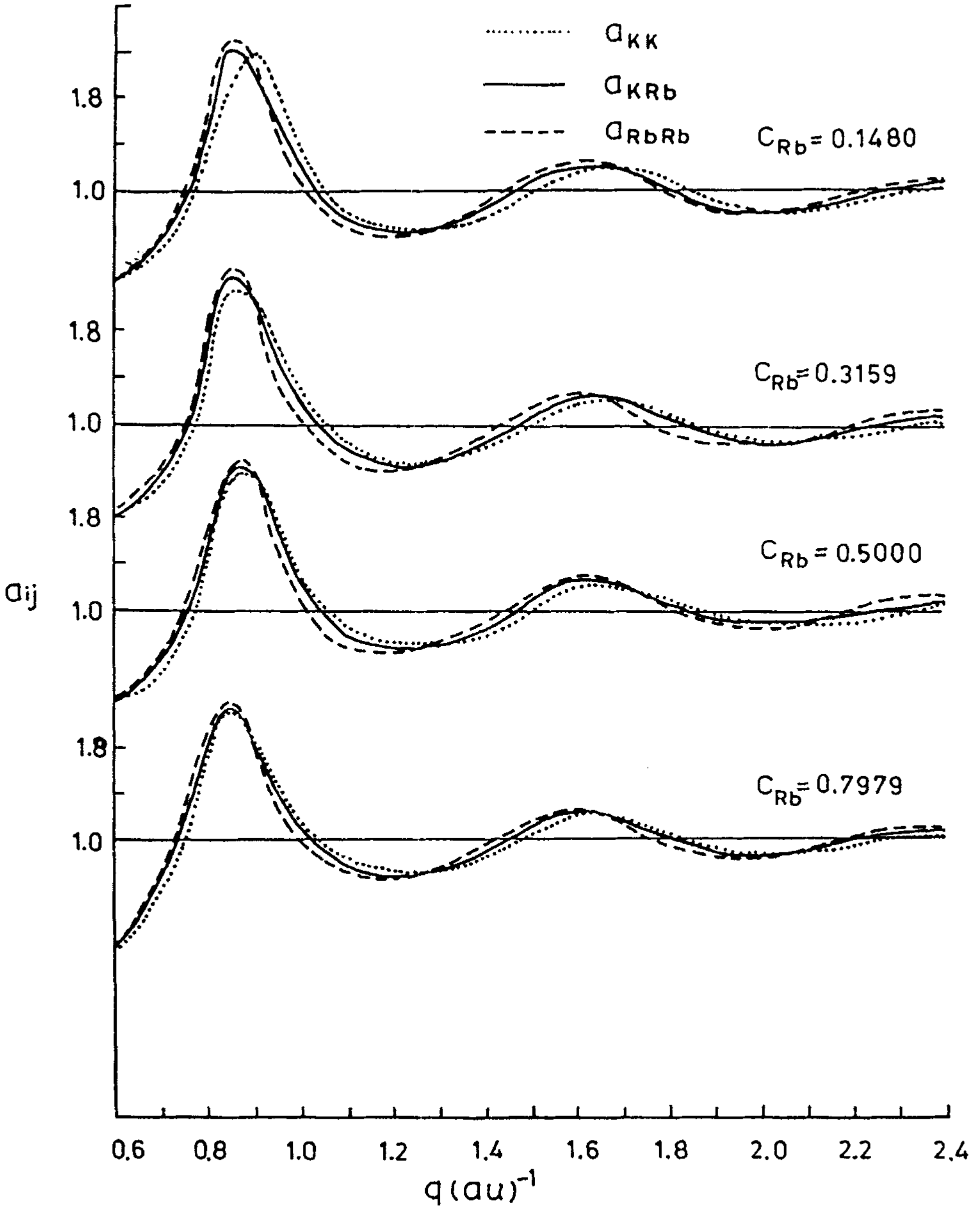

Figure 3 Partial structure factors for KRb liquid alloy at 373°K. ····· (a_{KK}), – – – – – (a_{RbRb}) and ——— (a_{KRb}).

the constituent species of binary alloys. The different contributions may be expressed as

$$R_{11} = (3\pi/\hbar|e|^2)(\Omega/NV_F^2)4\int_0^1 C_1 W_1^2 S_{11}(q/2K_F)^3\, d(q/2K_F) \tag{15}$$

$$R_{22} = (3\pi/\hbar|e|^2)(\Omega/NV_F^2)4\int_0^1 C_2 W_2^2 S_{22}(q/2K_F)^3\, d(q/2K_F) \tag{16}$$

and

$$R_{12} = (3\pi/\hbar|e|^2)(\Omega/NV_F^2)4\int_0^1 2(C_1C_2)^{1/2} W_1 W_2 S_{12}(q/2K_F)^3\, d(q/2K_F) \tag{17}$$

where e is the electronic charge, V_F is the Fermi velocity. K and q are electron and phonon wave vectors; W_1 and W_2 are the screened pseudopotential matrix elements which have been obtained using the energy dependent nonlocal optimised model potential of Shaw[8] because the latter has proved very successful in the study of electrical transport properties of liquid metals. The screened nonlocal matrix elements of the constituent species can be expressed as

$$W = f(K, q) + \left\{\frac{4\pi}{\Omega_0 q^2}\,\varepsilon^*(q)\right\}\left[1 - G(q)\rho + g(q)\left(1 - \frac{G(q)}{\varepsilon^*(q)}\right)\right] \tag{18}$$

with

$$f(K, q) = N\sum_{l=0}^{l_0} \langle K + q|\left(A_l(E) - \frac{Z}{r}\right)p_l|K\rangle \tag{19}$$

$$g(q) = \frac{4}{\pi^2 q^2 \varepsilon(q)}\int_{k \leqslant k_F} \frac{f(K, q)}{K^2 - |K + q|^2}\, d^3K \tag{20}$$

In the above expression ρ is the depletion hole and l_0 is the highest angular momentum to be modelled. For a given angular momentum, the energy dependent model parameters $A_l(E)$ and $R_l(E)$ are determined by matching the logorithmic derivative of the wave function at the boundary, which in turn yield crystal parameters at $E = E_F$. The depletion hole ρ has been computed following the work by Shaw and Harrison[28].

$$\rho = \frac{4}{\pi}\sum_{l=0}^{l_0}(2l + 1)\int_0^{K_F} K^2 dK \int_0^{R_l} j_l(K \cdot r)\left[\left(\frac{\partial A_l}{\partial E}\right)_{E=E_F}\right]\gamma^2 dE \tag{21}$$

where j_l $(k \cdot r)$ stands for Bessel function and $(\partial A_l/\partial E)_{E=E_F}$ is the derivative of parameter A_l with respect to energy evaluated at $E = E_F$. W_i have been computed through equation (18) in cylindrical coordinates following the work of Harrison[29] at $|K + q| = |K| = K_F$. The modified dielectric function $G(q)$ have the same meaning as in Eq. (11) and (12) respectively. The atomic volume and K_F have been chosen appropriate to the concentration of the alloy. The partial structure factors are taken from the work of Section 2.

The various contributions to the electrical resistivity i.e., R_{11}, R_{22} and R_{12} are computed via Eqs (15) to (17) for NaK, NaCs and KRb. These are plotted in Figures 4 to 6 and are compared with the experimental observation of Van der Lugt *et al.*[30] for NaK and NaCs. The computed results for NaK are in very good agreement with experimental observation for the whole range of concentration. The computed results of NaCs are however smaller than the observed values. None the less, the asymmetry of the electrical resistivity in the case of NaCs is appropriately reproduced. The results for KRb could not be compared because, to the best of our knowledge, no experimental measurement exist for the system.

It is evident from the figures that the same particle correlation (Na–Na, K–K, Rb–Rb and Cs–Cs) contribute positively to the absolute value of resistivity while the cross terms of NaK, NaCs and KRb give negative contribution. The magnitude of the cross terms (R_{12}) are always greater than the other contributions.

The concentration dependence of the electrical resistivity of NaCs is much more asymmetrical than NaK alloys. The resistivity of KRb varies almost linearly with respect to concentration. Our results reveal that the asymmetry in NaCs is brought about by all the three contributions i.e., R_{NaNa}, R_{NaCs} and R_{CsCs}. The greater asymmetry in the electrical resistivity in NaCs can be attributed to the large size effect in the alloy. We recall that the size effect in NaCs is maximum followed by NaK and minimum in the case of KRb.

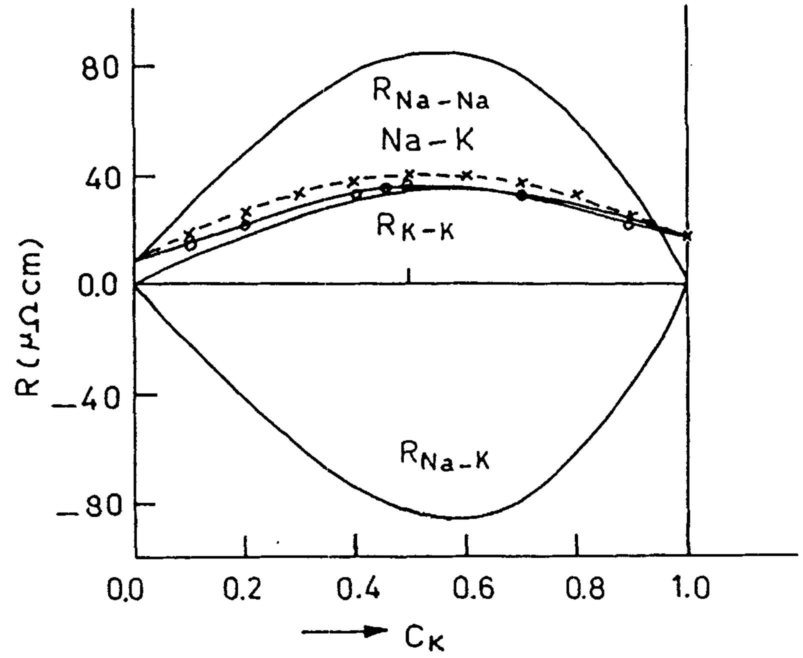

Figure 4 Electrical resistivity of NaK liquid alloy at 373°K. For R_{NaNa}, R_{NaCs} and R_{CsCs}, see text. R(O—O—O—O) Corresponds to the computed values of electrical resistivity and (x – – x – – x –) stand for experimental observation (Vander Lugt *et al.* 1973).

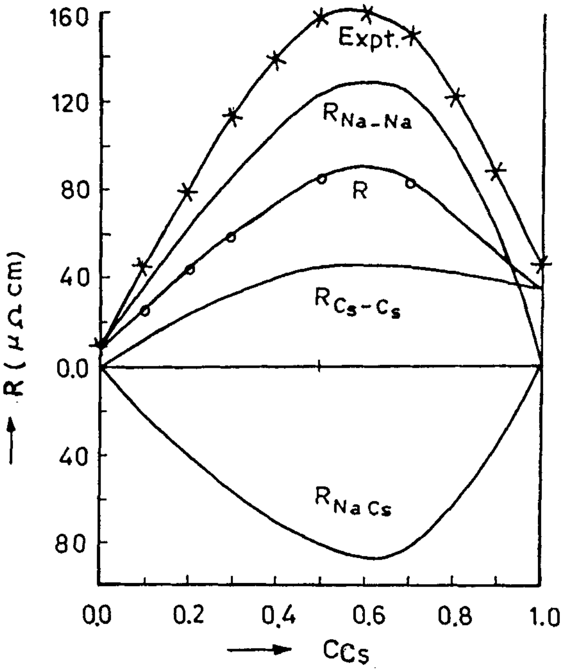

Figure 5 Electrical resistivity of NaCs liquid alloy at 373°K. For R_{NaNa}, R_{CsCs} and R_{NaCs}, see text. R(—O——O——O—) corresponds to the computed values of electrical resistivity of NaCs alloy and (×——×——×—×—) stand for experimental observation (Van der Lugt *et al.* 1973).

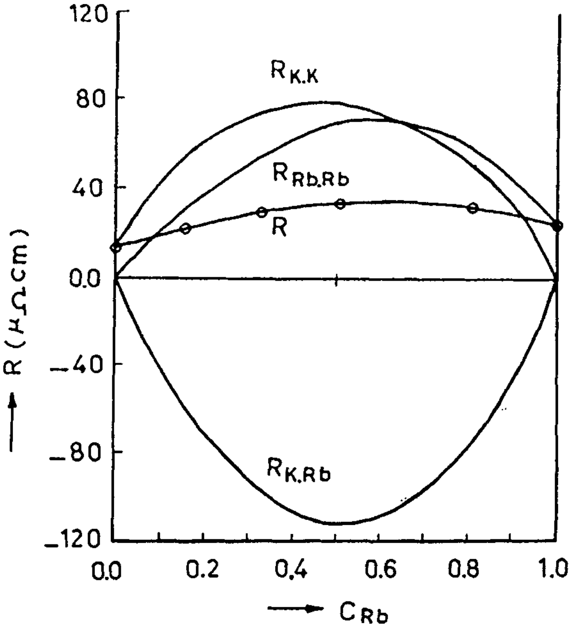

Figure 6 Electrical resistivity of KRb liquid alloy at 373°K. For R_{KK}, R_{RbRb} and R_{KRb}, see text. R(—O——O——O——O—) corresponds to the computed values of electrical resistivity of KRb alloy.

4 SUMMARY AND CONCLUSION

The structure and the electrical resistivity of NaK, NaCs and KRb have been studied as a function of concentration. The two important ingredients i.e., the partial structure factors and the form factors are obtained in a rigorous fashion. The present approach is free from any adjustable parameter.

The partial structure factors are obtained for hard sphere potential in the Percus–Yevick approximation. The concentration dependence of the hard sphere parameters is determined from the variational thermodynamics by minimising the Helmholtz free energy of the system. The present approach is entirely different from the earlier workers (see Shimoji[16]) where the hard sphere parameters are determined by fitting the observed structure factors of pure liquid metals. Also the hard sphere diameters and the atomic volumes of the alloys were assumed to vary linearly with concentration which was later proved[31] to be only approximate. In order to overcome these difficulties, we consider an approach where hard sphere parameters are determined by minimising the Helmholtz free energy of the system, data on volume of mixing of alloys are taken from experimental observation and the form factors are evaluated through a full nonlocal pseudopotential.

The computed values of hard sphere parameters indicate that the sizes of the atoms of the pure elements readjust, on alloying, to attain an equilibrium value. The heavier atoms undergo contraction while the lighter atoms experience expansion. This has been qualitatively explained by considering the redistribution of electronic charges at the Fermi surface.

The three partial structure factors (a_{11}, a_{22} and a_{12}) of liquid alloys differ considerably among themselves. The difference is maximum in NaCs but of least significance in case of KRb. The difference of the three partial structure factors are shown to have direct relevance to the size factor. Our results also indicate that the partial structure factors depend considerably on concentration.

With a view to obtaining greater insight the Faber–Ziman formula[2] for electrical resistivity of binary liquid alloys has been expressed (see Eq. 14) in a convenient form where the different contributions to the electrical resistivity can be identified separately. The same particle correlation contributions (R_{11} and R_{22}) are always positive whereas the cross term R_{12} has been found to be always negative. The asymmetry in case of NaCs and to some extent in case of NaK are brought about by all the three contributions. Further our results suggest that among the positive contributions, the lighter atoms correlations are larger in magnitude than the heavier atoms correlation. For example in case of NaCs, R_{NaNa} is greater than R_{CsCs}. Similarly in case of NaK, R_{NaNa} is greater than R_{KK}.

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