# Structure and Inter-Diffusion Coefficients of Liquid Na$_x$K$_{1-x}$ Alloys

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**Structure and atomic transport properties of liquid Na-K alloys are reported. Inter-diffusion coefficients of liquid Na$_x$K$_{1-x}$, alloys are calculated using scaling law proposed by Samanta et al. following Dzugutov which express the possible relationship between the excess entropy and diffusion coefficient. The interatomic interactions are described from the individual version of the electron-ion potential proposed by Fiolhais et al. The partial pair distribution functions and structure factors are calculated from the solution of Ornstein-Zernike integral equation with Rogers-Young closure. The evaluation with the composition of static structure and inter-diffusion properties are discussed.**

## 1. Introduction

Knowledge of diffusion coefficients is required to understand such important material processing techniques as binary solidification and glass formation. Also many of industrially important reactions are controlled by the diffusion of reactant species. On the other hand, it is difficult to determine the diffusion coefficient experimentally at high temperature and it is not fully understood how they depend on the structure and the thermodynamics of liquids as well as the solidus. To find a relationship between transport properties (diffusion, viscosity, and electrical resistivity) and structural properties which remain one of the most challenging tasks in the field of condensed matter, some attempts have been made since the late 1970s. Dzugutov[1,2] has proposed a scaling law which assumes a proportionality between the reduced diffusion and excess entropy. A relationship was obtained using microscopic reduction parameters (collision frequency and interparticle distance).

The Dzugutov scaling law[3-16] was tested for different liquid metals using different interaction pair potentials with computer simulation methods for diffusion coefficients was formulated for a binary mixture by Hoyt[3] and Samanta et al.[4] In this study, we have calculated diffusion coefficients by using the scaling laws proposed by Hoyt[3] and Samanta et al.[4] for liquid Na$_x$K$_{1-x}$, metal alloys near the melting point. We have used the individual version of a local pseudopotential proposed by Fiolhais and coworkers[17,18]

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which was developed for the solid state and can be transferable to liquid metal alloys[19-23] as interaction potentials. The pair distribution function $g_{ij}(r)$ is determined from the solution of Ornstein-Zernike equation with Rogers-Young closure[24] giving access to the excess entropy. To the best of our knowledge, previously no one has reported such a study to investigate inter-diffusion coefficients of liquid Na-K metal alloys using a partial pair distribution factor from this transferable pseudopotential with the Rogers-Young closure.

The manuscript is organized with a theory section, a calculated results section, and a conclusion section: In the theory section, we briefly describe the effective interatomic interaction. Partial pair distribution functions and partial structure factors of liquid Na$_x$K$_{1-x}$ alloys, and scaled diffusion coefficients $D^*$, together with total excess entropy, $S_T$, and the inter-diffusion coefficient $D_{Na-K}$ of liquid Na$_x$K$_{1-x}$ alloys. The second section gives results of numerical calculations and then compares with other available calculated data. Lastly, concluding remarks are presented in the final section.

## 2. Theory

### 2.1 Effective Pair Potential

We use the well-established second-order perturbation determination of the effective pair potential, $u_{ij}(r)$, which can be written as

$$u_{ij}(r) = \frac{Z_i Z_j}{r}\left[1 - \frac{2}{\pi}\int_0^\infty F_{N_{ij}}(q)\frac{\sin qr}{q}dq\right], \quad \text{(Eq 1)}$$

where

$$F_{N_{ij}}(q) = \left(\frac{q^2}{4\pi}\right)^2 \frac{1}{Z_i Z_j} w_i(q) w_j(q)\left[1 - \frac{1}{\varepsilon(q)}\right]\left[1 - G(q)\right]^{-1}.$$

$$\text{(Eq 2)}$$

In these expressions, $Z_i$ denotes the valences of the ions of the $i$th species. $\varepsilon(q)$ is the Hartree dielectric function and $G(q)$ is a local field correction. Here we employ the well known local field correction of Ichimaru and Utsumi.[25] $w_i(q)$ denotes pseudopotential form factor described by Fiolhais et al.[17] as

$$w_i(q) = 4\pi Z_i R_i^2 \rho \left[ -\frac{1}{(qR_i)^2} + \frac{1}{(qR_i)^2 + \alpha_i^2} \right.$$
$$\left. + \frac{2\alpha_i\beta_i}{\left[(qR_i)^2 + \alpha_i^2\right]^2} + \frac{2A_i}{\left[(qR_i)^2 + 1\right]^2} \right] \quad \text{(Eq 3)}$$

where $\rho = (c\rho_i + (1-c)\rho_j)$ is the number density of the system and $R_i$, $\alpha_i$, $\beta_i$, and $A_i$ denote the parameters of the potential tabulated by the authors.[18] This local pseudopotential, which was developed for solid state in requiring the main electronic features to be correctly predicted, could be transferable to other environments as checked for liquid metal alloys.[19-23]

### 2.2 Partial Pair Distribution Functions and Partial Structure Factors

With the partial pair potential known, the total correlation function $h_{ij}(r)$ of a binary alloy can be determined from the solution of the Ornstein-Zernike equation as

$$\gamma_{ij}(r) \equiv h_{ij}(r) - c_{ij}(r) = \sum_{k=1}^{2} c_k \rho \int h_{ik}(r) c_{kj}(r) dr, \quad \text{(Eq 4)}$$

where $h_{ij}(r) = g_{ij}(r) - 1$ and $c_{ij}(r)$ is the direct correlation function. To solve the Ornstein-Zernike integral equation, one needs a closure between $h_{ij}(r)$ and $c_{ij}(r)$. In our case we use Rogers-Young approximation[24] defined as

$$g_{ij}(r) = \exp[\beta u_{ij}(r)] \times \left[ 1 + \frac{\exp\{f_{ij}(r)\gamma_{ij}(r)\} - 1}{f_{ij}(r)} \right] \quad \text{(Eq 5)}$$

where $\beta = 1/k_B T$, $k_B$ is the Boltzmann constant, $T$ is temperature, and $f_{ij}(r)$ is the mixing function given by

$$f_{ij}(r) = 1 - \exp(a_{ij}r) \quad \text{(Eq 6)}$$

In this work we place $a_{ij} = a$ and we calculated from the relation suggested by Lai et al.[26] After the calculation of pair distribution function, we computed the Ashcroft-Langreth's partial structure factors[27] by

$$S_{ij}(q) = 1 + \sqrt{c_i c_j}\rho \int \left[ g_{ij}(r) - 1 \right] \exp(-i\vec{q} \cdot \vec{r}) d\vec{r} \quad \text{(Eq 7)}$$

where $c_i$ is the concentration of the $i$th components. From the knowledge of partial structure factor of $S_{ij}(q)$, we are able to compute the total structure factors by

$$S(q) = \frac{c_1 f_1^2 S_{11}(q) + 2\sqrt{c_1 c_2} f_1 f_2 S_{12}(q) + c_2 f_2^2 S_{22}(q)}{c_1 f_1^2 + c_2 f_2^2} \quad \text{(Eq 8)}$$

where $f_1$ and $f_2$ are atomic scattering factors and are taken from the literature.[28]

### 2.3 Scaling Law and Diffusion Coefficients

Hoyt et al.[3] proposed a new scaling law for a binary mixture of two components $\mu$ and $\nu$ given by

$$D^* = \left(\frac{D_\mu}{\chi_\mu}\right)^{c_\mu} \left(\frac{D_\nu}{\chi_\nu}\right)^{c_\nu} = A\exp(S_T) \quad \text{(Eq 9)}$$

where $D_\mu$ and $D_\nu$ represent the self diffusivity of the respective components with mole fractions $c_\mu$ and $c_\nu$, and scaling factor is given by

$$\chi_\mu = 4(\pi k_B T)^{1/2} \sum_\nu \sigma_{\mu\nu}^4 \rho_\nu g_{\mu\nu}(\sigma_{\mu\nu}) \left(\frac{m_\mu + m_\nu}{2m_\mu m_\nu}\right)^{1/2}. \quad \text{(Eq 10)}$$

The total excess entropy is given by

$$S_T = c_\mu S_\mu + c_\nu S_\nu \quad \text{(Eq 11)}$$

where $S_\mu$ is the partial molar entropy for the $\mu$th component as given by[3]

$$S_\mu = -\frac{1}{2}\sum_\nu \rho_\nu \int dr \left[ g_{\mu\nu}(r) \ln g_{\mu\nu}(r) - (g_{\mu\nu}(r) - 1) \right]. \quad \text{(Eq 12)}$$

Scaled diffusivity of $\mu$th component in a binary mixture is given by[4]

$$D_\mu^* = \frac{D_\mu}{\chi_\mu} = 0.049 \exp(S_\mu) \quad \text{(Eq 13)}$$

and the inter-diffusion coefficient of liquid binary alloys can be obtained by

$$D_{\mu\nu} = c_\nu D_\mu + c_\mu D_\nu. \quad \text{(Eq 14)}$$

## 3. Results and Discussion

### 3.1 Interactions

The effective pair potentials are computed by using individual versions of Fiolhais pseudopotential with parameters for Na $\alpha = 3.499$, $R = 0.494$ and for K $\alpha = 3.421$, $R = 0.683$. To calculate the number density of system, we use number density data for Na and for K from Waseda[29] at 373 K.

The three pair potentials obtained for each composition show usual potential behaviors of metallic systems. In Fig. 1 we display the three pair potentials $u_{ij}(r)$ obtained for three concentrations of $Na_xK_{1-x}$ alloys namely $Na_{0.3}K_{0.7}$, $Na_{0.5}K_{0.5}$, and $Na_{0.7}K_{0.3}$ alloys. As can be seen in Fig. 1, a sharp repulsive part at short distances is followed by a first negative minimum at about the first neighbor's distance and decreasing Friedel's oscillations at medium range which become negligible at about three times the interatomic distance. In fact, in an alloy, examining a single pair potential is irrelevant and it is more interesting to consider the features of the whole set of three partial pair potentials.
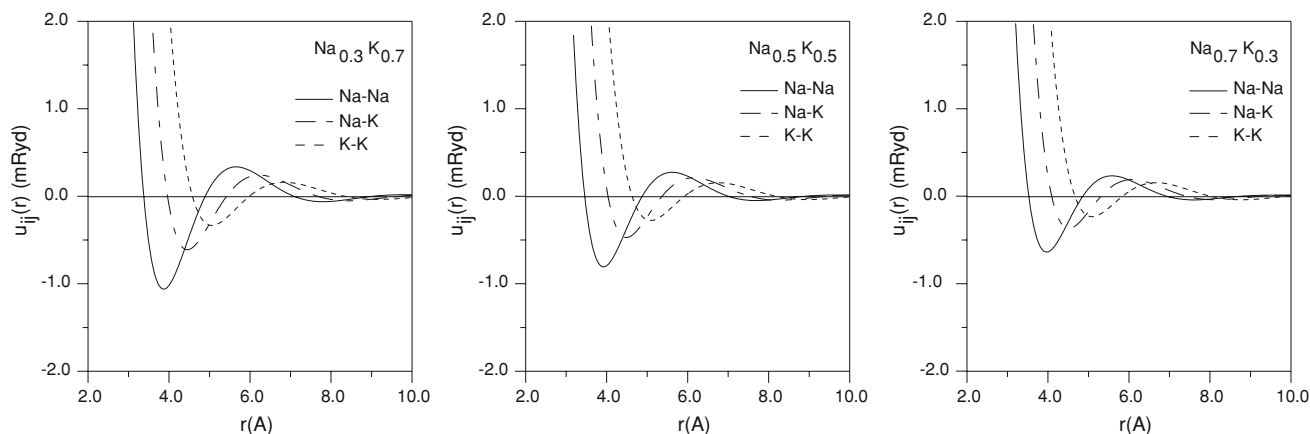
**Fig. 1** Pair potentials of the liquid $Na_{0.3}K_{0.7}$, $Na_{0.5}K_{0.5}$, and $Na_{0.7}K_{0.3}$ alloys at $T = 373$ K. Solid, dot-dashed, and dotted lines represent Na-Na, Na-K, K-K functions, respectively

**Table 1  The characteristic of the pair interaction potentials for each alloy studied in this work**

| Alloy | $\sigma_{11}$, Å | $\varepsilon_{11}$, $10^{-3}$ Å | $\alpha = \frac{\sigma_{11}}{\sigma_{22}}$ | $\beta = \frac{\varepsilon_{11}}{\varepsilon_{22}}$ | $\gamma$ | $\theta$ |
|---|---|---|---|---|---|---|
| $Na_{0.1}K_{0.9}$ | 3.80 | −1.47 | 1.32 | 0.27 | −0.0022 | 1.030 |
| $Na_{0.2}K_{0.8}$ | 3.84 | −1.24 | 1.31 | 0.29 | −0.0045 | 1.033 |
| $Na_{0.3}K_{0.7}$ | 3.86 | −1.06 | 1.31 | 0.31 | 0 | 1.031 |
| $Na_{0.4}K_{0.6}$ | 3.90 | −0.92 | 1.30 | 0.32 | −0.0022 | 1.008 |
| $Na_{0.5}K_{0.5}$ | 3.92 | −0.80 | 1.29 | 0.33 | −0.0044 | 1.011 |
| $Na_{0.6}K_{0.4}$ | 3.92 | −0.80 | 1.29 | 0.33 | −0.0044 | 1.011 |
| $Na_{0.7}K_{0.3}$ | 3.96 | −0.63 | 1.28 | 0.36 | 0 | 0.945 |
| $Na_{0.8}K_{0.2}$ | 3.98 | −0.57 | 1.27 | 0.36 | −0.0022 | 0.924 |
| $Na_{0.9}K_{0.1}$ | 4.00 | −0.51 | 1.27 | 0.37 | 0 | 0.931 |

Therefore, we will discuss the four parameters which are gathered in Table 1: $\alpha = \sigma_{22}/\sigma_{11}$ and $\beta = \varepsilon_{22}/\varepsilon_{11}$ related to size and attraction asymmetry where $\sigma_{ij}$ and $\varepsilon_{ij}$ denote the position and depth of the first minimum of $u_{ij}(r)$, and $\gamma = 2\sigma_{12}/(\sigma_{11} + \sigma_{22}) - 1$ and $\theta = \varepsilon_{12}/(\varepsilon_{11}\varepsilon_{22})^{1/2}$ related to the deviation from additive potentials. We recall that size asymmetry generates heterocoordination tendencies,[30] while attraction asymmetry causes homocoordination. Attraction non-additivity induces either heterocoordination (if $\theta > 1$) or homocoordination (if $\theta < 1$).[31]

Table 1 shows that an increasing tendency to homocoordination as $c_{Na}$ increases in $Na_xK_{1-x}$ alloys. Indeed, size asymmetry decreases while the attraction asymmetry goes simultaneously from 0.27 to 0.37.

### 3.2 Structure

The pair distribution functions of the metals studied in this work are determined from the solution of Ornstein-Zernike equation. Labik, Malijevsky, and Vonka algorithm[32] is used for the numerical solution of the Ornstein-Zernike equation given by Eq (4) with the closure relation given by Eq (5, 6) in all cases. Each computation is carried out by using 1024 data points with a step size $\Delta r = 0.02$ Å.

In Fig. 2 we display the partial pair distribution functions $g_{ij}(r)$ obtained for nine concentrations of $Na_xK_{1-x}$ alloys.

Partial pair distribution functions behave in the same way as the total one of pure liquids. The positions of first peaks are related to the size of the atoms. The first peak of $g_{Na-K}(r)$ lies in the middle between $g_{Na-Na}(r)$ and $g_{K-K}(r)$ first peaks. It is observed that $g_{Na-Na}(r)$ undergoes important changes whereas both $g_{Na-K}(r)$ and $g_{K-K}(r)$ change slightly. The heights of the first peaks may exhibit the signature of chemical order. In fact, when the $x_{Na}$ is increased the height of first peak of $g_{Na-Na}(r)$ decreases, while its position remains practically unchanged. On the other hand, the $g_{Na-K}(r)$ remains practically constant while the height of the first peak $g_{K-K}(r)$ slightly increases and becomes for $x_{Na} = 0.5$ comparable to that of $g_{Na-K}(r)$. For this concentration the global configuration suggested by $g_{ij}(r)$ obtained from Fiolhais pseudopotential predicts a very weak tendency towards phase separation. Indeed, if the first peak of $g_{Na-K}(r)$ was much higher than both others, it would be the signature of the heterocoordinaion tendencies like compound forming. On the other hand if it were significantly lower than both others, it would reveal homocoordination tendencies.

It can also be noticed that for alloys with greater than 70 at.% of Na, the first peak of $g_{Na-K}(r)$ becomes slightly lower than both others indicating a slight tendency to homocoordination. This result is consistent with the conclusions drawn from the study of the pair potentials.

In Fig. 3 we present the Ashcroft-Langreth partial structure factors of nine $Na_xK_{1-x}$ alloys. Some usual features are recovered namely $S_{NaNa}(q)$ and $S_{KK}(q)$ oscillate around 1 as $q$ tends to infinity, while $S_{NaK}(q)$ oscillates around 0 in the limit. The curves are very sensitive to the composition.

In Fig. 4 we present the total structure factors according to Eq (8) in comparison with available experimental x-ray data[33,34] for three composition of Na-K.

The calculated total structure factors in the low-$q$ region and the position of principal peaks are in good agreement with experiment for each composition of Na-K displayed in
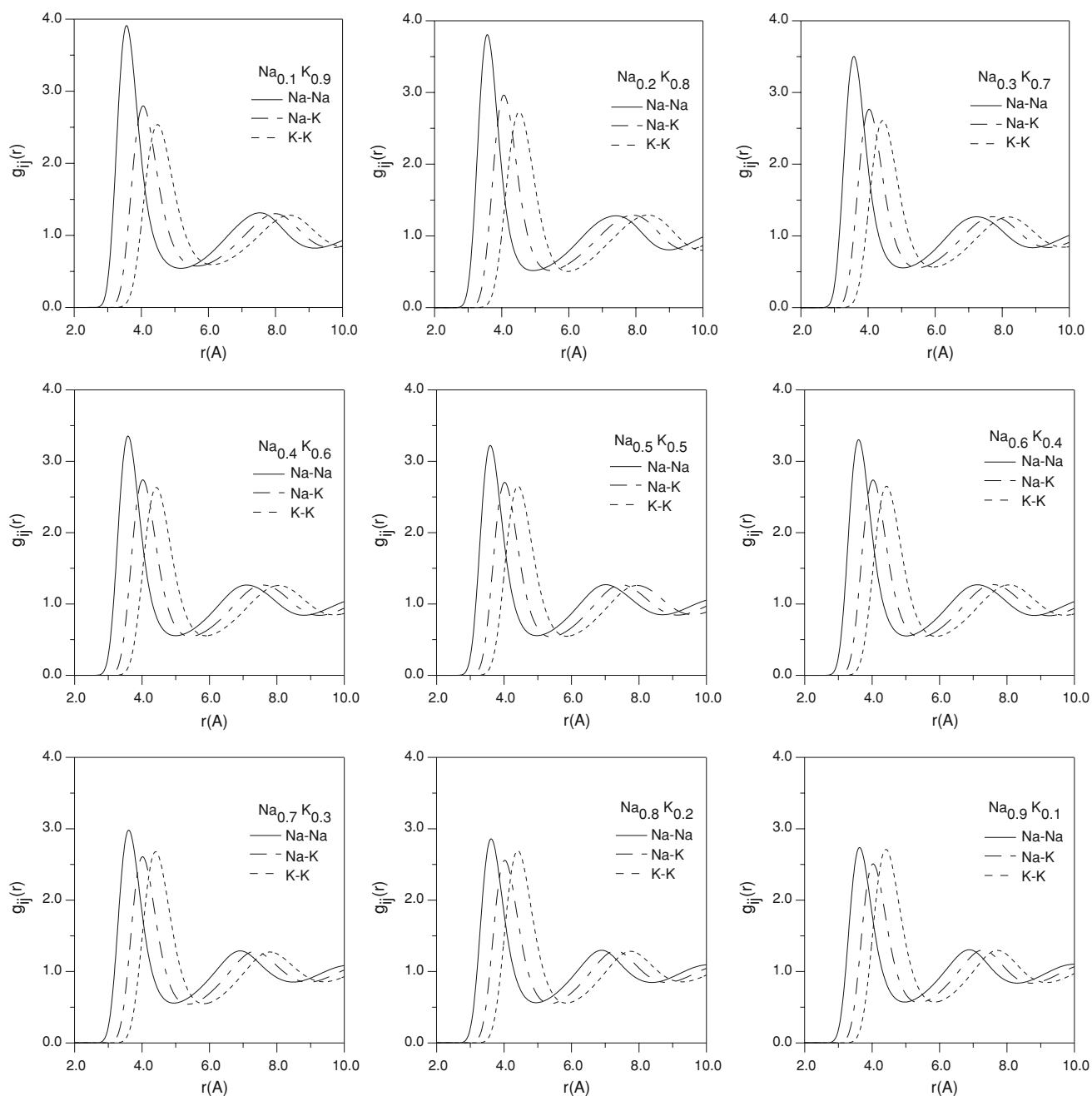
**Fig. 2** Partial pair distribution functions for the nine alloys under consideration. Solid, dot-dashed, and dotted lines represent Na-Na, Na-K, K-K functions, respectively

Fig. 4. It should be noted that the amplitude of first peaks of $S(q)$ in $Na_{0.3}K_{0.7}$ and $Na_{0.7}K_{0.3}$ cases agree well with experimental data while it is overestimated in case of $Na_{0.5}K_{0.5}$. The greatest discrepancy is observed in oscillations of calculated $S(q)$ especially in case of $Na_{0.7}K_{0.3}$. The ability of these effective pair potentials to describe the interactions in these alloys has already been demonstrated by Wax and co-workers in their MD study.[22,23] Our results have also supported them. The reasonable good agreement with x-ray results is an indication of the reliability the

description of the interactions used. For this alloy, Fiolhais' model of interactions confirms its transferability to the liquid state.

### 3.3 Thermodynamic and Diffusion Properties

The important aspect of scaling laws is that they connect the dynamical quantity diffusivity to the total excess entropy which is the difference between system's thermodynamic entropy and that of the equivalent ideal gas. The total excess
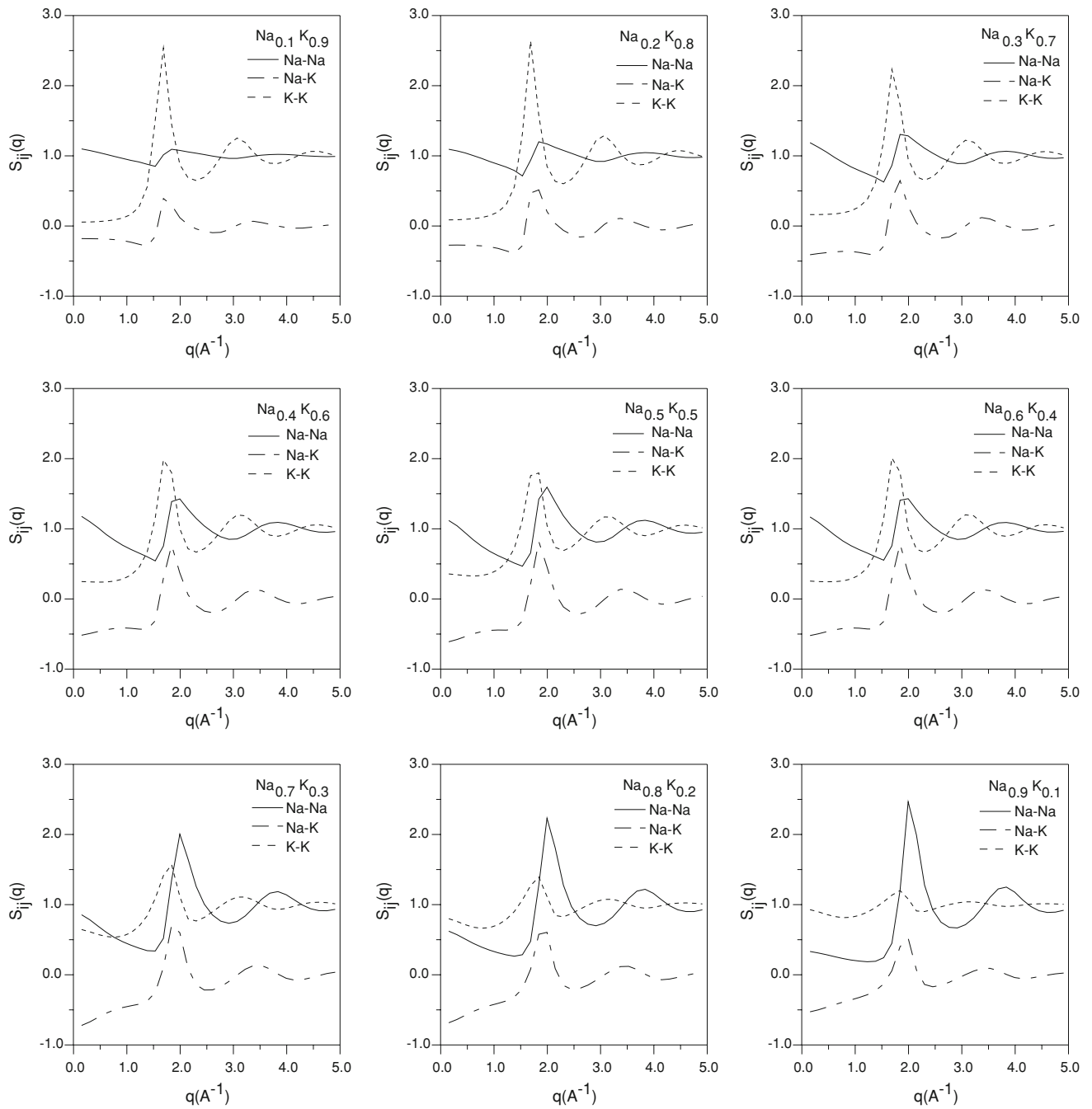
**Fig. 3** Ashcroft-Langreth partial structure factors for the nine alloys under consideration. Solid, dot-dashed, and dotted lines represent Na-Na, Na-K, K-K functions, respectively

entropy is calculated directly in terms of pair distribution functions by using Eq (9, 10). Thus the dynamical quantity of system namely diffusivity is connected with an equilibrium property partial pair distribution function. So, using computed $g_{\mu\nu}(r)$, we have calculated total excess entropies, for each system studied in this work using Eq (11, 12). Calculated values are summarized in Table 2.

As is seen Table 2 calculated total excess entropy values changes in the interval between $-3.24$ and $-3.64$. We could

not get experimental excess entropy data for the systems studied in this work but we could get one calculated data recently published by Yokoyama et al.[16] for $Na_{0.5}K_{0.5}$ at 373 K. Their calculated excess entropy result which is equal to $-3.41$ in $k_B$ is very near to our result for that composition.

After the computation of total excess entropy, we have calculated scaled diffusion and inter-diffusion coefficients of nine composition of Na-K. Our results are gathered in
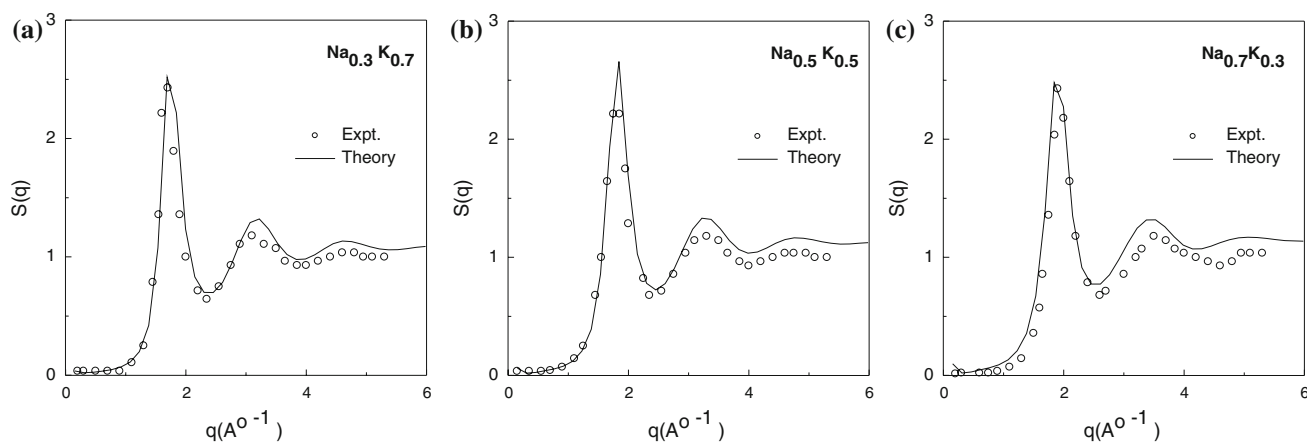
**Fig. 4** Total x-ray structure factors $S(q)$ for the liquid $Na_{0.3}K_{0.7}$, $Na_{0.5}K_{0.5}$, and $Na_{0.7}K_{0.3}$ alloys at $T = 373$ K in comparison with experimental data[33,34]

**Table 2** Scaled diffusion coefficients, total excess entropies, and inter-diffusion coefficients for Liquid $Na_xK_{1-x}$ alloys are together with available the other calculated data[23]

| Alloy | $D^*$ $(10^{-3})$ Calc. | $S_T$ $(k_B)$ Calc. | $D_{Na-K}$, $10^{-9}$ m²/s Calc. | Calc.(a) |
|---|---|---|---|---|
| $Na_{0.1}K_{0.9}$ | 1.91 | −3.24 | 3.63 | 4.36 |
| $Na_{0.2}K_{0.8}$ | 1.28 | −3.64 | 3.19 | 4.13 |
| $Na_{0.3}K_{0.7}$ | 1.73 | −3.33 | 3.69 | 3.62 |
| $Na_{0.4}K_{0.6}$ | 1.67 | −3.37 | 3.70 | 3.43 |
| $Na_{0.5}K_{0.5}$ | 1.65 | −3.38 | 4.08 | 3.27 |
| $Na_{0.6}K_{0.4}$ | 1.60 | −3.41 | 3.85 | 3.11 |
| $Na_{0.7}K_{0.3}$ | 1.70 | −3.35 | 3.47 | 2.95 |
| $Na_{0.8}K_{0.2}$ | 1.76 | −3.37 | 3.27 | 2.71 |
| $Na_{0.9}K_{0.1}$ | 1.85 | −3.27 | 3.16 | 3.01 |

(a) Taken from Wax[23]

Table 2. Since we are not aware the experimental data for inter-diffusion coefficient in the literature for these systems, we have compared our results with available simulation data obtained with the same potential and at the same temperature. The molecular dynamics simulation results for self inter-diffusion coefficients $D_{Na-K}$ obtained by Wax[23] are also tabulated in Table 2. As is seen Table 2, our results of inter-diffusion coefficient calculated from scaling law proposed by Samanta et al.[4] are different from the simulation result of Wax.[23] While in the cases of $Na_{0.9}K_{0.1}$ and $Na_{0.8}K_{0.2}$, they are smaller than those of Wax,[23] in the other cases our results are bigger. We think that the differences between our results of and those of Wax could occur because of two reasons. One of them is related to number density of the system which is the input parameter of potential. We have calculated the number density of each composition from the relation $\rho = c\rho_i + (1-c)\rho_j$ using the number density data for Na and for K from Waseda[29] while Wax has used experimental

density data. The other reason is related to the calculation method of inter-diffusion coefficient. In the MD study, the cross correlation between velocities of distinct particles in the diffusion process are not neglected.

## 4. Conclusions

In this work we have investigated the structure and atomic transport properties of liquid metal alloys Na-K at three different concentration using possible relationships between the excess entropy and transport properties of liquids namely scaling laws. To calculate excess entropy, we have computed the partial pair distribution functions using the individual version of pseudopotential proposed by Fioalhais et al. with well known local field correction of Ichimaru and Itsumi and Ornstein-Zernike integral equation with Rogers-Young closure. The analysis of structure properties of liquid Na-K system clearly showed that for alloys with less than 80 at.% of Na, the first peak of $g_{Na-K}(r)$ becomes slightly lower than both others indicating a slight tendency to homocoordination.

Considering the predicted values of inter-diffusion coefficients, we have concluded that the experimental uncertainty being unknown, the discussion would be speculative. Nevertheless, it would be interesting to compare the simulation predictions with experimental data on a large concentration range. To our knowledge, such experimental data have never been published to date.

On the other hand, a scaling law proposed by Samanta et al. for diffusion coefficients is a simple way to calculate inter-diffusion coefficients of metal alloys and it can be used to estimate an approximate value for liquid $Na_xK_{1-x}$ alloy for different temperatures and different compositions when experimental data do not exist. However, the existence of experimental data would be helpful. In order to check the reliability of the scaling law, we have started a similar study for the other liquid simple metal alloys. The results will be published subsequently.

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