STRUCTURE OF LESS SIMPLE LIQUID ALLOYS: Ag_x-In_{1-x}

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The transferability of the local evanescent core (EC) pseudopotential to less-simple liquid binary alloys is assessed. The structural properties of liquid Ag-In alloys at different compositions are calculated using the Variational Modified Hypernetted Chain (VMHNC) integral equation theory of liquids with the effective pair potentials derived from the evanescent core electron-ion potential constructed by Nogueira, Fiolhais and Perdew for the solid state. Comparison with the results those obtained by other different forms of the model pseudopotentials and experimental data confirms the ability of the universal density dependent version of the EC potential to be used in the case of liquid less-simple metals and metal alloys.

1. Introduction

From a theoretical of view, the study of simple metals is closely related to pseudopotentials [1]. Structure of the simple metals in their liquid state are well described using the effective inter-ionic interaction derived from the pseudopotential theory [1-3]. In principle the pseudopotentail can be of local or non-local character. Although some researchers have been preferred non-local pseudopotentials, it has been noted that, in some cases the local model pseudopotentials describe the some liquid state properties even better than those of norm conserving non-local ones [4,5].

In this work we have concerned with a local evanescent core (EC) type model pseudopotential of Fiolhais *et al.* [6], whose parameters are fitted to the dominant electronic density features for 16 simple metals in the solid state. (i) the valence Z, (ii) the radius r_s of the sphere, (iii) the electron number N_{int} averaged over the interstitial region between the Wigner-Seitz polyhedron and the largest inscribed sphere. Two possible routes are available to determine these characteristics. The pseudopotential contains two parameters R and α, which are chosen by using either the conventional crystal structure (individual parameters) or fcc structure (universal parameters). These versions of Fiolhais' pseudopotentials [6] are so-called namely EC(I) and EC(U1) respectively. Another version of the universal evanescent pseudopotential [EC(U2)] model in which the parameters R and α depend on the valence Z and the average electron density ρ, namely. $R(r_s, Z)$ and $\alpha(r_s, Z)$ was proposed by Nogueira, Fiolhais and Perdew [7]. It has been obtained that a second-order perturbative calculation with these pseudopotentials are in good agreement with the predicted physical properties in the solid state and the individual pseudopotential is better choice for each sixteen simple metal in generally [6]. It has been applied to finite systems for dimers, clusters and metallic slabs [8] and noted that its transferability is high for ten metals (K, Rb, Cs, Mg, Al, Ga, In, Tl, Sn and Pb), poor for Li, Be, Ca, Sr and Ba [9]. All these works doesn't prove this pseudopotential is applicable to liquid state in spite of successful calculations in solid state. This is the main aim of the presented paper.

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In one of our previous work [10], it has been shown that the EC(I) version of this model potential is transferable for liquid alkaline and alkaline earth metals using very accurate integral equation of liquids, the variational modified hypernetted chain (VMHNC) approximation [11-13]. The resistivity [14] and ionic-structure calculations [15-18] and atomic transport properties [19-20] in liquid metals have been studied with different versions of this potential. Structural and dynamic properties of liquid alkaline and alkaline-earth metals have also been investigated [15-17] using these versions of EC pseudopotential by Brettonet and co-workers but not polyvalent ones. Related to this, we have presented the results for liquids Fe, Co and Ni, using the density dependent universal parameters EC(U2) which has been obtained with the proposed parameterization in that work [21]. The results in that work are in good agreement with experimental data [22]. We have also check this parametrization for liquid alkaline earth metals and metal alloys [10]. It has been noted that its transferability is a cause of concern for the charge transferred alloys, such as Li-Ba liquid alloys in the zero alloy case. On the other hand, in a recent work Dalgic and co-workers have been carried out the structural calculations for the liquid hcp rare-earth metals using the effective pair potential derived from the EC(U2) type of Fiolhais' pseudopotentials with the VMHNC liquid state theory [23]. In that work, the validity of the EC(U2) model potential has been checked by using the standart pseudopotential theory.

Motivated by the success of the transferable local pseudopotential of Fiolhais *et al*. [6,7] to predict the static structure of liquid simple metals and metal alloys, we examine the extent to which it can be transferred successfully from the solid state to less simple liquid metals and metal alloys for considering the structural properties of liquid Ag-In alloys. To the best of our knowledge, this model potential has not been extended to the case of liquid less-simple binary alloys. The second aim of this paper is thus to present theoretical results for the structural properties of liquid Ag-In alloys. For this reason, we took interest liquids Ag, In and Ag-In liquid alloys for which some authors have the successful results for their structural properties using the Brottenet-Silbert (BS) model potentials [4,5,24,25]. According to our knowledge, there is no published parameters of EC(U1) and EC(I) for liquid Ag. Therefore we only present the results for Ag and Ag-In with EC(U2) model potential. We have also obtained the structural properties of liquid Ag-In alloys in comparison with the experimental data [26] and the molecular dynamics calculations [27]. We show that the universal choices of Fiolhais' potential predicts more reasonable structural properties for liquid Ag, In and liquid Ag-In alloys than others.

2. Theory

The effective inter-atomic pair potential in simple metals $\phi(r)$ is based on the use of pseudopotentials to describe the interaction between an ion and a second ion and its screening cloud of electrons from second order pseudopotentail perturbation theory, obtained by,

$$\phi(r) = \frac{Z_{eff}^2}{r} + \phi_{ind}(r) \tag{1}$$

where Z_{eff} is the effective number of valence electrons per atom and here Fourier transform (FT) of the indirect part is given by

$$\tilde{\phi}_{ind}(q) = \chi(q)|\tilde{v}(q)|^2 \tag{2}$$

Where $\tilde{v}(q)$ is the pseudopotential local form factor and $\chi(q)$ is the response function of the electron gas. The effects of exchange and correlation between the electrons are accounted for by the introduction of a local field factor $G(q)$ in the response function as

$$\chi(q) = \frac{\chi^0(q)}{1 - \frac{4\pi}{q^2}[1 - G(q)]\chi^0(q)} \tag{3}$$

Where $\chi^0(q)$ is the response function of a non-interacting electron gas. Here we employ the well known local field corrections of the Ichimaru-Utsumi (IU) [28] and the local density approximation (LDA) version of the local-field function G(q) with the correlation energy of Vosko-Wilk and Nussair (VWN) [29]. In the present work, we use the recent local pseudopotential proposed by Fiolhais *et al*. This model pseudopotential has the core repulsion represented by an exponential factor, so called evanescent core (EC) pseudopotential. An analytic expression for the form factor of this pseudopotential in Fourier space

$$\tilde{v}(q) = 4\pi Z_{eff} R^2 \left[-\frac{1}{(qR)^2} + \frac{1}{(qR)^2 + \alpha^2} + \frac{2\alpha\beta}{\left[(qR)^2 + \alpha^2\right]^2} + \frac{2A}{\left[(qR)^2 + 1\right]^2} \right] \tag{4}$$

Where R is the core decay length, β and *A* parameters are given in terms of α namely,

$$\beta = \frac{\alpha^3 - 2\alpha}{4(\alpha^2 - 1)} \quad , \qquad A = \frac{\alpha^4}{4(\alpha^2 - 1)} \tag{5}$$

The values α and R can be obtained from the equilibrium condition of the solid state. For this reason this model potential has the advantage to be free of adjustable parameters. In this work, we consider the other pseudopotentials for comparison. The first one to be considered is Brettonet-Silbert (BS) pseudopotential [4,5]. This is most popular local pseudopotential and proved to be successful in the study of atomic [30], electronic [31], structural [5,32] and atomic transport properties [25] of liquid less-simple metals and metal alloys. We have also used the local Heine-Abarenkov (LHA) pseudopotential [33] which was applied successfully for the structural and thermodynamic properties of liquid metals and metal alloys [3]. Another pseudopotential proposed by Sharma [34] for noble metals is similar to LHA model potential.

A simple liquid metallic alloy, $A_x B_{1-x}$, may be regarded as an assembly of A-type and B-type bare ions with charges Z_v^A and Z_v^B respectively, where x is the concentration of the A-type component. Moreover, the ions attract the valence electrons which pile up around them, thus screening the ionic potentials and leading to effective interactions between the ions. Now, once the A-type and B-type effective local pseudopotentials, $v_{ps}^A(q)$, $v_{ps}^B(q)$ have been obtained, application of standard second-order perturbation pseudopotential theory leads to the effective interionic pair potentials, $\phi_{ij}(r)$, (i, j = A, B) given by

$$\phi_{ij}(r) = \frac{Z_v^i Z_v^j}{r} + \phi_{ps}^{ij}(r) \tag{6}$$

where the Fourier transform of $\phi_{ps}^{ij}(r)$ is given as

$$\phi_{ps}^{ij}(q) = \chi(q) \tilde{v}_{ps}^i(q) \tilde{v}_{ps}^j(q) \quad . \tag{7}$$

Here, $\chi(q)$ is the response function of the electron gas as described above.

With the effective pair potential known, integral equations are able to provide us the liquid structure for metals and alloys. In our structural calculations, one of the integral equation theory which has shown to be very reliable theory of liquids VMHNC has been carried out [11-13]. Like most liquid state theories the VMHNC solves the Ornstein–Zernike (OZ) equation, which for a homogeneous, isotropic, binary system reads (i, j =1, 2)

$$h_{ij}(r) = c_{ij}(r) + \sum_{l=1}^{2} \rho_l h_{il}(r) * c_{lj}(r) \tag{8}$$

Which defines the partial direct correlation functions, $c_{ij}(r)$, in terms of the total correlation functions $h_{ij}(r) = g_{ij}(r) - 1$, where $g_{ij}(r)$ denote the partial pair distribution functions and ρ_1 denote the partial ionic number densities. The O-Z equation can be solved by minimizing the configurational Helmholtz free energy functional $f^{VMHNC}(\beta, \rho, x_1, \eta_\alpha)$ by the variational condition

$$\frac{\partial f^{VMHNC}(\beta, \rho, x_1, \eta_\alpha)}{\partial \eta_k} = 0 \qquad , \ k = 1, 2, ..., m \tag{9}$$

with the exact closure relation as

$$c_{ij}(r) = h_{ij}(r) - \ln g_{ij}(r) - \beta \phi_{ij}(r) - B_{ij}(r) \tag{10}$$

In the above equations $\phi_{ij}(r)$ are the partial interatomic pair potentials and the $B_{ij}(r)$ denotes the Percus-Yevick (PY) hard sphere bridge functions for binary system. Related to this, Ashcroft-Langreth (AL) definition for the partial structure factors $S_{ij}(q)$ can be given as,

$$g_{ij}(r) = 1 + \frac{1}{8\pi^3 (n_i n_j)^{1/2}} \int (S_{ij}(q) - \delta_{ij}) \exp(-i\vec{q}.\vec{r}) dq \tag{11}$$

with n_i being the number density of i species. For useful details about the VMHNC calculations of the partial structure factors, the reader is referred to Ref. [13].

3. Results and discussion

The presentation of the results is divided into two parts: the first one concerns with the pure simple metals. The structural properties of liquid Ag and In for which experimental results near their melting points are available and the second one deals with structure of Ag-In liquid alloys at different Ag compositions that the experimental results for % 20 and % 70 Ag [26] can only be available and others can be compared with previous theoretical works [27]. For the purpose of the discussion, we show in Table 1 the relevant input data concerning the two sets of thermodynamic states for each liquid metal, Ag and In. The input temperature and corresponding number densities n are taken from Waseda [22] given in Table 1. As already indicated in the preceding section, the calculation of the liquid structure requires, as a first step, the calculation of the interatomic pair potentials. In this work, we have calculated the effective inter-ionic pair potentials using the three version of the EC pseudopotential, namely EC(U1), EC(U2) and EC(I). Note that the EC(U2) pseudopotential parameters are extracted from an AIP document in Ref. [54] of Ref. [7]. However we could only work with EC(U2) for liquid Ag. According to our knowledge, there is no published parameter of EC(U1), EC(I) for Ag. Firstly, we choose the Z_{eff} values of liquids Ag and In for the parametrisation of the density dependent universal version of EC pseudopotential, namely EC(U2), it is well known that the effective valence Z_{eff} takes non-integer values in transition and less simple metals to account for s-d hybridisation [2]. For the choice of Z_{eff} values, we have searched which values of Z_{eff}, within the above range, predict the best result for g(r) comparing with experiment. For this purpose, we have changed Z_{eff} from 1.3 to 1.1 for In, 1.5 to 1 for Ag. We have noted that Bhuiyan and co-workers have studied with the Z_{eff} values of 1.3 for In in their BS model potential calculations [24]. Thus for comparison, we shall use a couple of sets of α, Z_{eff}, R values of EC(U2) model potential for each metal. The obtained the EC(U2) parameters for liquids Ag and In are reported in Table 1.

Table 1. Thermodynamic states studied in this work, temperature T, number density n and pseudopotential parameters for EC (U2) model, α and R (a.u: atomic units).

Metal	T(K)	n (atoms/Å^3)	Z_{eff}	α (a.u.)	R (a.u.)
In	433	0.0369	1.1	3.984	0.402
			1.3	3.734	0.409
Ag	1273	0.0518	1.0	4.575	0.326
			1.5	3.915	0.345

Fig. 1 shows the calculated effective pair potentials for In issued from the three specified version of the Fiolhais' potential comparing with those obtained from other local pseudopotentials such as BS and LHA using the IU screening function where we have changed Z_{eff} from 1.3 to 1.1.
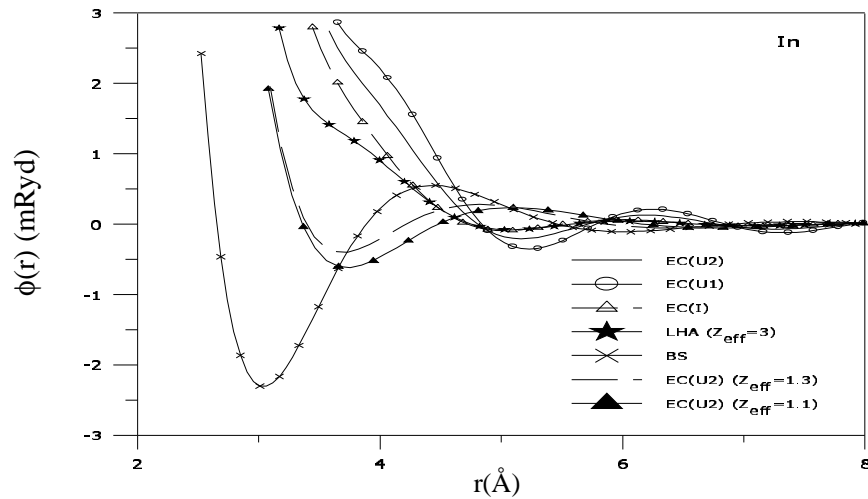
Fig. 1. Interatomic pair potentials for liquid In.

The input parameters of the EC(I) and EC(U1) model potentials are taken from Fiolhais *et al.* [6] without changing the values of the parameters for $Z_{eff} = 3$. For the LHA and BS model potential parameters are taken as the same as in Ref. [14] and Ref. [24], respectively. We have noted that IU screening give rise to a deep potential well for all model potentials for In while LDA yields a shallow well. It appears in Fig. 1 that a noticeable positive first minimum also present in the case of LHA, EC(U1) but not so pronounced for EC(U2) with $Z_{eff} = 3$. We have also pointed out in our previous calculations [21,23] that this is a typical feature of the Fiolhais' potentials. It was reported in the literature that the positive first minimum on the interionic potential has been observed for liquid polyvalent metals with suitable combination of pseudopotentials and local field corrections [35]. However this typical feature has not been observed for the effective pair potentials calculated with $Z_{eff} = 1.1$ and 1.3 using the EC(U2) and EC(I) model potentials and BS pseudopotential. It can be seen in Fig. 1 that the positive first minimum of LHA potential and the first minimum of both calculated EC(U2) pair potentials for $Z_{eff} = 1.1$ and 1.3 are around 3.7A. It is seen that Fiolhais *et al.* effective pair potentials are shallower than that of BS potential. It can be pointed out that the parametrization (individual or universal) modifies both the depth of the potential and the hardness of the repulsive part or the core size in the case of In.
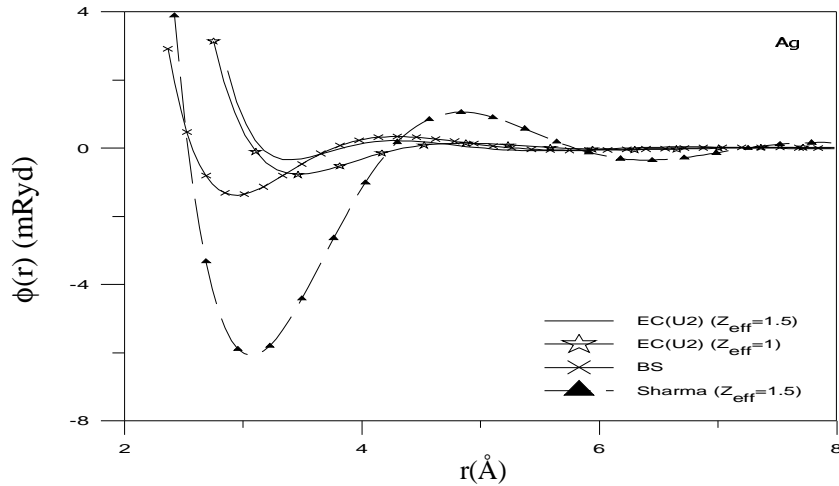
Fig. 2. Interatomic pair potentials for liquid Ag.

In Fig. 2 we have also compared the calculated the EC(U2) effective pair potentials of liquid Ag with those obtained from both the BS [4] and Sharma [34] model potentials using IU screening where we have changed Z_{eff} from 1.5 to 1. Those potential parameters are from Ref. [5] and Ref. [34], respectively. It appears in Fig. 2, the depth of the EC(U2) potentials are shallower than those of BS and Sharma. The position of the EC(U2) potentials are displaced towards slightly larger values of r. To test the adequacy of the Fiolhais' potentials, it is now desirable to use the three calculated interionic potentials in order to obtain some structural properties of liquid In and Ag such as the static structure factors and pair distribution functions. We would like to make a qualitative comparison of the structure evaluated by employing the VMHNC liquid state theory with other published studies. These EC potentials are used as input data in our structural calculations. We have used the VMHNC liquid state integral equation theory for simple metals to solve the OZ equation with MHNC closure relation using Zerah's algorithm [36]. In order to show the influenced of the effective valence on g(r), in Fig. 3 we present the pair distribution function g(r) of liquid In calculated with the pair potentials corresponding to $Z_{eff} =1.3,\ 1.1$, comparing with the experimental data of Waseda [22]. Fig. 3 shows that the height of the first peak of g(r) with $Z_{eff} =1.1$ seems to be underestimated while it is overestimated in the case of $Z_{eff} =1.3$. For the results of BS model potential, it is shifted slightly toward smaller q values as compared with experimental data. We note that the effective pair potentials with $Z_{eff} =3$ give unsatisfactory results for liquid In using the presented parameters of EC potential. However the EC(U2) version with $Z_{eff} =1.1$ gives the best prediction of g(r) for liquid In.
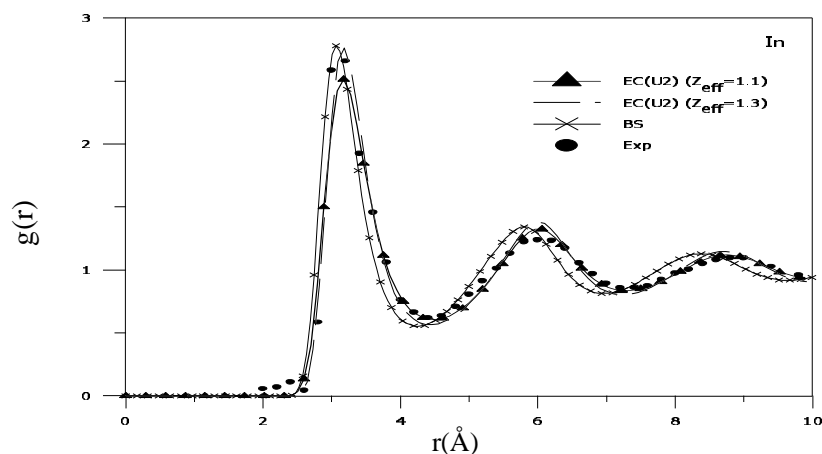

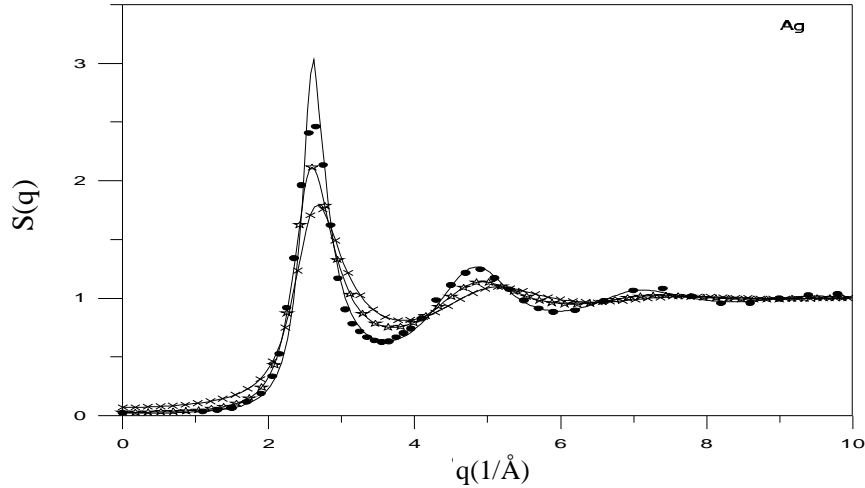Fig. 3. Pair distribution functions for liquid In at T= 433 K.

Fig. 4. Structure factors for liquid Ag at T=1273 K. (same labeling as in Fig. 2).

The VMHNC results of S(q) for liquid Ag are shown in Fig. 4. Except the height of the first peak, the agreement between our VMHNC results and those obtained with the EC(U2) model potential for $Z_{eff} = 1.5$ and experiment is very good. We can see in Fig. 4 that the low-q behavior of S(q) is well described whatever the density dependent universal version of Fiolhais *et al.* potential used. As compared to other theoretical works for Ag, our results of S(q) stemmed from the EC(U2) model are better than those of Bhuiyan *et al.* [24] obtained from the BS local pseudopotential. It should be noted that the position of the first peak of S(q) is quite well predicted by the universal EC potentials. The agreement between theoretical and experimental results of g(r) for liquid Ag- not shown here is reasonably good, especially for EC (U2) model. We have noted that the structure of both pure liquids Ag and In near their melting points are well described with the EC(U2) Fiolhais' pair potentials using the IU screening. The EC(U2) parameters with $Z_{eff} = 1.1$ for In and $Z_{eff} = 1.5$ for Ag predict the best result for g(r) comparing with experiment. These EC(U2) potential parameters are used in our liquid Ag-In alloy calculations. The largest difference between the results predicted by the different potentials appears at low q values. The experimental value of S(0) for liquid Ag and In is almost exactly reproduced by the EC(U2) potential. We also note that whereas the LHA and Sharma pseudopotentials underestimate S(0) the BS one overestimates it. We now turn to structural properties of liquid binary Ag_x-In_{1-x} alloys at the specific thermodynamic states given in Table 2.

Table 2. Input data for liquid $Ag_x In_{1-x}$ alloys.

Substance	Z_{eff}	T(K)	n_{alloy} (atoms/ Å^3)	α_1(a.u.)	α_2(a.u.)	R_1(a.u.)	R_2(a.u.)
$Ag_{80}In_{20}$	1.42	1123	0.0494	3.889	3.886	0.349	0.425
$Ag_{70}In_{30}$	1.38	1023	0.0490	3.889	3.886	0.349	0.425
$Ag_{70}In_{30}$	1.38	973	0.04792[a]	3.943	3.926	0.338	0.415
$Ag_{50}In_{50}$	1.30	873	0.0456	3.889	3.886	0.349	0.425
$Ag_{20}In_{80}$	1.18	623	0.04002[a]	3.981	3.964	0.331	0.407
$Ag_{20}In_{80}$	1.18	873	0.0363	3.889	3.886	0.349	0.425

[a]These values are the average number densites.

Where the alloy number densities for three composition of Ag-In system are taken from Ref. [4] into Ref. [27]. These values used in our effective pair potential calculations. Furthermore, for

comparison with previous calculations [5,26] we have obtained the pair potentials for x = 0.2 and 0.7 of Ag concentration in Ag_x-In_{1-x} alloy at 623 K and 973 K, respectively. The average number densities at there thermodynamic states are computed from the pure number densities of two component species. The corresponding number densities n_1 and n_2 of Ag and In at these two temperatures are taken from Brandes [37]. The parameters of the elemental systems for the EC(U2) potential given in Table 1 have been adopted for the further use in the present study of alloy.

The interatomic partial pair potentials $\phi_{AgAg}(r)$, $\phi_{AgIn}(r)$ and $\phi_{InIn}(r)$ obtained from equation (6) with the EC(U2) potentials for different Ag compositions are shown in Figs. 5(a,b). The calculated pair potentials of Ag-In liquid alloy for $Ag_{20}In_{80}$ at 873 K using the number density given in Table 2 are illustrated in 5(a). In Fig. 5(b) we present the results of effective pair potentials for liquid $Ag_{70}In_{30}$ alloy at 973 K.

It can be seen in Fig. 5 that the pair potentials for two different alloy composition exhibit rather different trends with each other. From Figs. 5(a), it is clear that the depth of the primary potential well of $\phi_{InIn}(r)$ is shallower than that of $\phi_{AgAg}(r)$. This tendency is also observed in the case of $Ag_{20}In_{80}$ liquid alloy at 623K in which the EC(U2) pair potentials calculated with the average number density taken from Ref. [5].

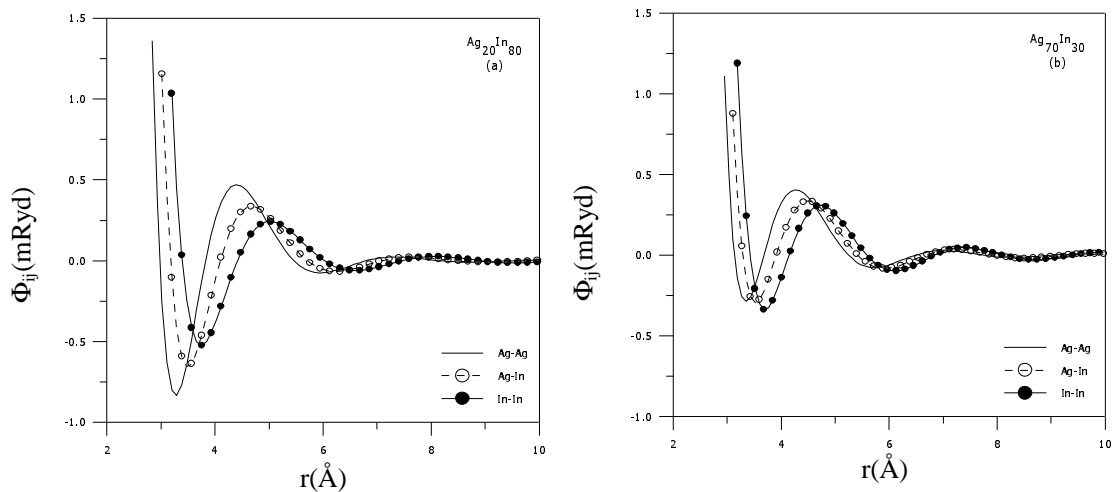Fig. 5. Interatomic pair potentials: (a) $Ag_{20}In_{80}$ at 623K, (b) $Ag_{70}In_{30}$ at 973 K.

We have to note that these observations disagree with Khaleque and co-workers but agree with the analysis of the profiles of pair distribution functions calculated at the same thermodynamic states. On the other hand, it can be seen in Fig. 5(b), the potential $\phi_{InIn}(r)$ is deeper than that of $\phi_{AgAg}(r)$. Our results presented for $Ag_{70}In_{30}$ liquid alloy are in good agreement with those obtained with BS model potential by Khaleque *et al.* [5]. We have also found the same trend in the pair potentials calculated with the alloy density taken from [27] for $Ag_{70}In_{30}$ liquid alloy.

The AL partial structure factors for Ag_xIn_{1-x} liquid alloys have been calculated by using the EC(U2) pair potentials with the VMHNC liquid state theory. In Fig. 6, we present the AL partial structure factors $S_{ij}(q)$ for $Ag_{20}In_{80}$ at 623 K along with the experimental data of Arai [26].

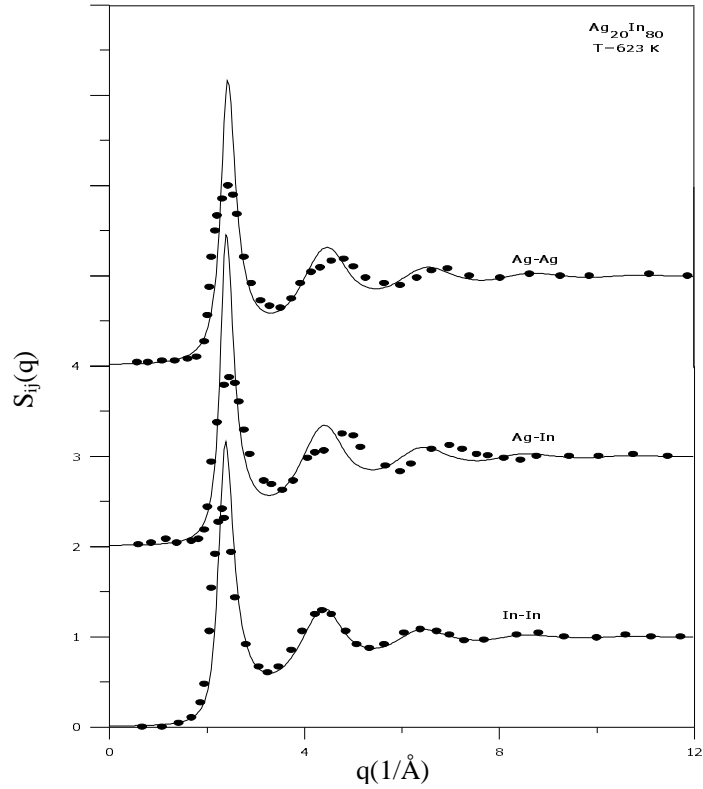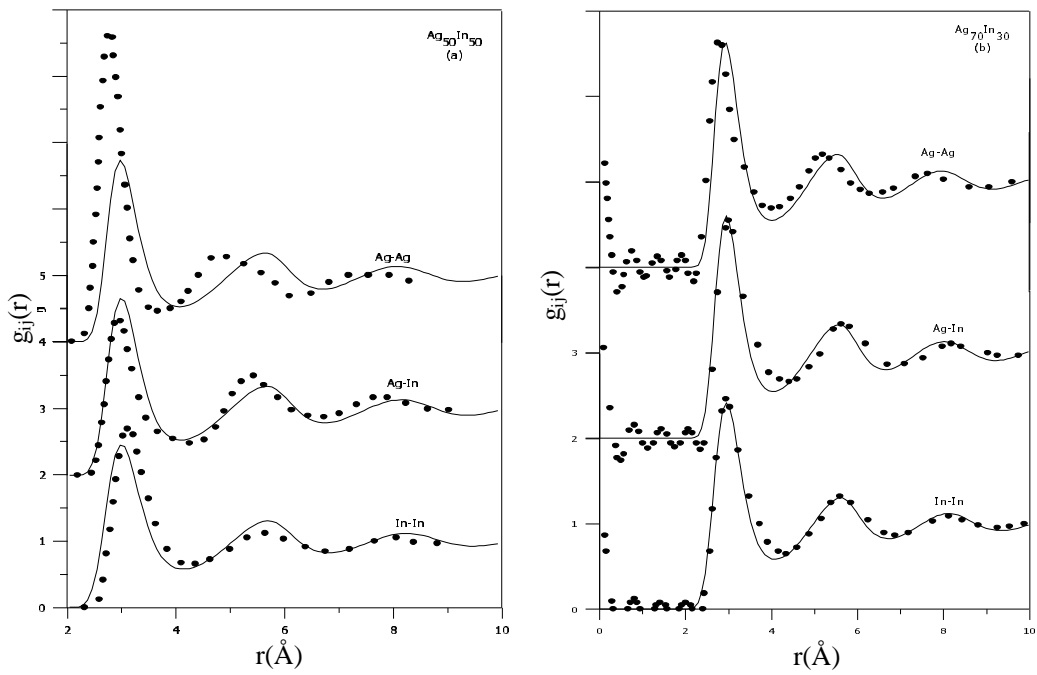Fig. 6. The partial structure factors for $Ag_{20}In_{80}$ liquid alloy at 623 K.

Fig. 7. The pair distribution functions (a) $Ag_{50}In_{50}$ at 873 K, (b) $Ag_{70}In_{30}$ at 973 K.

The pair distribution function $g_{ij}(r)$ for Ag-In binary alloys are shown in Figs. 7(a,b) for x=0.5 and 0.7, respectively. For x= 0.7, $g_{AgAg}(r)$ has the largest peak, $g_{InIn}(r)$ has the smallest and $g_{AgIn}(r)$ has values in between. The reason is that the alloy is rich in Ag for x= 0.7, thus the probability of finding a Ag ion near another Ag ion is larger. It is expected that x decreases $g_{InIn}(r)$ increases and consequently $g_{AgAg}(r)$ decreases. We have found for x= 0.5, $g_{InIn}(r)$ has the largest peak. This behaviour is observed for the hard sphere partial distribution functions with BS model potentials [25]. However Mendelev [27] has presented in the computer simulation of Ag-In liquid alloys structure that $g_{AgAg}(r)$ has the largest height of the first peak and its increase as the Ag fraction is decreased in the range from 60% to 10%. For x= 0.2, it is found that $g_{AgIn}(r)$ has the largest peak, as expected with experimental data of Arai [26]. Anyway, the universal version of EC potential with VMHNC can explain the correct behaviour of Ag-In liquid alloys.

4. Conclusions

We have examined the test of the transferability of EC potential in the case of less simple liquid metals and metal alloys. We have also calculated the static structure for different Ag concentration of liquid Ag-In alloys in conjunction with the VMHNC. The overall agreement with experimental data is good. The analysis of the results confirms the ability of the EC(U2) potential to describe the interactions in less simple metals and alloys. In this work, the density dependent universal version of Fiolhais *et al*. pseudopotential and IU screening with VMHNC seem to be a good association since they provide a quite satisfactory description of the structural properties for Ag-In liquid alloys in the whole set of thermodynamic states studied. It is the first time that the correct tendency is shown for $Ag_{20}In_{80}$ liquid alloy, as expected from the experimental data.

Acknowledgements

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