OPTOELECTRONİCS AND ADVANCED MATERİALS – RAPİD COMMUNİCATİONS Vol. 1, No. 3, March 2007, p. 108 - 112

Structure of liquid CdTe alloys using local evanescent core pseudopotential

S. DALGIC*, M. COLAKOGULLARI
Department of Physics, Trakya University, 22100, Edirne, Turkey

There are presented the results of a test of transferability of the local evanescent core (LEC) pseudopotential proposed by Fiolhais *et.al.* to the chalcogen liquid alloys. The test is a comparison of the static structure of simple liquid metals and liquid CdTe alloys with the experimental results. The structural properties are calculated using the Variational Modified Hypernetted Chain (VMHNC) liquid state theory. It has been found that the liquid structure obtained using the LEC pseudopotential is in better agreement with the experimental data than other potentials.

(Received November 12, 2006; accepted February 14, 2007)

Keywords: Liquid Cadmium Telluride, Local evanescent core, Liquid structure

1. Introduction

Among II-VI semiconductors, CdTe is of special technological interest. Cadmium, Telluride and its alloys are employed to fabricate a wide array of electro-optic devices, high-performance infrared detectors and room-temperature radiation detectors. The II-VI compounds are materials which exhibit many interesting solid-state phenomena of considerable practical importance. The compound CdTe can be considered as quite representative of this group. Indeed, the recent growing scientific and technological interest on CdTe arises from its peculiar physical properties. For example, its mechanical, chemical and thermal stability. Moreover, CdTe is a promising material for electronic and optical devices made of can be used in photovoltaic energy conversation, infrared, X- and γ-ray detectors and solar cell [1,2].

Besides being a technologically important compound, liquid CdTe (l-CdTe) also presents an interesting subject for fundamental studies. In the liquid phase CdTe is among those II-VI semiconductors that exhibit properties which are quite different from those of liquid IV and III-V semiconductors. Liquid CdTe was studied by neutron diffraction near its melting point [3] and the structure of melts was simulated by statistical thermodynamics techniques with use the Monte Carlo Method [4]. Note that CdTe only weakly dissociates in molten state. Therefore the interatomic bonds exhibit a predominantly covalent character of [5].

In this work, we are concerned with a local evanescent core (LEC) type model pseudo-potential of Fiolhais *et.al.* [6]. The pseudo-potential contains two parameters R and α which are chosen by using either the conventional crystal structure (individual parameters (LEC(I))) or fcc structure (universal parameters (LEC(U1))). Another version of the local evanescent pseudopotential [LEC(U2)] model in which the parameters R and α depend on the valence Z and the average electron density ρ, namely $R(r_s,Z)$ was proposed by Nagueira, Fiolhais and Perdew [7].

On the other hand, empirical interatomic potentials have proven to be efficient for calculations of physical properties of liquid semi-conductors such as CdTe. Three body Tersoff empirical potential has been developed in order to study the structural, elastic and thermodynamic properties of CdTe by molecular dynamics [8]. The Analytic Modified Embedded Atom Method (AMEAM) has been applied to the study of the structural and thermodynamic properties of CdTe using the Variational Modified Hypernetted Chain (VMHNC) with effective pair potentials based on AMEAM [9].

Motivated by the success of the transferable local pseudopotential of Fiolhais *et.al.* to predict the static structure of liquid metals and metal alloys, we examine to extent to which it can be transferred successfully from the solid state to liquid semiconductors for considering the structural properties of CdTe. According to our knowledge, the Fiolhais type pseudopotential has been first applied to liquid chalcogenide alloy. In the present paper, we have report first the results for the structure and thermodynamics of CdTe using Fiolhais type LEC(U2) potentials in conjunction with VMHNC approximation. In our previous works, we have been shown that the Fiolhais pair potential is transferable for liquid alkali and alkaline earth metals [10]. We have successfully applied to estimate the structural properties of liquid Li-Ba and Ag-In alloys very accurate integral equation of VMHNC [11, 12].

The structure of the article is the following: After this introduction a brief description of the theory is given in the next section. Moreover, in the third section, the results are presented and compared with the available experimental data and theoretical works. Finally, our conclusion is given in the last section.

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

$$\widetilde{\phi}_{ind}(q) = \chi(q) \left| \widetilde{v}(q) \right|^2 \ , \tag{2}$$

where $\widetilde{\mathrm{v}}(\mathrm{q})$ 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. We employ the well known local field corrections of the Ichimaru-Utsumi (IU) [13] and the local density approximation (LDA) version of the local-field function G(q) with the correlation energy of Vosko-Wilk and Nussair (VWN) [14]. 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 local evanescent core (LEC) pseudopotential. An analytic expression for the form factor of this pseudopotential in Fourier space

$$\widetilde{v}(q) = 4\pi Z_{eff} R^2 \left[-\frac{1}{(qR)^2} + \frac{1}{(qR)^2 + \alpha^2} + \frac{2\alpha\beta}{\left[(qR)^2 + \alpha^2\right]^2} + \frac{2A}{\left[(qR)^2 + 1\right]^2} \right] \tag{3}$$

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

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

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.

A simple liquid semiconductor alloy, A_xB_{1-x}, may be regarded as an assembly of A-type and B-type bare ions with charges Z_{eff}^A and Z_{eff}^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

$$\phi_{ij}(r) = \frac{Z_{eff}^i Z_{eff}^j}{r} + \phi_{ps}^{ij}(r) \tag{5}$$

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

$$\phi_{ps}^{ij}(q) = \chi(q) \widetilde{v}_{ps}^i(q) \widetilde{v}_{ps}^j(q) \tag{6}$$

Here, $\chi(\mathrm{q})$ 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. In our structural calculations, one of the integral equation theories which has shown to be very reliable theory of liquids, VMHNC, has been used [15-17]. 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)

$$h_{ij}(r) = c_{ij}(r) + \sum_{l=1}^{2} \rho_l h_{il}(r) * c_{lj}(r) \tag{7}$$

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_l denote the partial ionic number densities. The exact closure relation is given by

$$c_{ij}(r) = h_{ij}(r) - \ln g_{ij}(r) - \beta\phi_{ij}(r) - B_{ij}(r) \tag{8}$$

where $\phi_{ij}(r)$ are the interatomic pair potentials and the $B_{ij}(r)$ denotes the Percus-Yevick (PY) hard sphere bridge functions for binary system.

Formally, the generalization of liquid state from monatomic to binary fluids, we have now a set of three coupled integral equations relating the partial pair distribution functions $g_{ij}(r)$ to the pair potentials $\phi_{ij}(r)$. The partial pair distribution functions are related to Ashcroft-Langreth (AL) partial structure factors $S_{ij}(q)$ for i and j species in the following way

$$g_{ij}(r) = 1 + \frac{1}{8\pi^3 (\rho_i \rho_j)^{1/2}} \int \left(S_{ij}(q) - \delta_{ij} \right) \exp(-i\vec{q}.\vec{r}) dq \tag{9}$$

where ρ_i being the number density of *i* species. We obtain the total distribution function as a linear combination of the partial distribution functions and normalized by the scattering lengths for equiatomic concentration

$$g_{total}(r) = \frac{\alpha_i^2 g_{ij}(r) + 2\alpha_i\alpha_j g_{ij}(r) + \alpha_j^2 g_{ij}(r)}{\alpha_i^2 + \alpha_j^2} \quad (10)$$

where the α_i and α_j are the scattering length and these values are given 7.5 and 5.8 respectively.

3. Results and discussion

We have calculated the effective pair potentials based on LEC(U2) pseudopotential functions for liquid Cd and Te. The pair potential calculations are performed at T = 623 K for Cd and T = 843 K for Te, near melting temperatures of Cd and Te. The presentation of the results is divided into two parts: the first one concerns the pure simple liquid metals. The structural properties of liquid Cd and Te for which experimental results near their melting points are available and the second one deal with structure of Cd-Te liquid semiconductor alloy at equiatomic concentration. We show in Table 1 the relevant input data for liquid metals and alloy. The input temperature and corresponding number densities are taken from Waseda [18] given in Table 1 for liquid metals. Alloy density and temperature are taken from Glazov [19].

Table 1. The input parameters for potential.

Metals	$Z_{eff.}$	ρ (Atoms/A^3)	α	R (a.u.)	T (K)
Cd	1.50	0.0428	3.73718	0.38336	623
Te	2.00	0.0270	3.24210	0.49332	843
CdTe	1.05	0.0294	3.99784	0.42184	1373

The calculated the effective pair potentials are shown in Fig. 1 for liquid Cd and Te. We see that, whereas Cd has an attractive pair potential of about -0.21 mRyd at the nearest neighbours distance, Te has a repulsive pair potential of about +0.45 mRyd. Thus, the effective pair potential contribution to the total binding energy in Te is repulsive not attractive as for Cd. These potentials give the correct trend at larger r values.

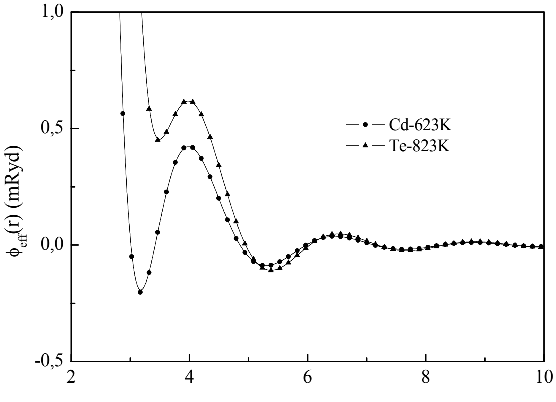

Fig. 1. The effective pair potentials for liquid Cd and Te.

Calculated static structure factors for liquid Cd and Te are shown in Figs. 2a and 2b together with experimental data of Waseda [18]. In the case of Cd, as shown in Fig. 2a, represented structure factor has a principle peak located at the same position of the experimental one. But for Te the calculated main peak is somewhat shifted. We also find that the oscillations in the calculated structure factor die out more rapidly than experimental data for liquid Te. Also in these figures insets show the pair distribution functions for liquid Cd and Te (experimental data). In contrast to Cd, the height of the calculated main peak of g(r) for Te is underestimated. The calculated g(r) of Cd is in good agreement with experiment.

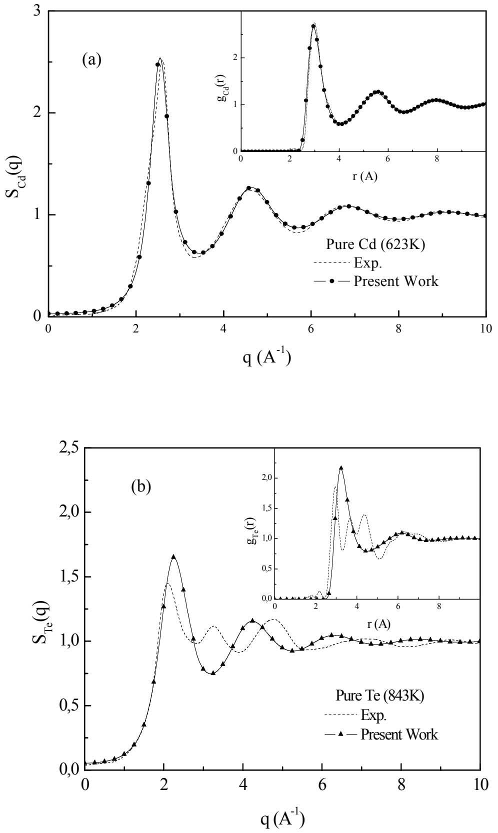

Fig. 2. The static structure factors for (a) liquid Cd and (b) liquid Te. Insets are shown the radial distribution functions.

Using the number density and Z_{eff} given in Table 1 for l-CdTe, the effective pair potentials $\phi_{CdCd}(r)$, $\phi_{CdTe}(r)$ and $\phi_{TeTe}(r)$ obtained from equation (5) with the LEC(U2) pseudopotentials for equiatomic concentration are shown in Fig. 3a. It is clear that the depth of the primary potential well of $\phi_{TeTe}(r)$ is shallower than that $\phi_{CdCd}(r)$. The $\phi_{CdTe}(r)$ is located between Cd-Cd and Te-Te potentials and this potential is the superposition both of them. To test adequacy of the Fiolhais' potentials, it is now desirable to be used to calculate effective pair potentials in order to obtain some structural properties of semiconductor liquid

CdTe such as the static structure factors and pair distribution functions.

The partial static structure factor for CdTe liquid alloy has been calculated by using the LEC(U2) pair potentials with the VMHNC liquid state theory. In Fig. 3b we present the partial structural factors for Cd-Te at 1373K along with the experimental data of Gaspard *et.al.* [3]. Qualitative similarity between Cd-Te partial structural factors and experimental curve is fairly obvious, although the amplitudes are radically different. We also find that the oscillations in our calculated $S_{CdTe}(q)$ die out more rapidly than in the experimental data. It is suggested a too soft repulsive potential. Anyway, the LEC(U2) pseudopotentials conjunction with VMHNC can explain the correct behaviour of CdTe alloy.

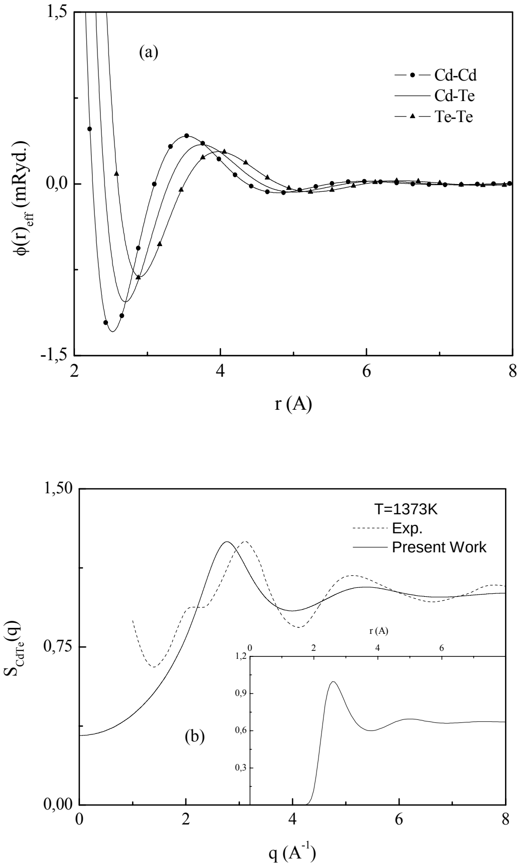

Fig. 3.(a) Effective pair potentials for liquid CdTe alloy (b) Partial static structure factor and total radial distribution function for l-CdTe alloy.

The total correlation function for CdTe alloy is plotted in inset of Fig. 3b. It was used to calculate to coordination number in l-CdTe. We used the known formula: $N = \int_0^{r_{\min}} r^2 g_{Total}(r)\,dr$ where $r_{\min}$ is usually taken to be the position of the first minimum in the $g_{total}(r)$ for a given temperature. Here $r_{\min}$=3.76A. It gives the coordination number: N=3.94. This is very close to the number for a tetrahedral structure and corresponds to zinc-blende structure. The values obtained from two different experimental data given in Refs. [3,20] are 3.3 and 4.4, respectively.

4. Conclusion

We have examined the test of the transferability of LEC(U2) pseudopotential in the case of II and VI metals respectively and II-VI semiconductor liquid alloy. The structural calculations were carried out using Fiolhais' potential with the VMHNC theory of liquid. We have also calculated the static structure for l-CdTe alloy in conjunction with VMHNC. Comparison between the results of the VMHNC theory and available experimental data show that the proposed LEC pseudopotential formalism for l-CdTe alloy system is able to give a good description of the liquid state of the CdTe.

Acknowledgments

We gratefully acknowledge S. S. Dalgic and L. E. Gonzalez for discussions on all aspects on this work.

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[*] Corresponding author: dseyfe@yahoo.co.uk