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Molecular dynamics simulations of liquid GeSe alloy: the first application of Modified Analytic Embedded Atom Method (MAEAM)

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We present the results of molecular dynamics (MD) simulations of liquid GeSe alloy near melting point using an effective pair potential based on modified analytic embedded atom method (MAEAM). The potential functions of MAEAM are parameterized by fitting to both solid and liquid state properties of pure Ge and Se. MD simulations have been performed to investigate the structure and the dynamical properties of liquid GeSe alloy. We have compared the total structure factor and pair correlation function, obtained in the MD simulations to the results of self consistent integral equation theory of Variational Modified Hypernetted Chain (VMHNC), experiment and other MD results. To describe the atomic dynamics in l-GeSe, we calculate the diffusion coefficient D which is directly related to the mean square atomic displacement. Viscosity of the liquid alloy is estimated by Stokes-Einstein formula. On the other hand, the MD results of dynamics in l-GeSe are compared with those obtained by the viscoelastic theory of fluids. The collective dynamic properties such as the intermediate scattering function and the dynamic structure factor have determined. We have analyzed the behaviour of self dynamic-structure factor computed in the frame of the viscoelastic model.

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1. Introduction

Liquid mixtures of the chalcogenide systems such as Ge-Se, are preferred semiconducting materials for applications. They have well-defined niches in optics [1], optical recording [2] and other technologies. For several decades, the GeSe compounds have attracted the interest of many researchers because of high glass-forming ability of materials, e.g. most experimental as well as theoretical studies dealt with $GeSe_2$, for which the glass formation is easiest [3, 4]. The GeSe system was the first in which formation of an intermediate phase was demonstrated experimentally by Boolchand *et. al.* [5] and further developed theoretically by Thorpe *et. al.* [6]. Upon melting, GeSe remains semiconductor, which distinguishes it from all III-V and some II-VI semiconductor compounds. Ge and Se have close atomic numbers and sizes and for natural isotropic abundances their coherent neutron scattering lenghts are similar It is not therefore possible to resolve the local coordination environments of Ge and Se by using conventional neutron or x-ray diffraction methods to measure total structure factors. A recent *ab initio* molecular dynamics study by Raty *et.al.* [7] analyzed distance correlations and dynamics of liquid GeSe, confirming the local order of the liquid to be close to that of low-temperature crystalline phase.

The object of this paper is to present the structure factors, pair correlation function and dynamics of the liquid semiconductor GeSe by molecular dynamics simulation and an integral equation theory. Both of methods used in this work, the construction of effective potential plays the most important role to explain of interaction between interacting particles. Empirical descriptions of interatomic potentials have been widely used in computer simulations and theoretical calculations of various crystalline structures of metals. Many of scientists in material science great interest many body potentials based on the embedded atom method (EAM) which was originally proposed by Daw and Baskes [8]. In literature there are several versions of EAM which differ by parameterisation methods and functions involved. Recently Fang et al. [9] have been constructed interatomic potentials for binary immiscible alloys systems with modified analytic EAM (MAEAM) based on the Johnson's analytic EAM [10]. They have demonstrated that MAEAM may be a reasonable method for those systems by comparing with other EAM potential models. Although the EAM primarily developed for the solid phase has also been used in liquid structure calculations with molecular dynamics (MD) simulations or integral equation theories in order to check the accuracy of the forms chosen for the EAM potential functions and of the method used for their parameterisation. Some researchers have shown that one of the integral equation theories namely, the variational modified hypernetted chain liquid state theory (VMHNC) [11,12] successfully applied to liquid metallic systems in the EAM calculations [13-16]. However less attention has been devoted the structure and dynamics of liquid chalcogenide metals in the EAM calculations. At a more fundamental level, the first question is that the same EAM potentials fitted to the physical properties in the solid phase are capable of providing a good description of structure, dynamic and atomic transport properties of liquid chalcogenide metals and alloys. This problem concerning the EAM needs more work on these systems. For this reason, the principal aim of this paper is to examine the transferability of the EAM based effective potentials in the investigation of the structure and dynamic properties of liquid chalcogenides and their alloys within the molecular dynamics (MD) simulation and the liquid state theories.

In a recent series of articles [13-16], we were concerned in the issue transferability of EAM potentials for chalcogenides to the liquid environment. It appears to be successfully transferable of MAEAM and AMEAM versions in the case of some liquid chalcogenide alloys such as, K-Te, Cd-Te and As-Te alloys, respectively. This applicability was checked on structural properties and also on some dynamical ones such like the diffusion coefficient in conjunction with the VMHNC liquid state theory. However, the applicability of the EAM based effective potentials in the structural calculations of liquid chalcogenide alloys has not completed yet. To our knowledge, no liquid structural calculations have been performed on GeSe using the EAM based effective pair potentials coupled with integral equation theories. Our study comprises two steps: first, the construction of the effective interatomic pair potentials in the liquid alloy from EAM potentials, and, second, the calculation of the liquid structure from these interatomic interactions, by using both a liquid state theory and MD simulations.

In this paper we propose an effective pair potential based on the EAM which is capable of predicting both the structure and some atomic transport properties of liquid Ge, Se and equiatomic GeSe alloys. We report the results of MD and VMHNC calculations of the static and dynamic properties of liquid GeSe using the MAEAM model.

2. Theoretical formalism

2.1 Effective potentials and liquid state theory

In the original EAM, the total energy of atomic structure of the system can be expressed as sum of two terms, a many-body term, which depends on the electron density distribution function of atom f(r), a two-body term $\phi(r_{ij})$, which depends on the interatomic distances r. The different versions of EAM have been constructed by adding a modification term due to the difference between the actual total energy of a system of atoms and that calculated from the original EAM using a linear superposition of spherically averaged atomic electron densities [10].

In the MAEAM [9], a modified energy term M(P) is added to the total energy expression as,

$$E_{tot} = \sum F(\rho_i) + \frac{1}{2}\sum \phi(r_{ij}) + \sum M(P_i) \tag{1}$$

where energy modification term $M(P_i)$ is taken from Ref. [9] and $F(\rho_i)$ is the embedding energy function,. The argument of the energy modification term P_i is given in terms of the one electron density function of f(r) as in ref [9]. The embedding function $F(\rho_i)$ takes the same form as those used by Johnson and Oh [17]:

$$F(\rho_i) = -F_0\left[1 - n\,ln\left(\frac{\rho_i}{\rho_e}\right)\right]\left(\frac{\rho_i}{\rho_e}\right)^n \tag{2}$$

where $F_0 = E_c - E_{1f}$. E_c is the cohesive energy and E_{1f} is the unrelaxed vacancy formation energy of metal. ρ_e takes its equilibrium value and can be determined from $\rho_e .= 12f_e$ as Ref[18]. In order to describe the interactions between particles, we used two different pair potential forms. The first form of these pair potentials used in the theoretical calculations based on integral equation theory are given as:

$$\phi(r_{ij}) = \sum_{m=-1}^{6} k_m \left(\frac{r_{ij}}{r_{1e}}\right)^m \tag{3a}$$

where r_{1e} is the value of the nearest neighbour distance at equilibrium. In order to perform MD simulations, we proposed a new pair potential formed as :

$$\phi(r_{ij}) = k_1\left(\frac{r_{ij}}{r_{1e}}\right)^{-1} + k_2\left(\frac{r_{ij}}{r_{1e}}\right)^{2} + k_3\left(\frac{r_{ij}}{r_{1e}}\right)^{4} \tag{3b}$$

We reparameterized potential functions based on the MAEAM proposed by Fang *et.al.* [9] to apply liquid GeSe. In the present model, the atomic interactions up to r_c distance are considered. $\phi(r)$ is truncated at r_c about 1.9a. At this point, the pair potential and electron density function and their slopes are zero at cut-off distance:

$$\begin{aligned} \phi(r_c) &= 0, \qquad \phi'(r_c) = 0 \\ f(r_c) &= 0, \qquad f'(r_c) = 0 \end{aligned} \tag{4}$$

There is an equation for cohesive energy E_c as follows:

$$-E_c = \frac{1}{2}\sum_m \Phi(r_m) - F_o \tag{5}$$

In above equations, α and n can be determined from the following equations:

$$E_{EOS}(a^*) = \frac{1}{2}\sum \Phi(r_c) + F(\rho_c) + M(P_c) \tag{6}$$

where $E_{EOS}(a^*)$ is Rose's equation of state [19] for the cohesive energy and a* is the reduced lattice constant. In order to construct the effective interatomic pair potential from the EAM, second and higher derivatives of the embedding function F are ignored. The recently proposed effective pair potential form based on the Finnis – Sinclair (FS) approximation from the MAEAM can be given as in Refs. [13-16] by

$$\phi_{eff}^{AB}(r)=\phi_{AB}(r)-2F'_{AB}(\rho)f_{AB}(r)M_{AB}(P_{AB}) \qquad (7)$$

where the alloy pair potential $\phi^{AB}(r)$ between different atomic species is taken as:

$$\phi^{AB}(r)=\frac{1}{2}\left[\frac{f^{B}(r)}{f^{A}(r)}\phi^{AA}(r)+\frac{f^{A}(r)}{f^{B}(r)}\phi^{BB}(r)\right] \qquad (8)$$

where *AA* and *BB* indicate *A* and *B*, type atoms in a binary alloy respectively. $\phi^{AA}(r)$ and $\phi^{BB}(r)$ are the monatomic potentials given by Eqs. (3a-b). In the above equations:

$$f_{AB}(r)=f_{e\,AB}\left(\frac{r_{1e\,AB}}{r}\right)^{6} \qquad (9)$$

where $r_{1eAB}=(r_{1eAA}+r_{1eBB})/2$, $f_{eAB}=(f_{eAA}+f_{eBB})/2$, The modification term of alloys can be given as

$$M_{AB}(P_{AB})=\alpha_{AB}\left\{1-exp\left[-\left(ln\left|\frac{P_{AB}}{P_{e\,AB}}\right|\right)^{2}\right]\right\} \qquad (10)$$

where $\alpha_{AB}=(\alpha_{AA}+\alpha_{BB})/2$, $P_{eAB}=(P_{eAA}+P_{eBB})/2$ and $P_{AB}=\sum_{j}f_{AB}^{2}(r_{ij})$.

With the effective pair potential known, integral equations are able to provide us the liquid structure for metals and alloy. In our structural calculations, one of the integral equation theories which have shown to be very reliable theory of liquids VMHNC has been carried out [11,12]. Like most liquid state theories the VMHNC solves the Ornstein – Zernike (OZ) equation for binary system 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. The OZ equation is supplemented by the exact closure relation. The partial static structure factor, $S_{ij}(q)$, for binary alloys can be written as Fourier transform of partial distribution functions:

$$S_{ij}(q)=\delta_{ij}+4\pi(\rho_i\rho_j)^{1/2}\int\left(g_{ij}(r)-1\right)\frac{sin(qr)}{q}rdr \qquad (11)$$

The theoretical calculations can be compared with neutron or X-ray scattering experiments if the appropriate scattering parameters are known. The total pair distribution for any concentration of alloy can be written by a linear combination of three partial pair distribution functions $g_{11}(r)$, $g_{12}(r)$ and $g_{22}(r)$.

The transport coefficients are the important parameters for characterizing of the liquids. We are interested in for one-component and binary systems. The basic magnitude to be considered is the intermediate scattering function F(q,t), which describes the collective dynamic behavior of the system and is defined as $F(q,t)=<\rho(t)\cdot\rho(0)>$, where $\rho(t)$ is the microscopic number density. The dynamic structure factor *S*(q,w) is obtained from the corresponding intermediate scattering functions, F(q,t) by passing to the Fourier domain:

$$S_{ij}(q,w)=\frac{1}{2\pi}\int dt\,F_{ij}(\vec{q},t)e^{iwt} \qquad (12)$$

The transport coefficients, namely self diffusion coefficient, D, and shear viscosity, η are related with the time correlation functions such as the velocity autocorrelation function, Z(t),[20,21].

The self diffusion coefficient can be written either by a Green-Kubo (GK) type equation in terms of Z(t),

$$D_i=\frac{k_BT}{M}\int Z_i(t)\,dt \qquad (13)$$

or by an Einstein (E) expression in term of the mean square displacement, $\langle\Delta r^2(t)\rangle$, as

$$D_i=\lim_{t\to\infty}\frac{\langle\Delta r_i^{\,2}(t)\rangle}{6t}. \qquad (14)$$

For the further information about dynamical calculation, the reader is referred Canales *et.al.* [22]. In the present work, the diffusivity for each constituent in the alloy has been found using the theory proposed by Gonzalez et al. [20]. The diffusion coefficient can be used to estimate viscosity of liquid by Stokes-Einstein formula

$$\eta=\frac{k_BT}{6\pi r_oD} \qquad (15)$$

where $D=(D_{Ge}+D_{Se})/2$ and r_o is the effective diameter of the diffusing particles which defined the as the average value of the nearest – neighbor distances of each species in the liquid alloy system.

2.2 Molecular Dynamics simulations

MD is a direct simulation technique at the atomic level. Almost all the physical properties of the material may be determined using molecular dynamics. It requires generally an interatomic potential. Our MD simulations are based on effective pair potentials constructed with FS approximation given in Eq. 3b. The pair potential term in Eq.3 is choosen by the fitting to give a short range order interactions. Based on the constant volume, temperature method (NVT), we began randomly placing 128 atoms (64 Ge and 64 Se atoms) in a cubic box and periodic boundary conditions with the minimum acceptable distance between atoms 2A. the size of cubic cells was choosen to make density of liquid close to experimental data. After an equilibration period of 10 000 time steps, we have computed the properties during a run of 10 000 configurations. The time step was 0.01 ps, and the Beeman algorithm [23] which is the most accurate of the supposedly "Verlet-equivalent" algorithms, with coupling thermal bath as proposed by Nosé.[24] was used. The partial radial distribution functions $g_{ij}(r)$ and the mean square displacements were computed during the simulations.

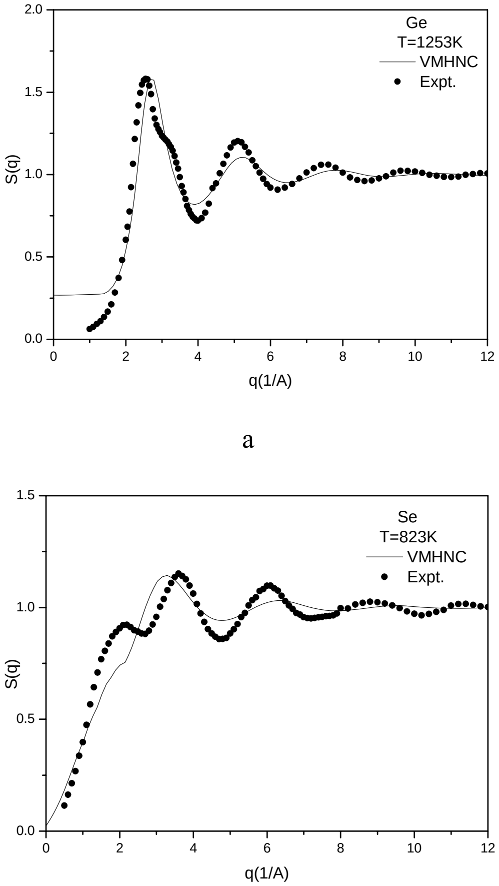
3. Results and discussion

First, we have calculated the effective pair potentials based on MAEAM potential functions for liquids Ge and Se at the thermodynamic states T=1253K; ρ=0.0461at./Å^3 and T=823K; ρ=0.0264at./Å^3, respectively [25]. The input physical data used in our liquid state calculations determined from the solid sate values of Kittel [26] are E_c^{liq} =3.85eV, a^{liq} =5.76Å for Ge; E_c^{liq} =2.46eV, a^{liq} = 4.37A for Se. All the parameters of potential functions are determined by not only fitting to solid but also liquid state properties using the parameterization procedure given in Ref. [13-16]. The model parameters used in our calculations are listed in Table 1.

Table 1. The MAEAM parameters for liquids Ge and Se.

Parameter	Ge	Se	Parameter	Ge	Se
F_o(eV)	2.15	1.58	r_c (A)	4.91	4.31
n	0.60	0.6	r_{1e} (A)	2.70	2.30
α(eV)	0.00142	0.0406	k_{-1} (eV)	135.479	50.497
			k_0 (eV)	-595.914	-222.113
			k_1 (eV)	1110.010	413.731
			k_2 (eV)	-1142.020	-425.662
			k_3 (eV)	703.209	262.105
			k_4 (eV)	-259.534	-96.735
			k_5 (eV)	53.174	19.819
			k_6 (eV)	-4.663	-1.738

In Table 1, the r_c is the cut-off distance determined by the cut-off procedure [13-16]. The values of r_{1e} are determined from the position of the first peak for the experimental pair distribution function. In Figs. 1a-b, the presently obtained static structure factors, S(q) for liquids Ge and Se have been illustrated along with the experimental data of Waseda [25], respectively. Although these calculated S(q)'s reasonably reproduce the experimental data, the agreement with experiment is much better for Ge. We also find that the oscillations in the calculated structure factors S(q) die out more rapidly than in the experimental data. The first sharp diffraction peak (FSDP) is presented in the experimental data 2.2Å^{-1} but it was unclear in the VMHNC result. Our calculated structure factor of Se show a FSDP at 2.1Å^{-1}. The first peak of S(q) is smooth which means that the chain-like structure remains in metallic structure



b

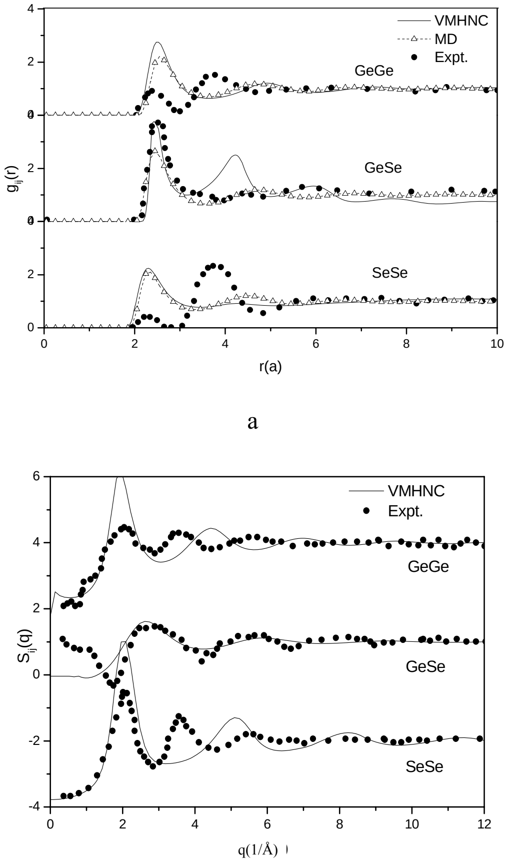
Fig. 1. The static structure factors, S(q) for liquids (a) Ge and (b) Se.

For liquid GeSe alloys, all calculations are performed with both VMHNC and MD simulations are performed at T=1053K and ρ=0.0377at/Å^3, near its melting. The parameters of our constructed MAEAM model used to perform MD simulation of liquid GeSe alloy are listed in Table 2.

Table 2. The MAEAM parameters used in our MD simulations for liquids Ge and Se.

	k_1	k_2	k_3	F_o(eV)	n	α(eV)
Ge	77.136	-49.223	12.562	2.55	0.80	0.0583
Se	53.274	-25.918	5.131	1.67	0.80	0.5423

The calculated partial pair distribution functions, $g_{ij}(r)$, from VMHNC and MD simulations are plotted in Fig 2a and calculated VMHNC Faber-Ziman partial static structure factors, $S_{ij}(r)$, for liquid GeSe alloy are displayed in Fig. 2b. In Figs. 2, we have also included the experimental data of Petri *et.al* [27].



a

b

Fig. 2. (a) The calculated partial pair distribution functions, $g_{ij}(r)$, and (b) static structure factors for liquid GeSe alloy.

It is observed that theoretical and simulated results of $g_{ij}(r)$ show same behaviour as the position of the mean peaks. The MD partial $g_{GeSe}(r)$ are not so different from the experimental data. The height and the position of the main peak for presented both calculations coincide with the experimental result of $g_{GeSe}(r)$. However, there is appear a second peak at around 4A in VMHNC result. We notice that the calculated first peak of $g_{ij}(r)$'s are higher than that of the experiment, except GeSe interactions from MD. This might be the sign of homocoordination tendency. It is seen in Fig. 2b that the positions of the main peaks of $S_{ij}(q)$ are well predicted using the effective potentials based on EAM, however the amplitudes of oscillations become radically different, except $S_{GeSe}(q)$. However, the calculated results of the $S_{ij}(q)$ are reasonable agreement with experimental data at larger q region.

The calculated total pair correlation functions, g(r), for liquid GeSe alloy are plotted along with the experimental data taken from Ref. [27] in Fig. 3. The values of neutron scattering lengths needed to estimate total distribution function are 8.185fm for Ge and 7.970fm for Se [28]. We find that the oscillations in our calculated g(r) die out more rapidly than in experimental one. It is suggesting too soft repulsive potential.

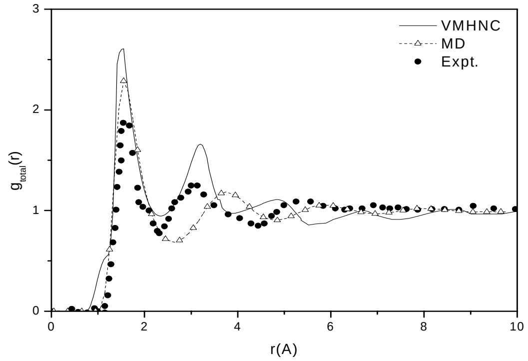


Fig. 3. The total pair correlation functions, g(r), for liquid GeSe alloy.

It is interesting to investigate the dynamic properties of equiatomic GeSe alloy in conjunction with the structural knowledge discussed above. We calculated the mean square displacements, $\langle r^2(t)\rangle$, and showed in Fig. 4 along with the other simulation study of Raty *et.al.* [7]. It is seen, from Fig. 4, time dependence of $\langle r^2(t)\rangle$ exhibits linear increasing by the time which is typical behaviour of simple liquids at higher temperatures. It has been noted that for longer times, as soon as the motions become diffusive, the $\langle r^2(t)\rangle$ has a linear dependence on time.

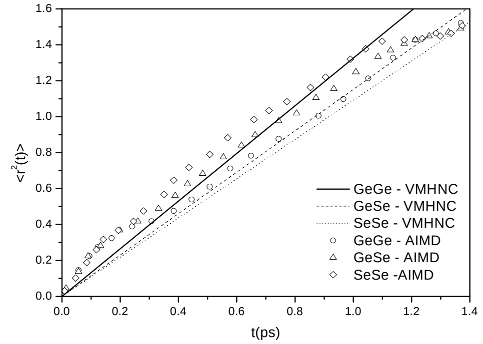


Fig. 4. Mean square displacement of GeSe alloy.

The calculated values of D for liquid GeSe alloy are listed in Table 3 compared with the available values in the literature. It is seen that both GK and E methods give consistent results with each other.

The present result of D for liquid Ge into the Se in GeSe alloy has been faster than that of Se into the Ge. The results obtained from E with MAEAM in GeSe alloy are close to other theoretical data. These values are typical of the liquid metals. This fact means that there is high probability of a rapid rearrangement of the Ge and Se chains, especially in the metallic state. Also, we have obtained the values of the shear viscosity coefficients for all interactions at liquid GeSe alloy, which is of the same order of magnitude as the experimental value at 1173K

Table 3. The calculated self diffusion coefficients D and shear viscosities η.

Metal	T(K)	D(Å^2/ps)			η (cP)	
		GK	E		E	
GeGe	1053	0.139	0.221	0.28[a]	3.2	
GeSe	1053	0.134	0.190	0.203[a]	3.6	1.9[a]
SeSe	1053	0.112	0.181	0.20[a]	4.2	
[a]Ref.[7]						

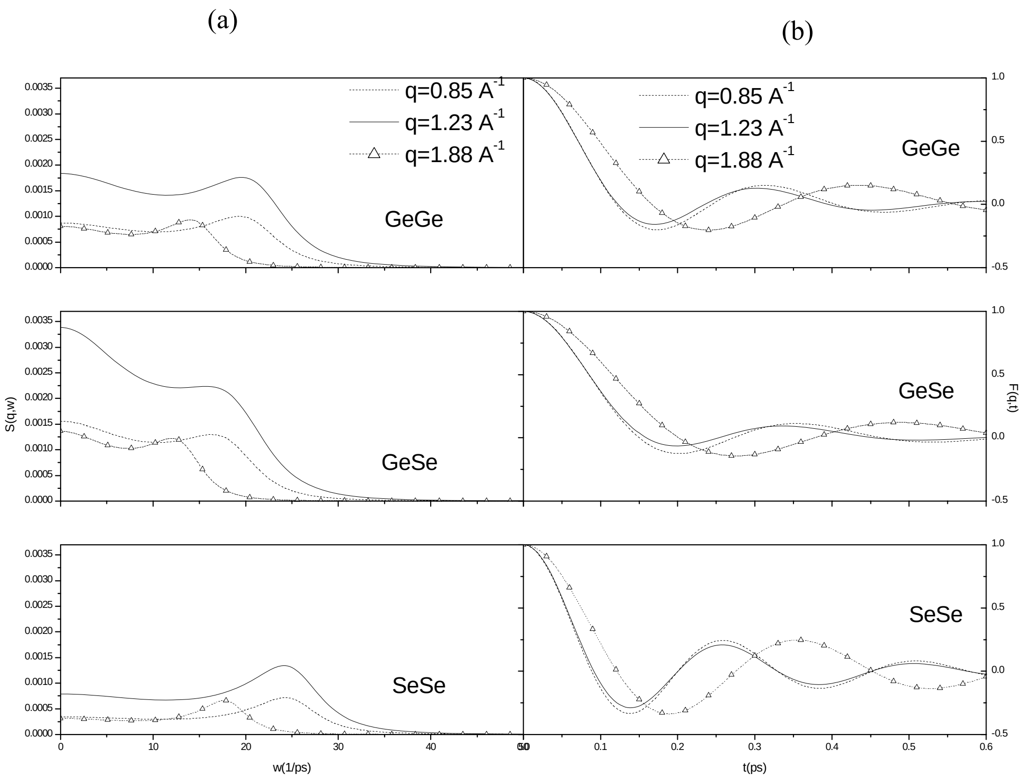


Fig. 5. (a) The calculated dynamic structure factors and (b) intermediate scattering functions for liquid GeSe alloy.

Figs. 5a and 5b show the partial dynamic structure factors, $S_{ij}(q,w)$ and partial intermediate scattering functions, $F_{ij}(q,t)$, respectively at three different q values for Ge-Ge, Ge-Se and Se-Se interactions in GeSe alloy. The $S_{ij}(q,w)$ provide information concerning the microscopic mechanisms of propagating longitudinal modes, e.g., the peaks in $S_{GeGe}(q,w)$ for the GeSe liquid alloy have been related to propagating fast modes supported by the Ge ions.

For the smaller q's, $S_{ij}(q,w)$ exhibit clear side peaks that for $q<q_{max}$ are located at very similar frequencies; this is the typical behavior of $S_{ij}(q,w)$ in the hydrodynamic regime and represents a propagating sound mode. For larger q, a typical increase in the height and narrowing in frequency is found (the de Gennes narrowing) whereas for larger q a monotonic decay of $S_{ij}(q,w)$, is obtained, leading to the free-particle behaviour. $F_{ij}(q,t)$ are obtained within a self-consistent scheme assumed Gaussian approximation, detailed in Ref.[20].The behavior of $S_{ij}(q,w)$ is of course a consequence of the time dependence of the intermediate scattering functions, $F_{ij}(q,t)$. It is observed that the $F_{ij}(q,t)$ exhibit an oscillatory behavior with the amplitude of the oscillations being stronger for the smaller k values.The fact that the amplitude of the decaying tail of $F_{ij}(q,t)$ is well reproduced implies that for small w the dynamic structure factor will increase significantly, as observed in the Fig. 5. On the other hand, the deficiencies in the description of the oscillations of $F_{ij}(q,t)$ around the decaying tail are reflected in the less accurate representation of the Brillouin peak of $S_{ij}(q,w)$. In the hydrodynamic regime ($q\rightarrow 0$), the decay of $F_{ij}(q,t)$ for binary mixtures is related to both entropy and concentration fluctuations, and the decay observed in Fig.

5b is mainly due to diffusion effects resulting from concentration fluctuations.

4. Conclusions

Several static and dynamic properties of the liquid GeSe alloy have been calculated at equiatomic concentration. The improved functional form of the effective pair potential for MAEAM have been applied to liquid Ge, Se and GeSe alloy. These calculations were performed with the potential functions that not only fit to solid data but also liquid state properties. The structural calculations were carried out using the Molecular Dynamic simulations and the VMHNC theory of liquids. In this work, we propose a new pair potential form of MAEAM to construct effective pair potentials within Finnis-Sinclair approximation which were used in our MD simulations of GeSe alloy. Comparison between the calculated results and available experimental data for partial structure factors and partial pair correlation functions show that the proposed MAEAM formalism for GeSe alloy system is capable of providing a good description in their liquid state. For the dynamical properties, we have analyzed several time dependent correlation functions, although comparison with the experiment could only be made at the level of some transport coefficients. There are reasonable agreement with the experiment of the calculated self-diffusion and viscosity coefficients. In the point of view, we have realized that MAEAM potentials can be apply to liquid Ge-chalcogenide systems in many aspects of computer simulations.

These results suggest that pair potentials constructed on the basis of MAEAM may also be capable of describing other single particle and collective dynamics properties of transition and chalcogenide liquid metals, such as intermediate scattering function (the Fourier transform of dynamic structure factor). In addition to this, these potentials may be used in theoretical calculation in order to understanding of dynamic properties of chalcogenide liquid metals and alloys.

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