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Dynamical correlations and collective excitations in liquid $K_{0.5}Cs_{0.5}$ alloy

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Abstract. A model developed by Glass and Rice for Brownian particles in liquids is employed for the computations of the velocity autocorrelation function and mean square displacement in liquid $K_{0.5}Cs_{0.5}$ alloy introducing the concept of the motion of 'effective atoms'. Further, collective excitations in this liquid metal alloy have been studied by computing the longitudinal and transverse phonon eigenfrequencies employing three different approaches. The computed results show good qualitative and quantitative agreement with each other. The effective interatomic pair potential used for the study of dynamics (single particle as well as collective motions) of $K_{0.5}Cs_{0.5}$ alloy is obtained using the empty-core pseudopotential given by Ashcroft. Also, some thermodynamical properties have been calculated using the longitudinal and transverse phonon velocities and are in good agreement with the available results.

1. Introduction

The problem of the study of liquid metals and their alloys has immense importance because of increasingly manifold interests of not only physicists but also chemists and engineers. During the past few decades, metallic liquids have been extensively studied [1] using the pseudopotential theories. Efforts [2, 3] have also been made to study the dynamics of liquid metals through the calculation of the zero-frequency transport coefficient, which characterizes the mass, momentum and energy flow in liquids under different conditions of velocity, density and temperature gradients in these liquids. On the other hand, neutron inelastic scattering measurements have provided some information concerning the dynamic structure of liquids [4]. These investigations of the dynamical structure factor $S(q, \omega)$ give us some idea of the collective excitations also. However, in practice, knowledge of $S(q, \omega)$ is restricted by experimental limitations to a finite range of the values of momentum transfer $\hbar q$ and the energy transfer $\hbar\omega$. This paper is divided into six different sections. Section 2 deals with the interatomic forces and effective interatomic potential in $K_{0.5}Cs_{0.5}$ alloy. The motion of effective atoms and its application to the computation of dynamical correlations in liquid metal alloy are discussed in section 3. The method of computation of longitudinal and transverse phonon eigenfrequencies is presented in section 4. Section 5 describes the calculation of some thermodynamical properties. Finally, the conclusions drawn from the study in the case of $K_{0.5}Cs_{0.5}$ alloy at 373 K are presented in section 6.

2. Pair potentials

The effective pair potentials between screened ions provide the basis for the calculations of the structural and thermodynamical properties of simple liquid metals. These pair potentials are commonly evaluated by treating the electron-ion coupling through the use of the pseudopotential concept and of linear screening theory. The usual form for the effective ion-ion interaction potential $V(r)$ in a pure liquid metal is given by [5]

$$V(r) = \frac{(Ze)^2}{r} + \frac{2\Omega}{(2\pi)^3} \int F(q) \exp(-iq \cdot r) dq. \quad (1)$$

The first term on the right-hand side represents the direct electrostatic repulsive interaction between two ions with valence Z and the second term comes from the indirect interactions associated with electron screening.

The density-dependent effective interatomic potential in the case of an alloy of type A_xB_{1-x} can be written as [6]

$$V_{\text{eff}}(r) = C_A^2 V_{AA}(r) + C_B^2 V_{BB}(r) + 2C_A C_B V_{AB}(r) \quad (2)$$

with concentrations C_A of A type and C_B of B type.

Alternatively, the effective interatomic pair potential, which has been computed treating the binary alloy as a one-component system consisting of effective atoms, is given by

$$V_{\text{eff}}(r) = \frac{(Z_{\text{eff}}e)^2}{r} + \frac{2(Z_{\text{eff}}e)^2}{\pi} \int_0^1 dq \frac{\sin(qr)}{qr} \cos(qr_{\text{c(eff)}}) (1/\epsilon_{\text{eff}}^{(q)} - 1). \quad (3)$$

The effective empty-core radius $r_{\text{c(eff)}}$ used in (3) is related to the Wigner-Seitz radius of the effective atom (alloy atoms) and is given by [7]

$$r_{\text{c(eff)}} = 0.51 r_{\text{alloy}} Z_{\text{eff}}^{-1/3}$$

where

$$\frac{4}{3}\pi r_{\text{alloy}}^3 = X \frac{4}{3}\pi r_A^3 + (1 - X) \frac{4}{3}\pi r_B^3$$

and

$$Z_{\text{eff}} = C_A Z_A + C_B Z_B.$$

Here r_A , r_B and r_{alloy} are the Wigner-Seitz radii of A, B and alloy, respectively. Another parameter, k_F , used in the calculation of effective potential through (3) is given by

$$k_{F(\text{eff})} = (3\pi^2 Z_{\text{eff}} \rho_{\text{eff}})^{1/3}$$

where $\rho_{\text{eff}} (= C_A \rho_A + C_B \rho_B)$ is the effective number density of the alloy.

2.1. Results

An especially simple and useful form of a model potential is the empty-core model pseudopotential proposed by Ashcroft [8] which is employed in the present computations. The effective interatomic pair potentials for the liquid binary $K_{0.5}Cs_{0.5}$ alloy have been calculated in two different ways. One is by using (2) and the other is by treating the binary alloy as a one-component system consisting of effective atoms with the help of (3). These effective interatomic pair potentials for liquid $K_{0.5}Cs_{0.5}$ alloy together with

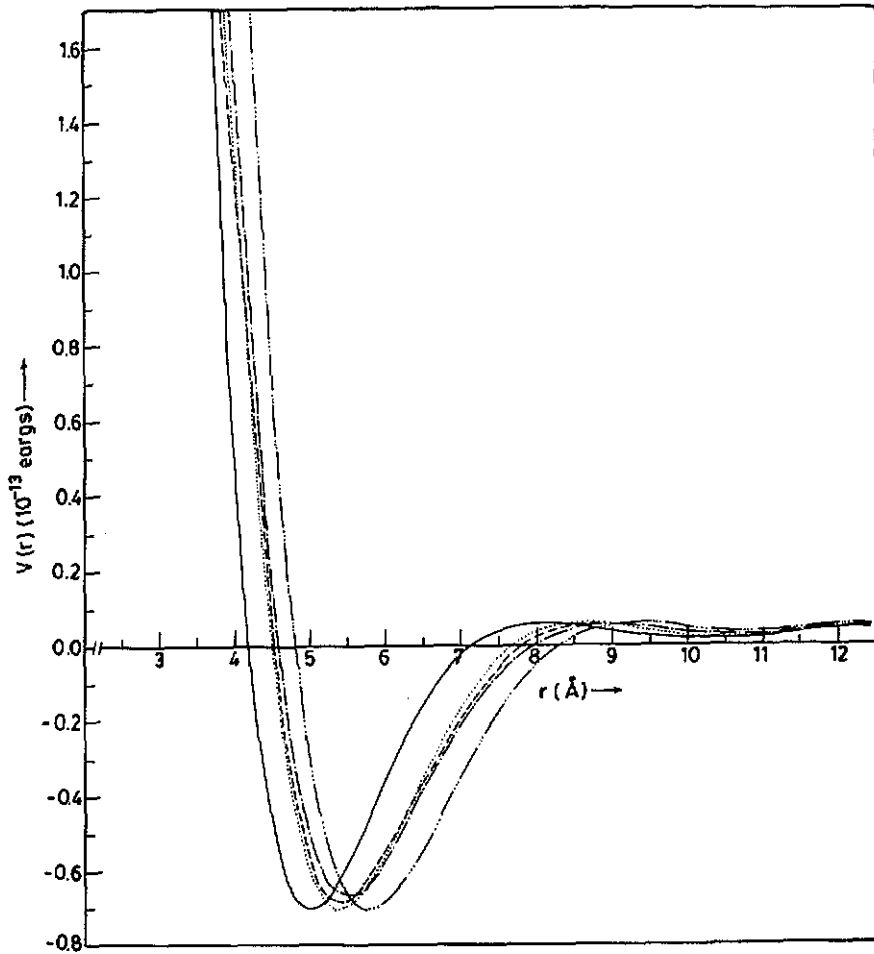


Figure 1. Pair potentials for liquid $K_{0.5}Cs_{0.5}$ alloy: —, $V(r)_{K-K}$; — · —, $V(r)_{Cs-Cs}$; — — —, $V(r)_{K-Cs}$; · · · · ·, $V_{eff}(r)$ computed using (2); - - - , $V_{eff}(r)$ computed using (3).

the pair potentials of $V_{K-K}(r)$, $V_{Cs-Cs}(r)$ and $V_{K-Cs}(r)$ are shown in figure 1. A close examination of the two interatomic potentials reveals that the potentials are almost similar as far as the repulsive nature is concerned. It can be observed from figure 1 that the effective potential obtained using the concept of 'effective atoms' shows slightly smaller well depths than the potential obtained using (2) does. Moreover, both these effective potentials show long-range oscillations converging towards a finite value instead of zero for $r \rightarrow \infty$. This may be because the repulsive part of the Coulomb potential dominates over the oscillations due to the ion-electron-ion interactions. The potential used for all further computations in the present paper is that obtained by (3) treating the binary alloy as a one-component system and consisting of 'effective atoms'.

2.2. Elastic constants

In the isotropic solids, three independent elastic constants exist. Because of the existence of central forces the Cauchy relationship has been assumed in these solids. The three independent elastic constants are then given by [9]

$$\begin{aligned}
 C_{11} &= \rho_{\text{eff}} k_B T (3 + 2I_1/5 + I_2/5) \\
 C_{12} &= \rho_{\text{eff}} k_B T (1 - 2I_1/15 + I_2/15) \\
 C_{44} &= \rho_{\text{eff}} k_B T (1 + 4I_1/15 + I_2/15)
 \end{aligned}
 \tag{4}$$

with ρ_{eff} the effective number density of the alloy. The integrals I_1 and I_2 are defined as [10]

$$\begin{aligned}
 I_1 &= \frac{\rho_{\text{eff}}}{2k_B T} \int_0^\infty g(r) r V'_{\text{eff}}(r) dr \\
 I_2 &= \frac{\rho_{\text{eff}}}{2k_B T} \int_0^\infty g(r) r^2 V''_{\text{eff}}(r) dr
 \end{aligned}$$

where $g(r)$ is the pair correlation function, and $V'_{\text{eff}}(r)$ and $V''_{\text{eff}}(r)$ are the first and second derivatives of the effective interatomic pair potential $V_{\text{eff}}(r)$ as calculated using (3).

The above-obtained effective pair potential is then further used to obtain the elastic constants. The values of these three independent elastic constants in $\text{K}_{0.5}\text{Cs}_{0.5}$ alloy at 373 K are $C_{11} = 3.52 \times 10^{10} \text{ dyn cm}^{-2}$, $C_{12} = 1.218 \times 10^{10} \text{ dyn cm}^{-2}$ and $C_{44} = 1.15 \times 10^{10} \text{ dyn cm}^{-2}$.

3. Single-particle motion

The most elegant method of determining the structure is to start from the description of single-particle motion. A whole class of theories of transport in dense fluids has been formulated on the basis of Brownian motion of particles. The simplest theory of Brownian motion describing single-particle motion is based on the phenomenological Langevin equation. A liquid is assumed to have a quasi-crystalline structure for the time smaller than the relaxation time (10^{-12} s) even at melting temperature and is characterized by a characteristic frequency ω_0 . In analogy with the theory of solids, a simple model which may be considered for liquids is that of a Brownian particle diffusing in a harmonic well of frequency ω_0 .

Following Glass and Rice [11] the simplified equation of motion in terms of the normalized velocity autocorrelation function $\psi(t)$ is written as

$$d^2\psi/dt^2 + \beta_0(d\psi/dt) + \omega_0^2\psi = 0. \tag{5a}$$

Using the boundary conditions (discussed elsewhere [11]) the velocity autocorrelation function can be written as

$$\psi(t) = [\exp(-\beta_0 t/2)] [\cos(\xi t) + (\beta_0/2\xi) \sin(\xi t)]. \tag{5b}$$

The diffusive motion of the atoms, always present in the liquids, is described in terms of the linear growth of the mean square distance travelled by the vibrating atoms over a time t . Hence the mean square displacement $\langle r^2(t) \rangle$ is given by [11]

$$\langle r^2(t) \rangle = \langle [R(t) - R(0)]^2 \rangle = 6\langle v^2 \rangle \int_0^t dt' (t - t') \psi(t'). \tag{6}$$

Here $\langle v^2 \rangle = 3k_B T/M$ is the average thermal velocity.

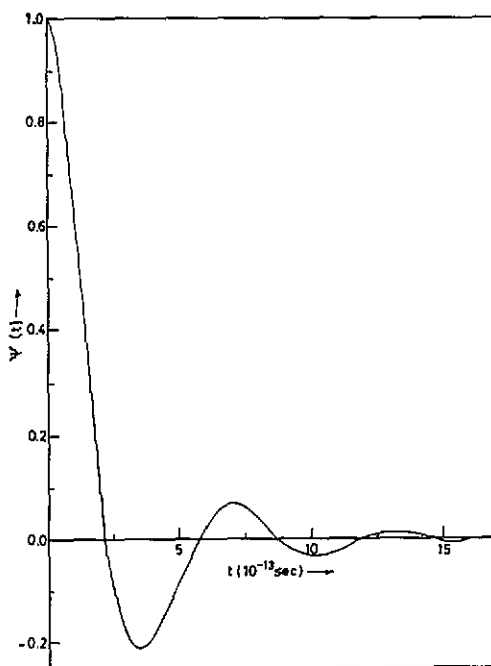


Figure 2. Present computed result for velocity autocorrelation function $\psi(t)$ in $K_{0.5}Cs_{0.5}$ alloy.

The above method, which was used earlier for the study of dynamical correlations in liquid metals [12–14], has been extended to the computation of the velocity autocorrelation function and mean square displacement in liquid $K_{0.5}Cs_{0.5}$ binary alloy in the light of the concept of the motion of effective atoms analogous to single-particle motion in liquid metals. The results of these computations have been discussed in section 3.1.

3.1. Results

The velocity autocorrelation function $\psi(t)$ computed using (5b) for $K_{0.5}Cs_{0.5}$ alloy at 373 K is shown in figure 2. It can be observed from figure 2 that the negative region indicates the backscattering of the effective atoms from the shell of their nearest neighbours arising from the short-range, strongly repulsive core collisions. The positive behaviour of $\psi(t)$ after the negative region indicates the redevelopment of the memory of the system.

The results of the mean square displacement $\langle r^2(t) \rangle$ for $K_{0.5}Cs_{0.5}$ alloy are shown in figure 3. For small times the values of the mean square displacement provide evidence of the fact that there is a vibratory component present in the atomic motions whereas for larger times the atoms diffuse freely like gases and the curve (for times greater than 8×10^{-13} s) becomes a straight line having a slope D (diffusion coefficient) which can be written as $\langle r^2(t) \rangle = 6Dt + C$. The diffusion coefficient D for liquid $K_{0.5}Cs_{0.5}$ alloy as calculated from the linear part of mean square displacement curve is $3.20 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$ and shows good agreement with the effective value [15] of the diffusion coefficient, $3.14 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$.

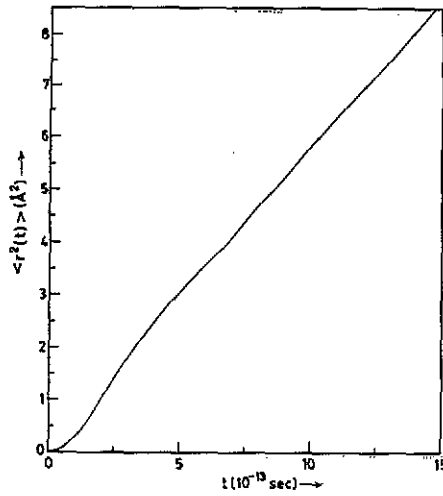


Figure 3. Present computed result for mean square displacement $\langle r^2(t) \rangle$ in $K_{0.5}C_{50.5}$ alloy.

4. Collective atomic motions

4.1. Theory of phonons in amorphous solids

Following Takeno and Goda [16] the secular equation for the phonon dispersion is given by

$$\det|\omega^2\delta(\alpha\beta) - D_{\alpha\beta}(q)| = 0 \quad (7)$$

where $D_{\alpha\beta}(q)$ is the dynamical matrix. Equation (7) is used in the lattice dynamics of the crystal lattice if the effective force constant is replaced by the bare force constant q . The effective force constants are derived from a spherically symmetric two-body potential; then the dynamical matrices giving eigenfrequencies are written in terms of effective pair potential and effective pair correlation function:

$$D_{zz}(q) = \omega_z^2(q) = \frac{4\pi\rho_{\text{eff}}}{M} \int_0^\infty dr g(r) \left[rV'_{\text{eff}}(r) \left(1 - \frac{\sin(qr)}{qr} \right) + [r^2V''_{\text{eff}}(r) - rV'_{\text{eff}}(r)] \left(\frac{1}{3} - \frac{\sin(qr)}{qr} - \frac{2\cos(qr)}{(qr)^2} + \frac{2\sin(qr)}{(qr)^3} \right) \right] \quad (8a)$$

$$D_{xx}(q) = D_{yy}(q) = \omega_x^2(q) = \frac{4\pi\rho_{\text{eff}}}{M} \int_0^\infty dr g(r) \left[rV'_{\text{eff}}(r) \times \left(1 - \frac{\sin(qr)}{qr} \right) + [r^2V''_{\text{eff}}(r) - rV'_{\text{eff}}(r)] \times \left(\frac{1}{3} + \frac{\cos(qr)}{(qr)^2} - \frac{\sin(qr)}{(qr)^3} \right) \right] \quad (8b)$$

where ρ_{eff} and M are the effective number density and effective mass of the alloy, respectively.

4.2. The model approach of Hubbard and Beeby

According to Hubbard and Beeby [17] who argued that the product of the static pair correlation function $g(r)$ and the second derivative $V''(r)$ of the potential peaks near the hard-sphere diameter, the expressions for $\omega_L(q)$ and $\omega_T(q)$ can be written as

$$\omega_L^2(q) = \omega_E^2 \{1 - [3 \sin(q\sigma)]/q\sigma - [6 \cos(q\sigma)]/(q\sigma)^2 + [6 \sin(q\sigma)]/(q\sigma)^3\} \quad (9a)$$

$$\omega_T^2(q) = \omega_E^2 \{1 + [3 \cos(q\sigma)]/(q\sigma)^2 - [3 \sin(q\sigma)]/(q\sigma)^3\} \quad (9b)$$

where

$$\omega_E = \left(\frac{4\pi\rho_{\text{eff}}}{3M} \int_0^\infty dr r^2 g(r) V''_{\text{eff}}(r) \right)^{1/2} \quad (9c)$$

is the maximum frequency and σ is the effective hard-core diameter of the effective atom in A_xB_{1-x} alloy.

4.3. Results

The eigenfrequencies of the longitudinal and transverse phonon modes, in $K_{0.5}Cs_{0.5}$ alloy, have been computed using (8a) and (8b) and are shown in figure 4. The dispersion curves show a linear variation in the low-wavevector transfer region and depict the characteristics of elastic waves. The first minimum in the ω - q curve for the longitudinal mode falls at the same value of q (1.6 \AA^{-1}) as the peak in the static structure factor $S(q)$ of $K_{0.5}Cs_{0.5}$ alloy [18]. It has been revealed through computer simulations and analytic calculations that this minimum arises from a process analogous to the Umklapp scattering in the crystalline solids. It is also evident from figure 4 that longitudinal phonon modes have more prominent oscillations than transverse phonon modes.

The longitudinal and transverse phonon eigenfrequencies obtained by the model approach of Hubbard and Beeby [17] have also been shown in figure 4. The phonon eigenfrequencies have been computed treating the system of $K_{0.5}Cs_{0.5}$ alloy as a one-component system. The effective hard-sphere diameter for $K_{0.5}Cs_{0.5}$ alloy is obtained using [19]

$$\eta = \eta_A + \eta_B$$

where $\eta_i = (\pi/6)\rho_i\sigma_i^3$ and $i \equiv A, B$. Here σ_i and ρ_i are the hard-sphere diameters and the number densities of the A and B components, respectively, in the liquid metal alloy. It is also observed from figure 4 that the longitudinal and transverse phonon modes as calculated by the approach of Hubbard and Beeby reproduce all the characteristic features of the dispersion curves.

4.4. The model calculation of Bhatia and Singh

An independent model approach given by Bhatia and Singh [20] has also been used for the computation of longitudinal and transverse phonon frequencies in the case of liquid metal $K_{0.5}Cs_{0.5}$ alloy. The model assumes that the ions in a simple metal with cubic symmetry interact with a central pairwise potential which is effective between nearest neighbours only. It also assumes that the force on an ion due to volume-dependent energies in the metal (kinetic and exchange energies of the conduction electrons, the ground-state energies of the electrons, etc) could be calculated using the Thomas-Fermi method. Under these assumptions, Bhatia and Singh [20] write the equations determining the ω - q relations in the case of liquids as

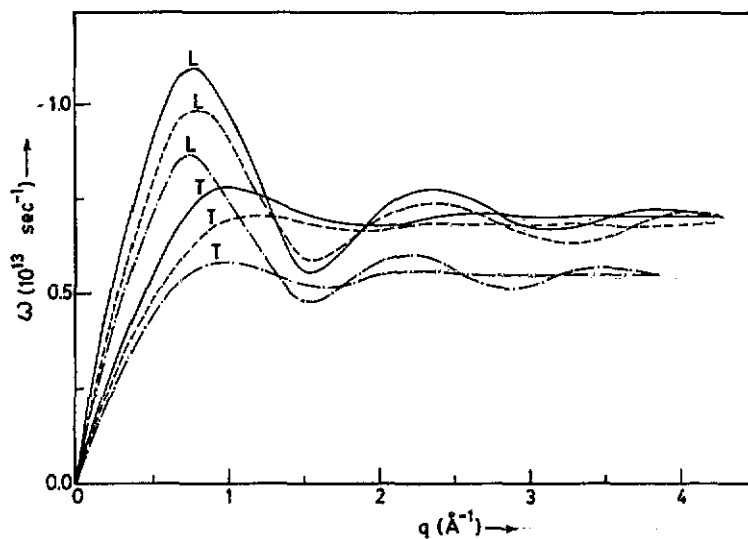


Figure 4. The longitudinal (L) and transverse (T) phonon frequency results for liquid $K_{0.5}Cs_{0.5}$ alloy: —, computed using the approach of Takeno and Goda [16]; ---, computed using the approach of Hubbard and Beeby [17]; ····, computed using the approach of Bhatia and Singh [20].

$$p\omega_l^2(q) = \{2N_c\delta[J_2(x) - J_0(x)/5]/a^2\} + K_e k_{TF}^2 q^2 [G(qr_s)]^2 / [q^2 + k_{TF}^2 \bar{g}(q)] \quad (10a)$$

$$p\omega_t^2(q) = (N_c\delta/a^2)[3J_0(x)/5 - J_2(x)] \quad (10b)$$

with

$$J_0(x) = 1 - [\sin(x)]/x$$

$$J_2(x) = \frac{1}{3} - \sin(x)[(1/x) - (2/x^3)] - [2 \cos(x)]/x^2$$

and

$$x = qa.$$

Here N_c is the number of nearest neighbours in the system, p is the density and a the nearest-neighbour distance. β and δ can be obtained for a body-centred cubic lattice from the relations [20]

$$C_{11} = 8\beta/3 + 8\delta/9 + K_e \quad C_{22} = -8\beta/3 + 8\delta/9 + K_e$$

$$C_{44} = 8\beta/3 + 8\delta/9.$$

4.5. Results

The model approach developed by Bhatia and Singh [20] as discussed in section 4.4 has also been used to estimate the eigenfrequencies of the longitudinal and transverse phonon modes in liquid $K_{0.5}Cs_{0.5}$ alloy. The parameters β and δ used in these calculations have been obtained through the use of elastic constants (equation (4)) for the liquid metal $K_{0.5}Cs_{0.5}$ alloy. These phonon dispersion curves are also shown in figure 4. A close examination of the longitudinal and transverse branches, as calculated by the model developed by Bhatia and Singh for the phonon dispersion, shows all the main characteristic features of the dispersion curves.

Because of the non-availability of any experimental results on phonon dispersion for $K_{0.5}Cs_{0.5}$ alloy, it has not been possible to compare the computed results with experiment. Nevertheless, the results obtained using three different theoretical approaches are in close agreement qualitatively as well as quantitatively.

5. Thermodynamical properties

From the long-wavelength limit of the dispersion curves, the longitudinal and transverse velocities of sound are estimated. The calculated values of the longitudinal sound velocity are $V_l = 1.70 \times 10^5 \text{ cm s}^{-1}$, $1.55 \times 10^5 \text{ cm s}^{-1}$ and $1.42 \times 10^5 \text{ cm s}^{-1}$ from the dispersion curves obtained using the three different approaches, i.e. the methods of Takeno and Goda, of Hubbard and Beeby, and of Bhatia and Singh, respectively. These values are then compared with the value of $1.58 \times 10^5 \text{ cm s}^{-1}$ obtained from the theoretical calculation [21] of the velocity of sound. Similarly from the linear part of the transverse phonon dispersion curves the values of the transverse phonon velocity V_t are also estimated. These are $V_t = 1.0 \times 10^5 \text{ cm s}^{-1}$, $0.85 \times 10^5 \text{ cm s}^{-1}$ and $0.76 \times 10^5 \text{ cm s}^{-1}$, respectively.

For an isotropic solid the isothermal bulk modulus B_T is given by [22] $B_T = \rho(V_l^2 - 4 \times V_t^2/3)$ where ρ is the density of the solid. For $K_{0.5}Cs_{0.5}$ alloy using the above-obtained values of V_l and V_t , the values of the isothermal bulk modulus are $2.22 \times 10^{10} \text{ dyn cm}^{-2}$, $2.06 \times 10^{10} \text{ dyn cm}^{-2}$ and $1.78 \times 10^{10} \text{ dyn cm}^{-2}$. These values of B_T are then compared with the value of $2.03 \times 10^{10} \text{ dyn cm}^{-2}$ obtained from the averaged value over the pure liquid metals. The results on B_T are further compared with the value of $2.05 \times 10^{10} \text{ dyn cm}^{-2}$ obtained by Gopal Rao and Gupta [23] and with the value of $1.98 \times 10^{10} \text{ dyn cm}^{-2}$ calculated using the elastic constant [24]. Further, these results have also been compared with the value of $2.03 \times 10^{10} \text{ dyn cm}^{-2}$ obtained from the long-wavelength limit of the structure factor, i.e. $S(0) = 0.02534$.

Further, following Hafner [22] and using these values of the longitudinal and transverse sound velocities, the Debye temperature Θ_D has been calculated for $K_{0.5}Cs_{0.5}$ alloy. The calculated values of the Debye temperature for liquid $K_{0.5}Cs_{0.5}$ alloy are $\Theta_D = 71.04 \text{ K}$, 60.77 K and 54.43 K , respectively. Using the Grimvall [25] formula the calculated average value of the Debye temperature in liquid $K_{0.5}Cs_{0.5}$ alloy is 51.25 K .

6. Conclusions

We have presented detailed theoretical calculations of $K_{0.5}Cs_{0.5}$ alloy at 373 K . The present study on the atomic structure and vibrational dynamics together with the thermodynamical properties reveals the following features.

(i) The study indicates that, in liquid alloys, long-range oscillations are also present in the ion-ion potential similar to the case of liquids and liquid metals.

(ii) The model proposed by Glass and Rice, assuming that liquids have a quasi-crystalline structure, yields a suitable description of the motion of effective atoms in liquid $K_{0.5}Cs_{0.5}$ alloy analogous to single-particle motion in liquid metals.

(iii) A perusal of section 4 shows that the thus-obtained dispersion relations from the three different theoretical approaches [16, 17, 20] reproduce all the broad features of the dispersions in liquid $K_{0.5}Cs_{0.5}$ alloy.

Acknowledgments

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