

Evaluation of total and partial structure factors, self-diffusion coefficients, and compressibilities of the cadmium-gallium melt

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The three partial structure factors $S_{11}(K)$, $S_{22}(K)$, and $S_{12}(K)$ defined by Ashcroft and Langreth are computed with a square-well potential as a perturbation over a hard-sphere potential for different atomic fractions or concentrations of cadmium for Cd-Ga melt at 296°C. Also, the number-number, concentration-concentration, and the cross-term number-concentration structure factors due to Bhatia-Thornton have been calculated for the seven concentrations of Cd-Ga melt at that temperature. From these partial structure factors total structure factors are computed and are compared with the experimental results. The total structure factors so computed are found to be in excellent agreement with the measured values except in the long-wavelength limit of $S(0)$. Using the partial structure factors in the long-wavelength limit the isothermal compressibilities have been calculated. From these partial structure factors and by using the linear-trajectory approximation of Helfand, the self-diffusion coefficients D_i 's have also been calculated for various atomic fractions of Cd for Cd-Ga alloy at 296°C. From these D_i 's, an estimate of the mutual diffusion coefficients has been made to a good approximation.

I. INTRODUCTION

From a phase diagram¹ one can easily see that the Cd-Ga system exhibits a closed miscibility gap with a long liquidus flat line. Extensive high-¹ and low-angle² x-ray scattering experiments have been carried out by Steeb *et al.* Furthermore, Cd exhibits an extremely large absorption cross section for thermal neutrons and hence conclusive results cannot be obtained alone by neutron diffraction studies. Because only x-ray diffraction experiments can be done for getting accurate data, it is not possible to obtain detailed partial structures from experiments. Therefore theoretical model potential calculations become important and necessary to get detailed information regarding the Cd-Ga melt.

It has been shown extensively³⁻⁸ that the structural properties of liquid metals can be explained on the basis of the mean-spherical model approximation (MSMA) with a square-well potential as a perturbation over the hard-sphere potential. Work under the MSMA has been carried out on pure metals^{9,10} and the potential parameters have been already obtained with these metals, i.e., Cd and Ga.

It is also important to note that Cd and Ga do not form any compound¹ but they have a strong segregation tendency, particularly around 50 at. % concentration of Cd as suggested by Steeb *et al.*² Thus it is proposed to apply the MSMA to these melts with a square-well potential and obtain the partial structure factors. In addition the Bhatia-Thornton correlation functions could also be calculated from these partial structures as they are linearly related.

From these partial structure factors the total structure factors at various concentrations of Cd have been calculated which in turn can be compared with the experi-

ment. Furthermore the isothermal compressibilities at different concentrations have been computed through the use of the Kirkwood-Buff equation by obtaining the partial structure factors in the long-wavelength limit.¹¹

II. THEORY

The direct correlation function (DCF) for binary mixtures can be defined as

$$C_{ij}(r) = \begin{cases} C_{ij}^0(r), & 0 < r \leq \sigma_{ij} \\ -\frac{\phi_{ij}(r)}{k_B T} = \frac{\epsilon_{ij}}{k_B T}, & \sigma_{ij} \leq r \leq A_{ij}\sigma_{ij} \\ 0, & r > A_{ij}\sigma_{ij} \end{cases} \quad (1)$$

where $C_{ij}^0(r)$ is the hard-sphere solution of the Percus-Yevick (PY) equation for liquid binary mixtures and are given by Lebowitz.¹² The Lebowitz solution of PY equation for the hard-sphere mixture is given by

$$-C_{ii}(r) = \begin{cases} a_i + b_i r + d r^3, & r < \sigma_{ii} \\ 0, & r > \sigma_{ii} \end{cases} \quad (4)$$

$$-C_{12}(r) = \begin{cases} a_1, & r < \lambda \\ a_1 + [b(r-\lambda)^2 + 4\lambda d(r-\lambda)^3 + d(r-\lambda)^4]r^{-1}, & \lambda < r < \sigma_{12} \\ 0, & r > \sigma_{12} \end{cases} \quad (6)$$

Here $\lambda = (\sigma_{22} - \sigma_{11})/2$. Furthermore, σ_{22} is chosen such that it is always greater than σ_{11} . a_1, a_2, b_1, b_2, d , and other symbols have been explained in detail⁶ already.

Here σ_{ii} , ϵ_{ii} , and A_{ii} stand for hard-core diameter, depth, and breadth of the square-well potential used for the species i , respectively. The mixed parameters are determined by using Lorentz-Berthelot mixing rules and are given by

$$\sigma_{12} = (\sigma_{11} + \sigma_{22})/2, \quad (9)$$

$$\epsilon_{12} = (\epsilon_{11}\epsilon_{22})^{1/2}, \quad (10)$$

$$A_{12} = (A_{11}\sigma_{11} + A_{22}\sigma_{22})/(\sigma_{11} + \sigma_{22}). \quad (11)$$

The Fourier transforms of $C_{ij}(r)$ have been given already^{5,6} and will not be repeated here. The $\hat{C}_{ij}(K)$ are linearly related to partial structure factors $S_{ij}(K)$ as

$$S_{11}(K) = \{1 - \rho_{11}\hat{C}_{11}(K) - \rho_{11}\rho_{22}\hat{C}_{12}^2(K)/[1 - \rho_{22}\hat{C}_{22}(K)]\}^{-1}, \quad (12)$$

$$S_{22}(K) = \{1 - \rho_{22}\hat{C}_{22}(K) - \rho_{11}\rho_{22}\hat{C}_{12}^2(K)/[1 - \rho_{11}\hat{C}_{11}(K)]\}^{-1}, \quad (13)$$

$$S_{12}(K) = (\rho_{11}\rho_{22})^{1/2}\hat{C}_{12}(K)\{[1 - \rho_{11}\hat{C}_{11}(K)][1 - \rho_{22}\hat{C}_{22}(K)] - \rho_{11}\rho_{22}\hat{C}_{12}^2(K)\}^{-1}. \quad (14)$$

The total structure factors $S(K)$ in terms of these partials is given by

$$S(K) = \sum_{i=1}^2 \sum_{j=1}^2 C_i^{1/2} C_j^{1/2} \frac{f_i(K) f_j(K)}{C_1 f_1^2(K) + C_2 f_2^2(K)} S_{ij}(K), \quad (15)$$

where $f_1(K)$ and $f_2(K)$ are atomic scattering factors of the i th species. C_i is the atomic fraction of the i th component.

In the long-wavelength limit, i.e., $K \rightarrow 0$, $\hat{C}_{ij}(K)$ can be written as

$$\begin{aligned} \rho_{ii}\hat{C}_{ii}(0) = & -24\eta_{ii} \left[a_{i/3} + \frac{b\sigma_{ii}}{4} + \frac{d\sigma_{ii}^3}{6} \right] \\ & + 8\eta_{ii}\epsilon_{ii}(A_{ii}^3 - 1)/k_B T \end{aligned} \quad (16)$$

and

$$\begin{aligned} \hat{C}_{12}(0) = & 4\pi\epsilon_{12}\sigma_{12}^3(A_{12}^3 - 1)/3k_B T - 4\pi a_1\sigma_{12}^3/3 \\ & - 4\pi\sigma_{11}^3[b(\sigma_{11} + 2\sigma_{22})/12 \\ & + \lambda d\sigma_{11}(3\sigma_{11} + 5\sigma_{22})/10 \\ & + d\sigma_{11}^2(2\sigma_{11} + 3\sigma_{22})/30]. \end{aligned} \quad (17)$$

One can then obtain the compressibility κ_T of the melt through Kirkwood and Buff's equation which can be written as¹¹

$$\begin{aligned} \kappa_T = & [1 - C_1\rho_{11}\hat{C}_{11}(0) - C_2\rho_{22}\hat{C}_{22}(0) \\ & - 2\rho C_1 C_2 \hat{C}_{12}(0)]^{-1}/\rho k_B T. \end{aligned} \quad (18)$$

In addition, one can also calculate the Bhatia-Thornton correlation functions since these are linearly related to the partial structure factors. The three correlation functions they have defined are as follows:

- (i) The number-number correlation function $S_{NN}(K)$.
- (ii) The concentration-concentration correlation function $S_{CC}(K)$.

(iii) The cross-correlation function $S_{NC}(K)$. These functions are given by

$$S_{NN}(K) = C_1 S_{11}(K) + C_2 S_{22}(K) + 2C_1^{1/2} C_2^{1/2} S_{12}(K), \quad (19)$$

$$\begin{aligned} S_{CC}(K) = & C_1 C_2 [C_2 S_{11}(K) + C_1 S_{22}(K) \\ & - 2(C_1 C_2)^{1/2} S_{12}(K)]; \end{aligned} \quad (20)$$

$$\begin{aligned} S_{NC}(K) = & C_1 C_2 [S_{11}(K) - S_{22}(K) \\ & + S_{12}(K)(C_2 - C_1)/(C_1 C_2)^{1/2}]. \end{aligned} \quad (21)$$

III. RESULTS AND DISCUSSIONS

Hermann *et al.* determined the structure factors (high-angle-scattering measurements) at 296°C and obtained the total structure factors at seven different concentrations of Cd. Through the present calculations we obtained the structure factors at all these concentrations. These are shown in Figs. 1 and 2. In the present calculations we assume ideal mixing and hence we can write the densities of the melt at various concentrations in terms of the densities of the pure metals as

$$\rho_{11} = C_1 \rho_{11}^0 \rho_{22}^0 [C_1(\rho_{22}^0 - \rho_{11}^0) + \rho_{11}^0]^{-1} \quad (22)$$

$$\rho_{22} = (1 - C_1) \rho_{11}^0 \rho_{22}^0 [C_1(\rho_{22}^0 - \rho_{11}^0) + \rho_{11}^0]^{-1}. \quad (23)$$

The potential parameters of the pure substances have been used in the present calculations of the partial structure factors of the melts. These were previously determined by Rao and co-workers.^{9,13} The input parameters are given in Table I. The concentrations have been expressed in atomic fractions of Cd.

The partial structure factors $S_{11}(K)$, $S_{22}(K)$, and $S_{12}(K)$ have been given for four typical concentrations only in Figs. 3-5, as experimentally determined partial structure factors are not found.

The peak height of $S_{22}(K)$ increases as the concentration of Cd increases. The behavior of $S_{11}(K)$ and $S_{22}(K)$ are in conformity with the fact that the structure factor of liquid Cd is higher than that of liquid Ga. Both

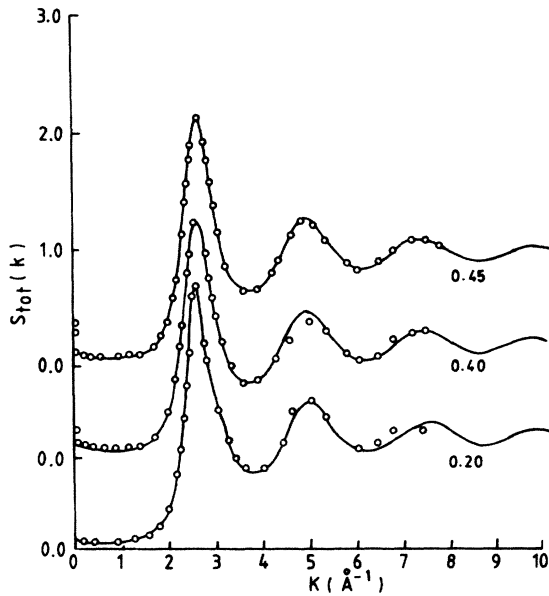


FIG. 1. Total structure factor $S_{\text{tot}}(K)$ vs K for Cd-Ga melt for different atomic fractions of Cd. Present calculated results (—). Experimental results (○).

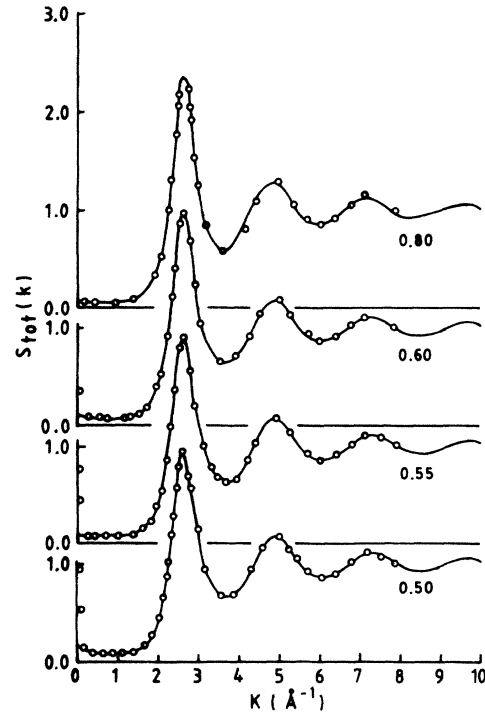


FIG. 2. Same as Fig. 1.

$S_{11}(K)$ and $S_{22}(K)$ go to unity for large K as seen from equations and at all these concentrations. For $S_{12}(K)$ at 20 at. % concentration of Cd a small shoulder appears at 3.15 \AA^{-1} and vanishes for higher concentrations of Cd. This is due to the peculiar nature of Ga, whose concentration is 80 at. %.

It is found from Figs. 1 and 2 that the first maximum in the total structure factor virtually remains unchanged at 2.55 \AA^{-1} and is shifted very slightly to a higher K value as the concentration of Cd increases. This is expected because the first maximum for Ga occurs at 2.52 \AA^{-1} while that for Cd (Ref. 14) is 2.62 \AA^{-1} . The peak height for Ga is 1.95 while that of Cd is 2.52. Thus the height of the principal maximum increases as the concentration of Cd increases. For mean concentrations the shape of the first maximum is nearly symmetric. For 20 at. % concentrations of Cd, which means 80 at. % concentration of Ga, the shoulder is visible at around 3.10 \AA^{-1} , as expected. However, this vanishes as the concen-

tration of Cd increases by more than 20 at. % of Cd. This appearance of a shoulder can be explained by assuming a special arrangement of Ga atoms in addition to the "free" Ga atoms which are considered to behave like hard spheres. The structure of this special arrangement is discussed in different ways¹⁵⁻¹⁷ and is, at present, not fully understood. Above 300°C the Ga melt does not show any shoulder¹⁰ and may be thought of merely consisting of "free" atoms.

The total structure factor at seven different concentrations of Cd has been compared with the experiment as determined by Hermann *et al.*¹ and is shown in Figs. 1 and 2. In every case the agreement is excellent except at low K values that is as $K \rightarrow 0$. As mentioned already the position of the first maximum of the structure factors of molten Ga and Cd occur nearly at the same K . Thus the structure factor of the molten alloys show no indication

TABLE I. Input parameters used for the present calculations.

Temperature (K)	Concentrations or atomic fraction of cadmium	σ_{11} (\AA)	σ_{22} (\AA)	ϵ_{11}/k_B (K)	ϵ_{22}/k_B (K)	A_{11}	A_{22}	ρ_{11}^0 (\AA^{-3})	ρ_{22}^0 (\AA^{-3})
569.0	0.20	2.500	2.700	218.00	282.79	1.77	2.00	0.0510	0.0430
	0.40	2.500	2.700						
	0.45	2.500	2.700						
	0.50	2.500	2.700						
	0.55	2.500	2.700						
	0.60	2.500	2.700						
	0.80	2.500	2.700						

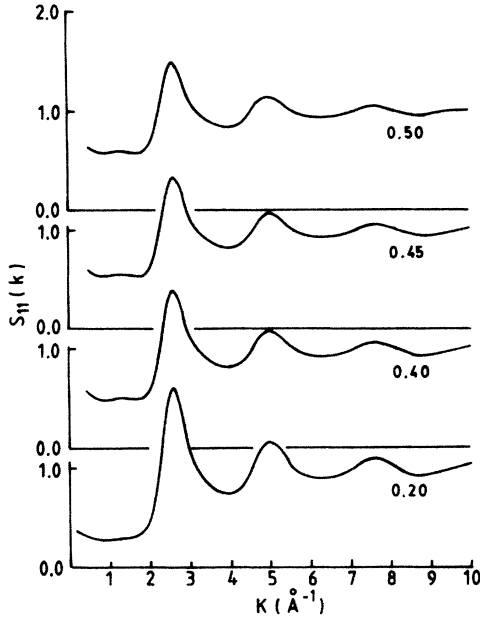


FIG. 3. $S_{11}(K)$ vs K for different atomic fractions of Cd for Cd-Ga melt.

for segregation and broadening or splitting of the alloy structure factor is not observed both from the present calculations or in the experimental results of Hermann *et al.*

However, Hermann *et al.*² performed small-angle x-ray scattering experiments at nine different concentrations of Cd and up to 440°C. An analysis of their small-

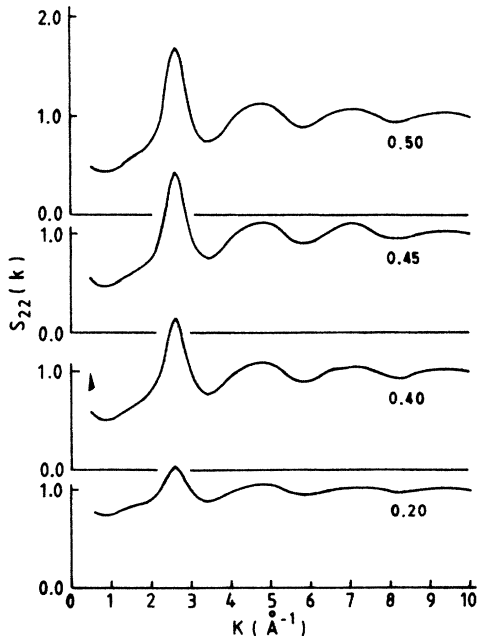


FIG. 4. $S_{22}(K)$ vs K for different atomic fractions of Cd for Cd-Ga melt.

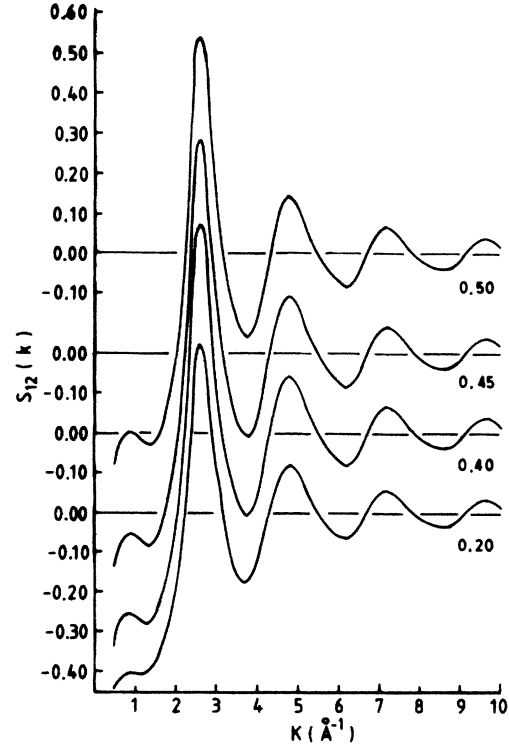


FIG. 5. $S_{12}(K)$ vs K for different atomic fractions of Cd for Cd-Ga melt.

angle x-ray diffraction experiment show that the melt at a critical concentration of 50.0 ± 1.0 at. % of Ga and at 296°C, the Bhatia-Thornton structure factor $S_{CC}(0)$ increases enormously up to 3500 times the ideal value namely $S_{CC}^{id}(0) = C_1 C_2$, where C_1 and C_2 are as usual atomic fractions of Ga and Cd. Thus they pointed out that there is a strong segregation as this concentration is approached.² It is also concluded by them that the scattering intensity at small momentum transfer is great whenever a segregation tendency occurs in the melt. As has been pointed by Bhatia and Thornton,¹⁸ the total coherent intensity can be separated into three parts and is given by

$$S(K) = \frac{I_{coh}(K)}{\langle f^2 \rangle} = \frac{\langle f \rangle^2}{\langle f^2 \rangle} S_{NN}(K) + \frac{\langle \Delta f^2 \rangle}{\langle f^2 \rangle} S_{CC}(K) + \frac{2\langle f \rangle \Delta f}{\langle f^2 \rangle} S_{NC}(K), \quad (24)$$

where f is the scattering amplitude,

$$\Delta f = f_1 - f_2, \quad \langle f \rangle = C_1 f_1 + C_2 f_2, \quad (25)$$

and the rest of the symbols have their usual connotation. Here (see Fig. 6) $S_{NN}(K)$ describes the contribution of the overall structure to the total structure factor while $S_{CC}(K)$ is due to the chemical short-range order. The $S_{CC}(K)$ increases for low K if the segregation tendency is present. For higher values of K it shows damped oscillations. Since $S_{NC}(0)$ can be expressed in terms of $S_{CC}(0)$ the coherent intensity can be written as

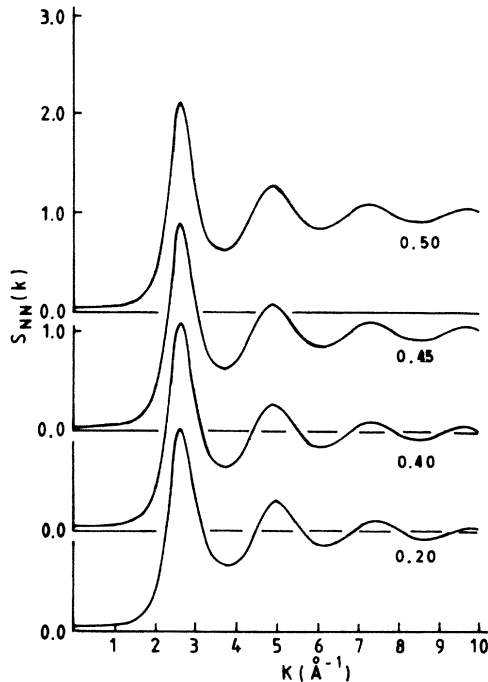


FIG. 6. $S_{NN}(K)$ vs K for different atomic fractions of Cd for Cd-Ga melt.

$$I_{\text{coh}}(0) = \rho k_B T \chi_T \langle f \rangle^2 + S_{CC}(0). \quad (26)$$

Here the terms have their usual significance. In the case of x-ray scattering the difference in the electron density of the constituents makes the concentration fluctuations visible. The first term in Eq. (26) yields only a small contribution to the scattering intensity and is independent of K for small K . So all the contribution to the scattering intensity comes from $S_{CC}(0)$ and its rise in the low- K region is expected because of the segregation tendency of Ga. All these characteristics can be observed in an excellent way from the present calculations shown in Fig. 7. Thus as the concentration is approached from 0.20 atomic fraction of Cd to 0.50 atomic fraction of Cd the $S_{CC}(0)$ rises rather steeply as observed in small-angle x-ray diffraction studies. This is not observed in normal simple alloys like Na-Cs alloy⁵ or K-Cs alloy.⁶ The same trend has been observed in the ultrasonic velocity measurements.^{19,20} These measurements clearly indicate structure changes in the melt at about 295 °C at which temperature the phase separation line appears as a discontinuity in the ultrasonic velocity.¹ The same observation was made for Bi-Ga system as well.²¹

Furthermore the ultrasonic absorption distinctly increases upon approaching the critical temperature. This rise is more distinct for lower frequencies, proving the existence of concentration fluctuations.

Since the present potential parameters have been fitted at the principal peak of the pure metal and no further parameters have been introduced for the small-angle behavior, it is not expected from the present calculations the rise of the total structure factor in the long-wavelength

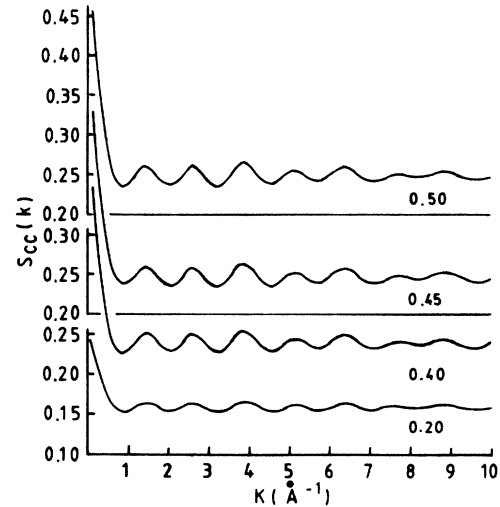


FIG. 7. $S_{CC}(K)$ vs K for different atomic fractions of Cd for Cd-Ga melt.

limit at these critical concentrations (that is around 0.50 atomic fraction of Cd).

Computations have been made from Eq. (18) for the compressibility κ_T as a function of concentration of Cd. It is not expected from the present calculations that κ_T as obtained now will agree with ultrasonic measurements because of the segregation tendency in the melts and consequent high value of $S(0)$ and nonideal behavior of the melt (see Table II).

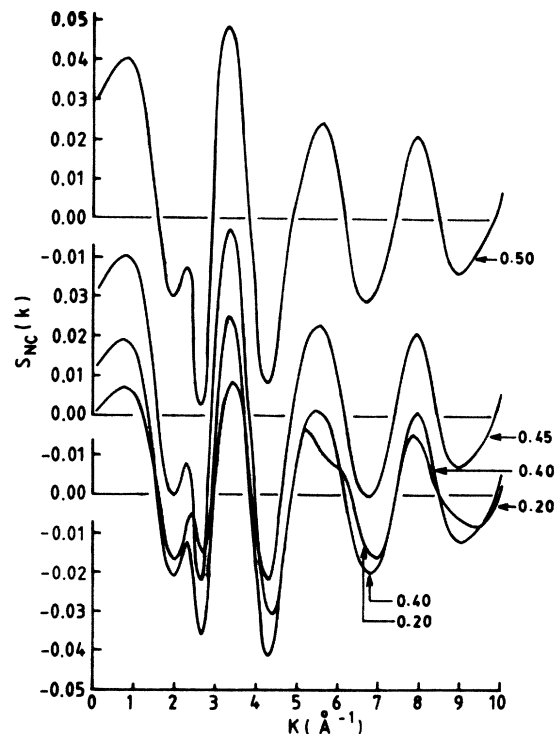


FIG. 8. $S_{NC}(K)$ vs K for different atomic fractions of Cd for Cd-Ga melt.

TABLE II. The first main peak height and its position and compressibility.

Temperature (K)	Concentrations or atomic fractions of cadmium	Calculated		Experimental		Compressibility $\kappa_T = 10^{12}$ (cm ² /dyn)
		Position K (Å ⁻¹)	Height $S(K)$	Position K (Å ⁻¹)	Height $S(K)$	
569.0	0.20	2.55	2.02	2.55	2.25	8.06
	0.40	2.55	2.05	2.55	2.07	8.19
	0.45	2.55	2.07	2.55	2.08	8.13
	0.50	2.55	2.09	2.55	2.10	8.03
	0.55	2.60	2.12	2.60	2.11	7.89
	0.60	2.60	2.15	2.60	2.14	7.73
	0.80	2.60	2.34	2.60	2.33	6.90

The Bhatia-Thornton correlation functions $S_{NN}(K)$, $S_{CC}(K)$, and $S_{NC}(K)$ have been computed and are given in Figs. 6–8. The variation of $S_{NN}(K)$ with K is similar to that of $S(K)$ for a pure liquid while $S_{NC}(K)$ shows a shoulder for 80 at. % concentration of Ga and this vanishes as Ga concentration decreases.

IV. COMPUTATION OF SELF-DIFFUSION COEFFICIENT

We evaluate the partial radial distribution function from the partial structure factors from the relation

$$h_{ij}(r) = g_{ij}(r) - 1 = \frac{1}{2\pi^2 r \rho} \int_0^\infty [S_{ij}(K) - \delta_{ij}] K \sin(Kr) dk. \quad (27)$$

Here δ_{ij} is the well-known Kronecker delta. Using the linear-trajectory principle of Helfand²² for binary mixtures due to Davis and Polyvos²³ we obtain the diffusion coefficient of the i th species as

$$D_i = \frac{k_B T}{\xi_i}, \quad (28)$$

where ξ_i is the friction constant. Furthermore ξ_i is written as

$$\xi_i = \xi_i^H + \xi_i^S + \xi_i^{SH}, \quad (29)$$

where ξ_i^H , ξ_i^S , and ξ_i^{SH} are the friction constants of the hard-sphere part, soft part, and the cross effects, respectively. These are given by

$$\xi_i^H = \sum_{j=1}^2 \frac{8}{3} \sigma_{ij}^2 g_{ij}(\sigma_{ij}) \rho_j (2\pi\mu_{ij} k_B T)^{1/2}, \quad (30)$$

$$\xi_i^S = - \sum_{j=1}^2 \frac{\rho_j}{3} \left[\frac{2\pi\mu_{ij}}{k_B T} \right]^{1/2} \times \frac{1}{(2\pi)^2} \int_0^\infty K^3 \hat{V}_{ij}^S(K) \hat{G}_{ij}(K) dk, \quad (31)$$

and

$$\xi_i^{SH} = - \sum_{j=1}^2 \frac{2\rho_j}{3} g_{ij}(\sigma_{ij}) \left[\frac{2\mu_{ij}}{\pi k_B T} \right]^{1/2} \times \int_0^\infty dk [K \sigma_{ij} \cos(K \sigma_{ij}) - \sin(K \sigma_{ij})] \hat{V}_{ij}^S(K). \quad (32)$$

Here ρ_j is the number density of the j th species. Furthermore, $\hat{G}_{ij}(K)$ and $\hat{V}_{ij}^S(K)$ are the Fourier transforms of total correlation function $[g_{ij}(r) - 1]$ and the soft part of the potential $V_{ij}^S(r)$. μ_{ij} is the reduced mass. Here $\hat{G}_{ij}(K)$ and $\hat{V}_{ij}^S(K)$ are given by

$$\hat{G}_{ij}(K) = [S_{ij}(K) - \delta_{ij}] (\rho_i \rho_j)^{-1/2}, \quad (33)$$

$$\hat{V}_{ij}^S(K) = \frac{3\pi\epsilon_{ij}}{K^3} [A_{ij} K \sigma_{ij} \cos(A_{ij} K \sigma_{ij}) - \sin(A_{ij} K \sigma_{ij}) - K \sigma_{ij} \cos(K \sigma_{ij}) + \sin(K \sigma_{ij})], \quad (34)$$

TABLE III. Friction coefficients in liquid Cd-Ga alloy.

Temperature (K)	Atomic fraction of Cd	$\xi_i^H/k_B T$ (10 ⁵ s/cm ²)		$\xi_i^S/k_B T$ (10 ⁵ s/cm ²)		$\xi_i^{SH}/k_B T$ (10 ⁵ s/cm ²)	
		Cd	Ga	Cd	Ga	Cd	Ga
569.0	0.20	0.2590	0.2100	0.1060	0.0713	0.3140	0.2170
	0.40	0.2660	0.2145	0.1200	0.0723	0.3360	0.2290
	0.45	0.2676	0.2154	0.1230	0.0726	0.3410	0.2320
	0.50	0.2692	0.2165	0.1250	0.0730	0.3460	0.2340
	0.55	0.2708	0.2175	0.1260	0.0733	0.3510	0.2370
	0.60	0.2724	0.2184	0.1310	0.0736	0.3560	0.2400
	0.80	0.2786	0.2220	0.1380	0.0748	0.3760	0.2500

TABLE IV. Self- and mutual diffusion coefficients in liquid Cd-Ga alloy at various concentrations.

Temperature (K)	Atomic fractions of Cd	D_{Cd} (10^{-5} cm ² /s)	D_{Ga} (10^{-5} cm ² /s)	$D_{\text{Ga-Cd}}$ (10^{-5} cm ² /s)	$D_{\text{Ga}}/D_{\text{Cd}}$
569.0	0.20	1.471	2.004	1.577	1.362
	0.40	1.385	1.939	1.606	1.400
	0.45	1.366	1.923	1.617	1.407
	0.50	1.349	1.908	1.628	1.414
	0.55	1.332	1.893	1.641	1.424
	0.60	1.316	1.879	1.654	1.427
	0.80	1.259	1.825	1.714	1.449

where ϵ_{ij} and A_{ij} are the depth and breadth of the square-well potential.

V. RESULTS AND DISCUSSIONS

In the Tables III and IV the computed results for the friction constant and diffusion coefficient are given. Unfortunately no experimental data are available for the Cd-Ga melt. From Table III it is clear that in the case of friction constant the hard-sphere part is maximum.

From the Table IV we observe that D_{Cd} and D_{Ga} decreases with increase in the concentration of Cd. The ratio $D_{\text{Ga}}/D_{\text{Cd}}$ varies slightly and can be considered as almost constant as in the case of ideal mixing of liquids throughout the range of calculations, that is, from 0.20 to 0.80 atomic fraction of Cd.

Evidently the volume changes due to various composition appears to be very small and hence the present method of calculation of the melt assuming ideal mixing gave exact number densities and hence correct total structure factors. Whenever there is not much of a variation in volumes from that of an ideal mixture, then the regular solution theory^{24,25} predicts the ratio of the diffusion coefficients of the constituents to be constant. Thus it is expected that $D_{\text{Ga}}/D_{\text{Cd}}$ should yield a constant

value and should be independent of composition of the constituents.

So far a good theory does not exist in the evaluation of mutual diffusion coefficient D_{12} .^{26,28} However, it can be approximately written as $D_{12} = C_2 D_1 + C_1 D_2 +$ correction term when C_i is the usual atomic fraction and the correction term accounts for the cross-correlation term between D_1 and D_2 . This correction term is generally negligible. We have given in Table IV the mutual diffusion coefficient $D_{\text{Ga-Cd}}$ calculated from the above equation.

It may be pointed out in conclusion that the various parameters used in these calculations have been obtained for pure metals in the computation of their (pure metal) structure factors and these are used conclusively to explain the total structure factors and also the diffusion coefficient. It may be pointed that the partial structure factors are very important in predicting several other transport properties like resistivity²⁹ and viscosities.^{30,31}

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