Indian Journal of Pure & Applied Physics
Vol. 46, June 2008, pp. 394-396

Electronic transport property of liquid Cd-Te alloys

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Received 28 October 2007; revised 22 February 2008; accepted 4 April 2008

The temperature dependent electrical resistivity of liquid $Cd_{0.6}Te_{0.4}$ alloys has been studied theoretically by employing Faber-Ziman formula. Also, the Faber-Ziman formulation is used to generate the partial structure factor of the liquid $Cd_{0.6}Te_{0.4}$ alloys at 1062°C. The electron-ion interaction is incorporated through a newly proposed local model potential alongwith Ichimaru-Utsumi (IU) dielectric screening function. Good agreement is achieved between the presently calculated results of resistivity with the experimental findings. Resistivity of liquid $Cd_{0.6}Te_{0.4}$ shows a semiconducting behaviour in the liquid phase. Thus, the resistivity data for Cd-Te system are in qualitative agreement with the nearly-free electron picture.

Keywords: Semiconductors, Liquid alloys, Electronic transport properties, Liquid structures, Pseudopotential

1 Introduction

Among II–VI semiconductors, cadmium tellurides (Cd_xTe_{1-x}) and its alloys have special technological interest. Due to large atomic number and high band gap at room temperature, CdTe alloys are employed to fabricate electro-optic devices, high-performance infrared detectors, gamma-ray detectors and room-temperature radiation detectors.

Experimentally, Ben Moussa *et al*[12]. had shown the temperature dependent electrical resistivity (ρ) and thermoelectric power (S) of liquid Cd_xTe_{1-x} and found that thermoelectric power is minimum at x=0.6 for the concentration of Cd. In the present study, we have investigated theoretically the temperature (T) dependent electrical resistivity (ρ) of liquid Cd_xTe_{1-x} near x=0.6 with the help of pseudopotential formalism. Recently, proposed model potential by Gajjar *et al.*[1,2] is used to describe the electron-ion interaction of the complex system is of the form.

$$V_B(q) = \frac{-4\pi Z \exp|2|}{\Omega_0 q^2 U (1+U^2)^4} \begin{Bmatrix} \cos(U)[2U^3 \exp|-1|(U^4+2U^2-23)]+ \\ \sin(U)[2U^2 \exp|-1|(23U^2+7U^4+ \\ U^6-7)+(1+U^2)^4] \\ +2U^3(11-14U^2-U^4) \end{Bmatrix} \quad \ldots(1)$$

where $U = qr_c$ Z, Ω_o, q and r_c are valency, atomic volume, magnitude of the momentum transfer vector and the parameter of the potential, respectively. In the present paper, the parameter of the potential given by Thakor *et al.*[3-5]. is determined using $q = q_0$ condition.

The approach of Faber and Ziman[6] is used to study the temperature dependence of the electrical resistivity of liquid $Cd_{0.6}Te_{0.4}$ binary mixture. In the present computation of electrical resistivity of liquid Cd-Te, the local field correction function due to Ichimaru and Utsumi[7] is employed for the first time to investigate the effect of exchange and correlation effects with reference to the static Hartree[8] (H) screening function. The mathematical expressions of these two local field correction functions used in the present computations are as follows.

$$f_{IU}(q) = AX^4 + BX^2 + C + \begin{Bmatrix} \left[AX^4 + \left(B + \frac{8}{3}B\right)X^2 - C\right] \\ \frac{(4-X^2)}{4X}\ln\left|\frac{2+X}{2-X}\right| \end{Bmatrix} \quad \ldots(2)$$

and

$$f_H(q) = 0 \quad \ldots(3)$$

where A, B and C are the constants of IU local field correction functions, and $X = q/k_F$ with $K_F = \left(3\pi^2 Z/\Omega_0\right)^{1/3}$ being the Fermi wave vector of the alloys, respectively.

2 Theory

Formulation of electrical resistivity for binary alloys given by Faber and Ziman[6]:

$$\rho = \frac{3\pi m^2}{4e^2 \hbar^3 k_F^6 n} \int_0^{\infty} S(q) \left| V(q) \right|^2$$

$$q^3 \theta(2k_F - q)\, dq \qquad \ldots(4)$$

where n is the electron density related to the Fermi wave number, θ the unit step function that cuts off the q-integration at $2k_F$ corresponding to a perfectly sharp Fermi surface, S(q) the structure factor and V(q) the screened ion pseudopotential form factor.

From the rearrangements of the various constants, one can write the formula for the electrical resistivity of the binary alloys in the following form:

$$\rho = \frac{12\ \Omega}{k_F^2} \int_0^{2k_F} \lambda(q)\, q^3\ dq \qquad \ldots(5)$$

with

$$\lambda(q) = (1-x) S_{11}(q) V_1^2(q) + 2\left[x(1-x)\right]^{1/2}$$

$$S_{11}(q) S_{22}(q) V_1(q) V_2(q) + x S_{22}(q) V_2^2(q) \ldots(6)$$

Here V_1(q) and V_2(q) denote the model potentials for elements *A* and *B*, S_{ij}(q) are the partial structure factors of the binary metallic complexes, x is the concentration of the first metallic component of A_xB_{1-x} mixture.

3 Results and Discussion

The input parameters used in the present computations are presented in Table 1. Moreover, packing fraction of liquid $Cd_{0.6}Te_{0.4}$ is kept at 0.45.

Faber and Ziman[9] (FZ) formulations has been used to generate the partial structure factors of the binary alloys calculated from the Ashcroft and Langreth[10] (AL) partial structure factors S_{ij}(q). Fig. 1 shows the partial structure factors of liquid $Cd_{0.6}Te_{0.4}$ along with neutron-scattering experimental data given by Prigent *et al.*[11] at temperature 1062°C.

The first and second peaks in the S_{ij} (q) of liquid $Cd_{0.6}Te_{0.4}$ is observed at 2.33 Å^{-1} and 4.52 Å^{-1}, respectively (experimentally[11] found at 2.88 Å^{-1} and 4.52 Å^{-1}, respectively). Thus, the oscillating behaviour of the S(q) suggest that there is a considerable ordering in the liquid $Cd_{0.6}Te_{0.4}$ which is induced by electron transfer from the Cd towards the Te atom. In particular, local order determination was made through analysis of neutron-scattering experiments[11] and suggests that liquid CdTe conserves its crystalline open structure environment with the coordination number of ~6.

Table 1 — Input parameters

Element	Z	T (°C)	Ω_0 (a u)	r_c (a u)
Cd	2	1080	168.3344	2.0658
		1090	168.4194	2.0661
		1100	168.5037	2.0665
		1110	168.5873	2.0668
		1120	168.6702	2.0672
Te	6	1080	260.7115	1.5968
		1090	260.8675	1.5971
		1100	261.0222	1.5975
		1110	261.1755	1.5978
		1120	261.3276	1.5981

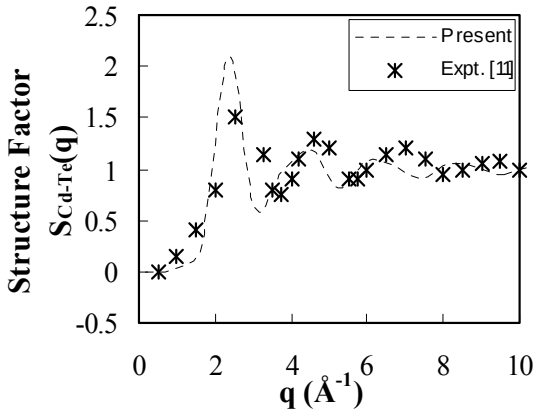

Fig. 1 — Structure factor of liquid $Cd_{0.6}Te_{0.4}$ at 1062°C

The temperature dependence of the electrical resistivity (ρ) is examined at the concentration of Cd; x = 0.6. In Figure 2, the present outcomes of ρ for liquid $Cd_{0.6}Te_{0.4}$ are shown along with the experimental results given by Ben Moussa *et al*[12]. The resistivity ρ decreases with increase in T indicates semiconducting nature; liquid $Cd_{0.6}Te_{0.4}$ has a negative temperature coefficient of ρ ($d\rho/dT < 0$).

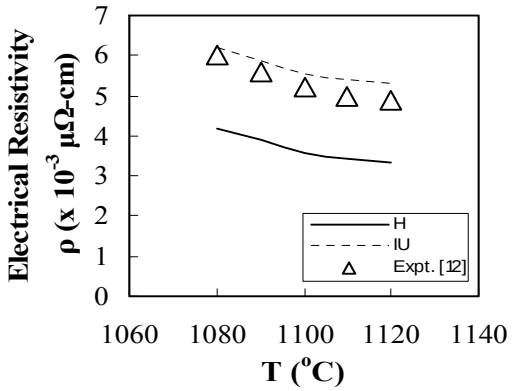

Fig. 2 — Temperature dependent resistivity of liquid $Cd_{0.6}Te_{0.4}$

4 Conclusions

The present results due to Ichimaru and Utsumi[6] local field correction function is found to be in good agreement with the experimental results. Liquid $Cd_{0.6}Te_{0.4}$ has a semiconducting behaviour in the liquid phase. The work is in progress to calculate temperature dependent resistivity and thermoelectric power of liquid Cd_xTe_{1-x} at various concentration of Cd alongwith different local field correction functions. The overall picture of the present computations thus, confirms not only the applicability of our model potential for study of the structure factor of II–VI semiconductor binary alloys but it also establishes the use of more prominent dielectric functions in the study of electronic transport properties of such complex binary mixtures.

Acknowledgement

The financial assistance from University Grants Commission, New Delhi, is duly acknowledged.

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