Theoretical Study of Electrical Transport Properties of $Bi_{1-X}Ga_X$ Binary Alloys using Pseudopotential Theory

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Abstract

In the present work, we report the electrical transport properties of $Bi_{1-X}Ga_X$ binary alloys theoretically by employing our well-known pseudopotential model. The screening influences are studied by using various exchange and correlation functions in the aforesaid study. The present results of electrical resistivity are found to be in qualitative agreement with available experimental data in the literature.

***Keywords*:** Electrical resistivity, Thermoelectric power, thermal conductivity, pseudopotential, exchange and correlation functions

I. INTRODUCTION

The semiconductor device technology is widely used in computationally control systems, computers, telephones, medical instruments, automobiles and household appliances etc. A proper understanding of the electronic properties of materials is only possible when the electrons are described by quantum mechanically. The properties of electronic materials and the interfaces between electronic materials can be used to explain the behavior of a variety of semiconductor devices such as light emitting diodes, solid state lasers, sensors, bipolar transistors and field effect transistors etc. Therefore, to understand the electronic structure of the semiconductor materials, the electronic transport properties plays an important role and show fascinating interest for research community [1-8] widely. The electronic transport properties of liquids can be extensively described by simple model suggested by Faber and Ziman (FZ) [4]. They have calculated the electrical resistivity of liquid metals using pseudopotentials and interference functions. Here, we report the electrical transport properties of liquid $Bi_{1-X}Ga_X$ binary alloys using FZ model [4] with our well-recognized model potential [9]. Seven different types of exchange and correlation functions viz. Hartree (H) [10], Hubbard-Sham (HS) [11, 12], Vashistha-Singwi (VS) [13], Taylor (T) [14],

Ichimaru-Utsumi (IU) [15], Farid *et al.* (F) [16] and Sarkar *et al.* (S) [17] are used to described the screening influences on the aforesaid properties.

2. THEORETICAL METHODOLOGY

The FZ's model is used for computation of electrical resistivity of binary alloys [1-8],

$$\rho = \frac{12\Omega_O}{k_F^2}\int_0^{2k_F}\begin{bmatrix}(1-X)S_{11}(q)V_{11}^2 + XS_{22}(q)V_{22}^2 \\ +2\sqrt{X(1-X)}S_{12}(q)V_{11}(q)V_{22}(q)\end{bmatrix}qdq. \quad (1)$$

Where, $V_{11}(q)$ and $V_{22}(q)$ represents the form factors of the model pseudopotential for two metallic elements A and B, while $S_{ij}$are the partial structure factors [3] with X the concentration of the second metallic component. The notation of the thermoelectric power (TEP) is narrated as [1-8],

$$TEP = -\left[\frac{-0.001795T(3-2\lambda(q)/q)}{E_F}\right] \quad (2)$$

The thermal conductivity is calculated by the following expression [1-8]

$$\sigma = \left(\frac{\pi^2 k_B^2 T}{3|e|^2\rho}\right) \quad (3)$$

Here, e, E_F, T and k_B are the electronic charge, Fermi energy, temperature and the Boltzmann's constants, respectively. Our well-known model pseudopotential [9] applied in the present computation is of the form

$$W(r) = \begin{cases} -\frac{Ze^2}{r_C^3}\left[2 - exp\left(1-\frac{r}{r_C}\right)\right]r^2 & for \quad r \le r_C \\ -\frac{Ze^2}{r} & for \quad r \ge r_C \end{cases}. \quad (4)$$

The detail of the model potential is narrated in our earlier paper [9]. Here r_C is the model potential parameter.

3. RESULTS AND DISCUSSION

The input parameters and constants used in the present work are shown in Table 1. The calculated results of the electrical transport properties of $Bi_{1-X}Ga_X$ binary alloys are presented in Figs. 1-3 with available experimental [5] data.

Table 1: The input parameters and constants.

Metal	Z	Ω_O (au)	η	r_C (au)
Bi	5	239.4	0.40	1.9644
Ga	3	131.4	0.43	1.6084

The electrical resistivity (ρ) at different concentration is displayed in Fig. 1 alongwith the available experimental results [5]. It is observed that the present results due to T-function are found in higher in comparison with other screening function. The relative impact of all exchange and correlation functions with H-function on the electrical resistivity (ρ) results is found in the range of 7.83%-

53.54%. The theoretical results are found to be in qualitative agreement with experimental data [5] and our data are not showing any type of parabolic nature in the results because of some limitations for fitting the potential parameter. The presently calculated thermoelectric power (TEP) is displayed in the Fig. 2. It is noted that, the H-function gives the extreme numerical value of the TEP, while those due to T-function gives the smallest value with the other functions. Also, the presently obtained results of the thermal conductivity (σ) is seen in Fig. 3. It can be observed that, the present yielding of it computed through H-function show higher fallouts while T-function produce lower values in comparison with the other functions. Absence of the experimental data of thermoelectric power (TEP) and thermal conductivity (σ), such calculated data may be considered as one of the proper choices for further examination or study. The improvement in the present results may be reached either by incorporating other forms of exchange and correlation effects or by suggesting the modification in determining the parameter of the potential.

4. CONCLUSION

The present effort of studying the electrical transport properties of $Bi_{1-X}Ga_X$ binary alloys not only confirms the importance of the pseudopotential theory, but it also establishes the proper choice of more promising exchange and correlation functions too. The presently computed results of electrical resistivity are found to be in qualitative agreement with the available experimental data.

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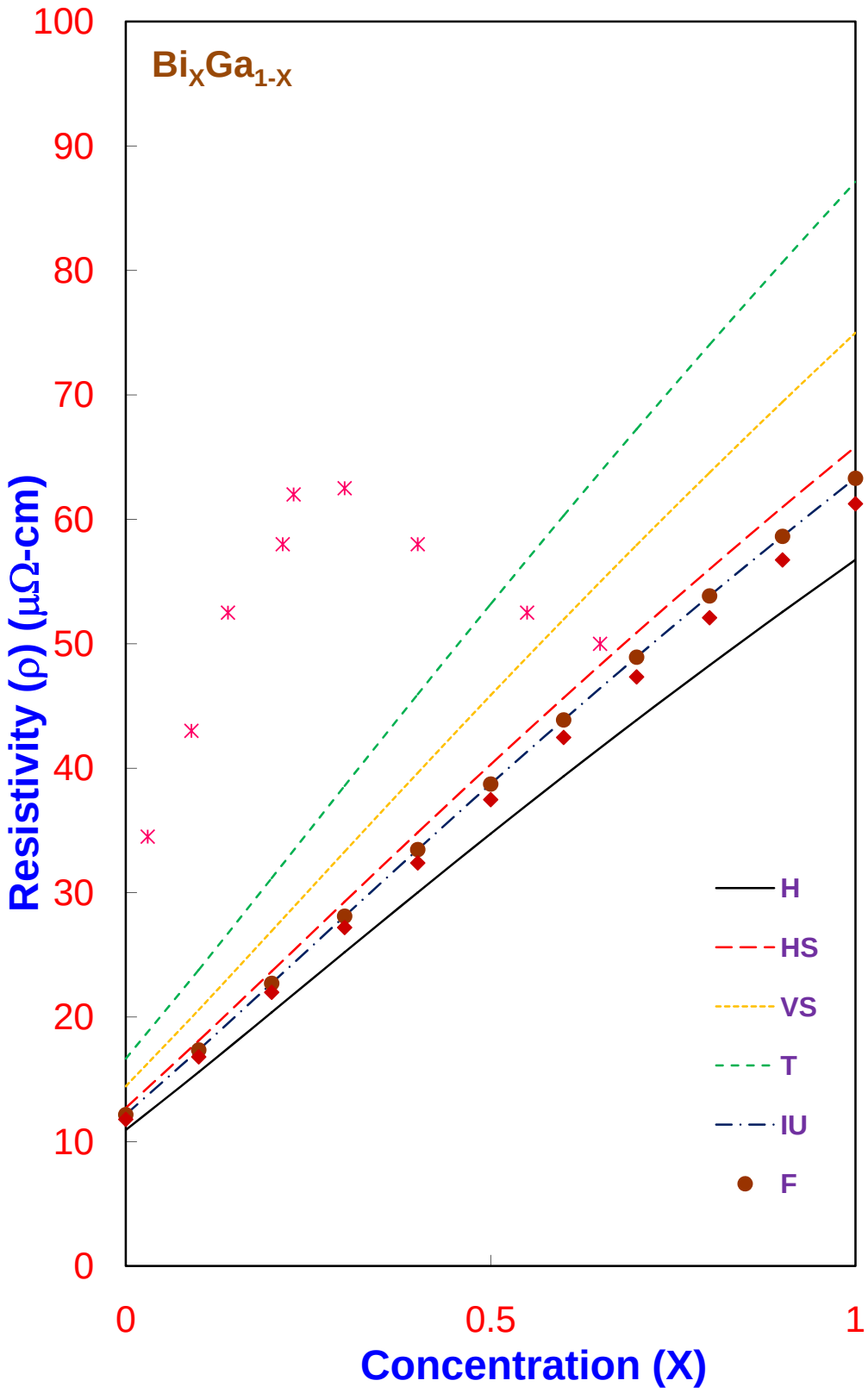

Figure 1. Electrical Resistivity (ρ) of $Bi_{1-X}Ga_X$Binary Alloys.

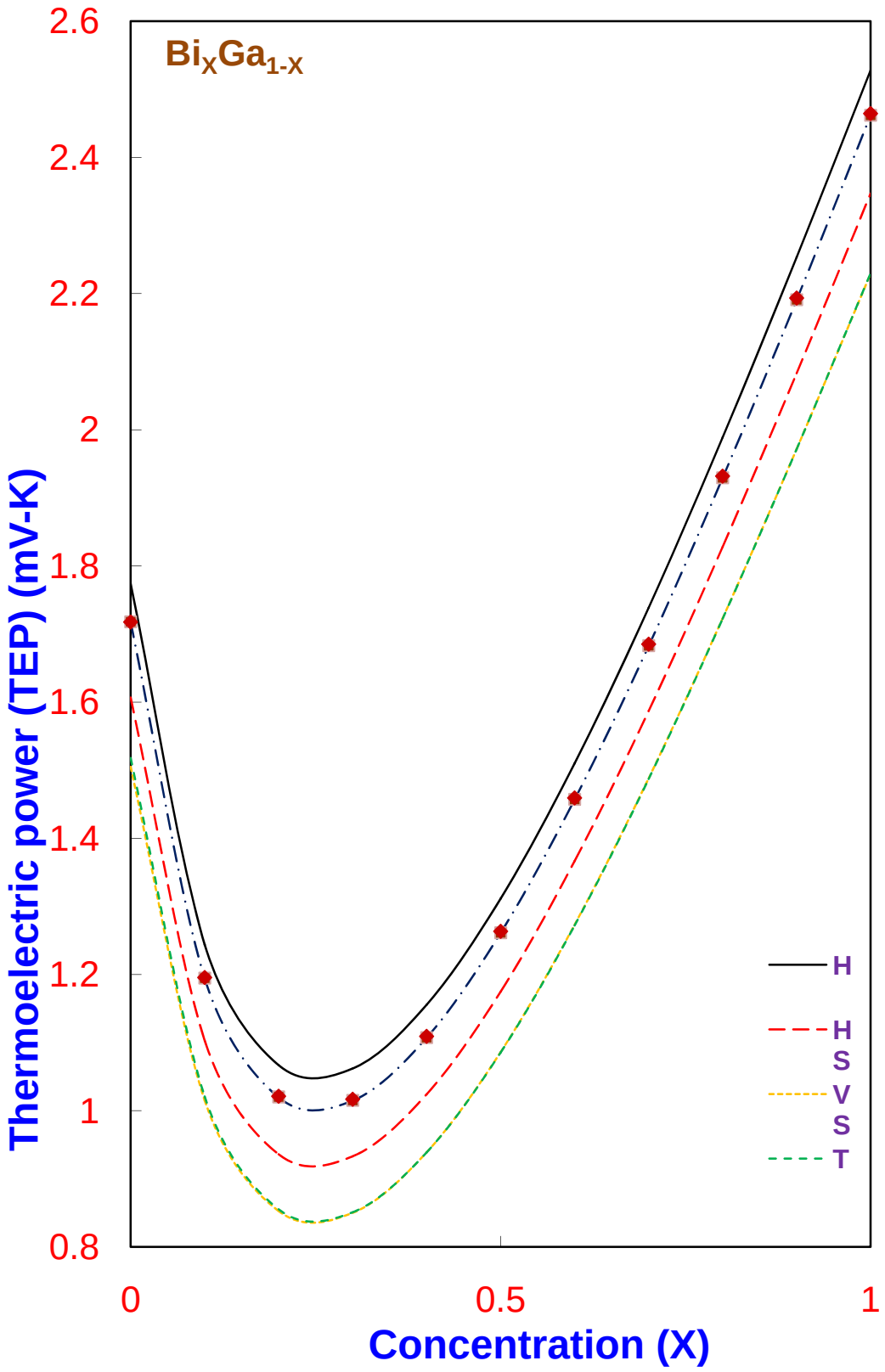

Figure 2. Thermoelectric Power (TEP) of $Bi_{1-X}Ga_X$ Binary Alloys.

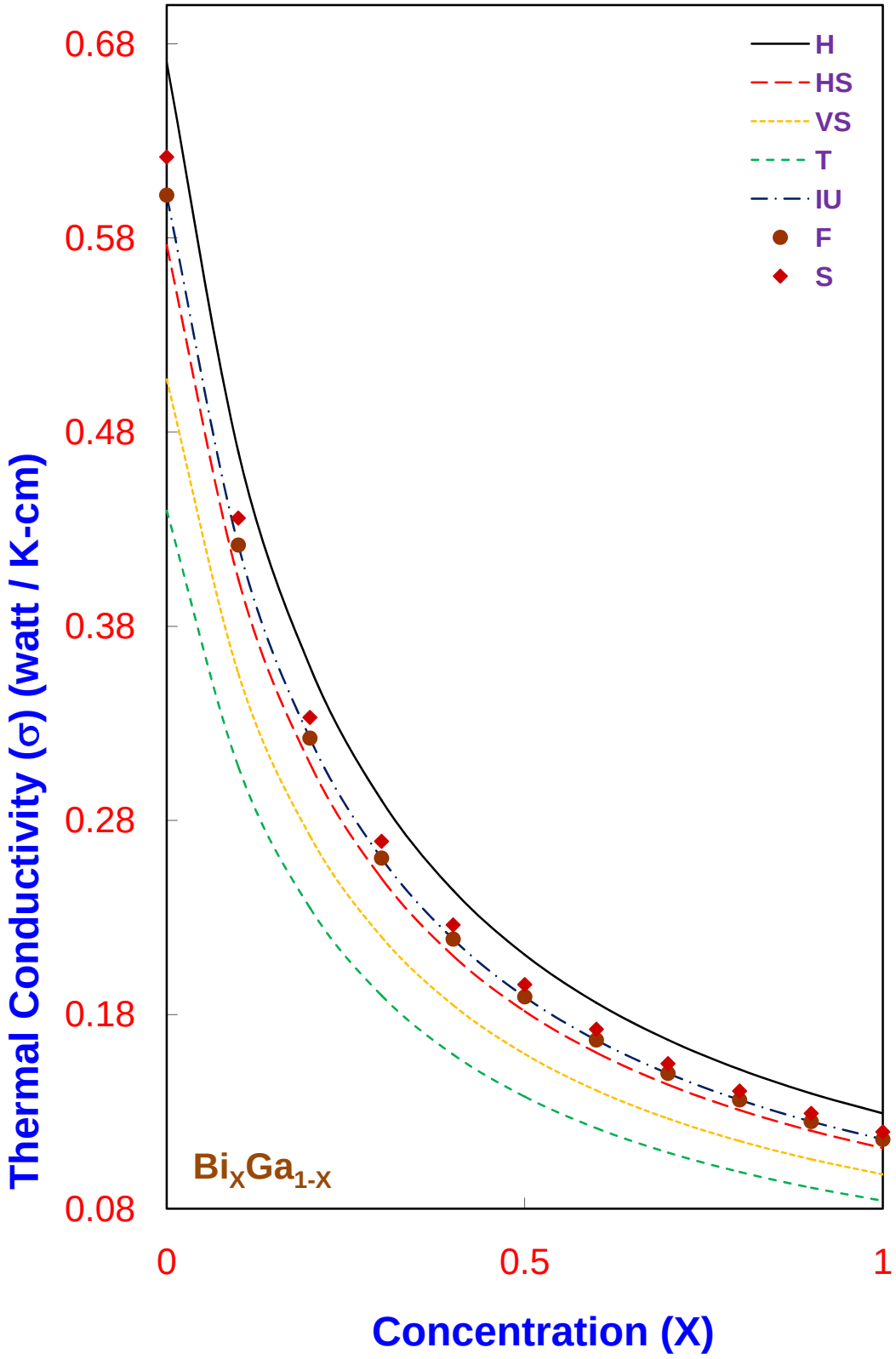

Figure 3. Thermal Conductivity (σ) of $Bi_{1-X}Ga_X$Binary Alloys.

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