

Pseudopotential-based study of electrical transport properties inherent to Bi-Ga alloys

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Abstract. In this paper, we account the electrical transport properties of Bi-Ga alloys studied theoretically by employing our well-known model pseudopotential. The impact of various screening functions was studied using various exchange and correlation functions in the aforesaid investigation. The obtained results on electrical resistivity are found to be in qualitative agreement with the experimental data in available literature.

Keywords: electrical transport properties, electrical resistivity, thermal conductivity, thermoelectric power, pseudopotential, exchange and correlation functions.

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1. Introduction

The semiconductor device technology is extensively used in computers, computational control systems, medical instruments, automobiles and household appliances, telephones *etc.* An appropriate consideration of the electronic transport properties of metals and their alloys is only conceivable when electrons are designated using quantum-mechanical approach. The properties of electronic materials and interfaces between electronic materials are used to elucidate behavior of a variety of semiconductor devices, namely: solid-state lasers, light emitting diodes, bipolar transistors, sensors and field effect transistors *etc.* Therefore, to understand the electronic structure of the semiconductor materials, the electronic transport properties play an important role and show fascinating interest for research community [1-8]. The electronic transport properties of liquids can be extensively described by the simple model suggested by Faber and Ziman (FZ) [4]. They have computed the electrical resistivity of liquid metals using pseudopotentials and interference functions. Here, we report the electrical transport properties of liquid Bi-Ga alloys using this FZ model [4] with our well-recognized model potential [9]. The different exchange and correlation functions proposed by 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 describe the screening influences on the aforesaid properties.

2. Theoretical basis

The FZ model is used for calculating the electrical resistivity of Bi-Ga alloy [1-8],

$$\rho = \frac{12\Omega_0}{k_F^2} \int_0^{2k_F} \left[(1-X)S_{11}(q)V_{11}^2 + X S_{22}(q)V_{22}^2 + 2\sqrt{X(1-X)}S_{12}(q)V_{11}(q)V_{22}(q) \right] q dq. \quad (1)$$

Here, $V_{11}(q)$ and $V_{22}(q)$ represent form-factors of our model pseudopotential [9] for two metallic substances *A* and *B*, while S_{ij} are the partial structure factors [3] with *X* being the concentration of the second metallic substance. The notation of the thermoelectric power (TEP) is narrated as [1-8]:

$$TEP = - \left(\frac{\pi^2 k_B^2 T}{3|e|E} \chi \right)_{E=E_F}, \quad (2)$$

with

$$\chi = 3 - \frac{2S(2k_F)V^2(2k_F)}{\langle S(k)|W(k)|^2 \rangle}. \quad (3)$$

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

$$\sigma = \frac{\pi^2 k_B^2 T}{3|e|^2 \rho}. \quad (4)$$

Here, e , E_F , T and k_B are the electronic charge, Fermi energy, temperature and the Boltzmann constant, respectively. Our well-known model pseudopotential [9] applied in the present computation is of the form:

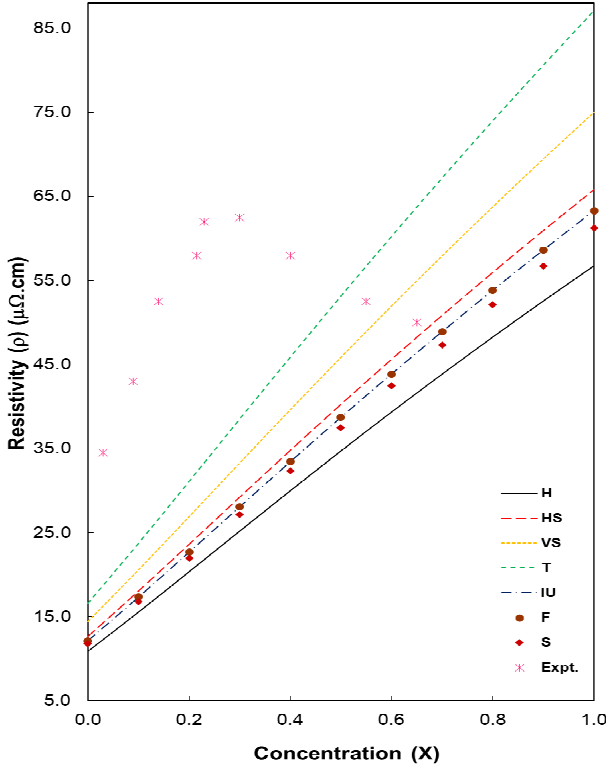


Fig. 1. Electrical resistivity (ρ) of Bi-Ga alloys.

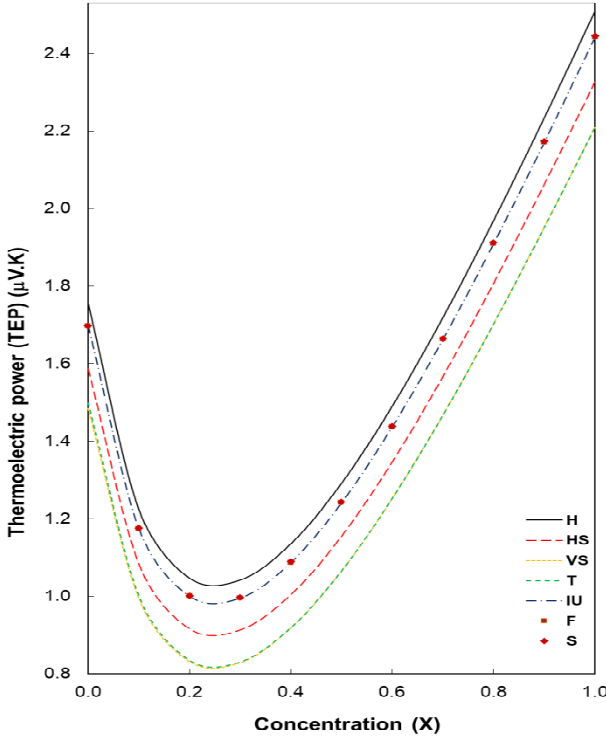


Fig. 2. Thermoelectric power of Bi-Ga alloys.

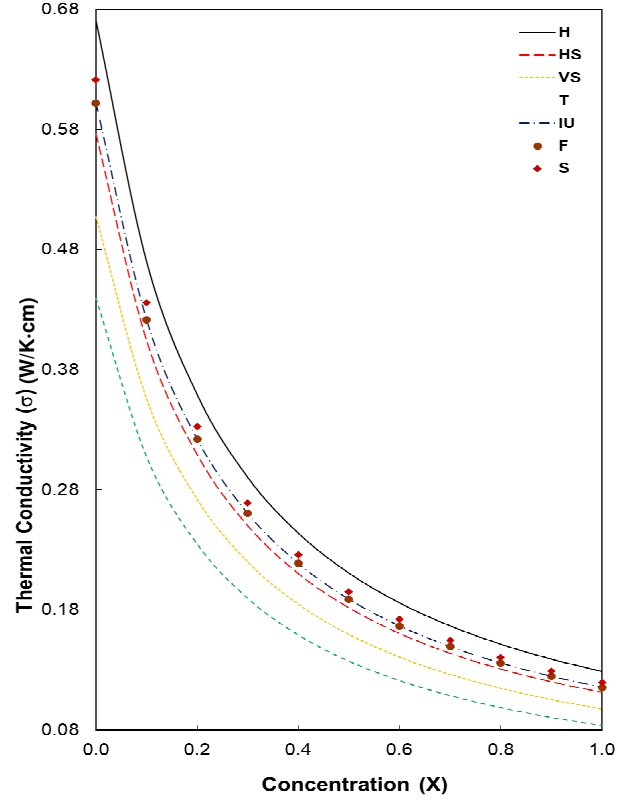


Fig. 3. Thermal conductivity (σ) of Bi-Ga alloys.

$$W(r) = \begin{cases} -\frac{Ze^2}{r_C^3} \left[2 - \exp\left(1 - \frac{r}{r_C}\right) \right] r^2 & \text{for } r \leq r_C \\ -\frac{Ze^2}{r} & \text{for } r \geq r_C \end{cases} \quad (5)$$

The details of such model pseudopotential have been discussed in our earlier paper [9]. Here, r_C is the model potential parameter.

3. Results and discussion

The input data and other constants used in the said work are shown in Table. While, calculated outcomes of the electrical transport properties inherent to Bi-Ga alloys are presented in Figs. 1 to 3 with experimental data [5] available in literature.

The electrical resistivity (ρ) at different concentrations is displayed in Fig. 1 along with the experimental results [5]. It is observed that the present yielding obtained from the T -function is shown above in comparison with other screening functions. The relative impact of all the exchange and correlation functions with respect to H -function on the electrical resistivity (ρ) results is found within the range of 7.83% to 53.54%.

The input parameters and constants.

Metal	Z	Ω_0 (a.u.)	η	r_C (a.u.)
Bi	5	239.4	0.40	1.9644
Ga	3	131.4	0.43	1.6084

However, the theoretical outcomes are shown to be in qualitative agreement with existing experimental yielding [5], and our data are not showing any kind of parabolic nature in the present results because of some limitations for fitting the potential parameter. The presently obtained thermoelectric power (TEP) is displayed in Fig. 2. It is noted that the H -function provides the extreme numerical value of TEP, while those due to T -function provides the smallest value as compared with the other screening functions. Also, currently obtained data of the thermal conductivity (σ) is seen in Fig. 3. It can be seen that the present yielding of it computed through H -function shows higher fallouts in comparison with other screening functions, while T -function produces lower outcomes. In absence of either theoretical or experimental data of TEP and thermal conductivity (σ), such calculated data may be considered as one of the proper choices for further examination or study. The enhancement in the current results may be reached either by including other types of the exchange and correlation functions or by signifying alteration in shaping the model pseudopotential parameter.

4. Conclusion

The present effort of obtaining the electrical transport properties of Bi-Ga alloys not only confirms the importance of the pseudopotential theory but also establishes the appropriate choice of more promising exchange and correlation functions, too. At the same time, the currently calculated outcomes of the electrical resistivity are observed in qualitative agree with existing experimental data.

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