Commun. Theor. Phys. (Beijing, China) **51** (2009) pp. 550–554
Vol. 51, No. 3, March 15, 2009

Transport Properties of Si and Ge Liquid Semiconductor Metals

Aditya M. Vora*
Humanities and Social Science Department, S.T.B.S. College of Diploma Engineering, Opp. Spinning Mill, Varachha Road, Surat 395 006, Gujarat, India

(Received June 5, 2008; Revised September 22, 2008)

Abstract *In the present article, we study the electrical resistivity ρ, the thermoelectric power (TEP) α, thermal conductivity σ, Knight-Shifts and temperature coefficient of the Knight-Shifts of the liquid Si and Ge using the well known model potential for the first time. The structure factor used in the present work is derived from the Percus–Yevick (PY) theory. Various local field correction functions are used to study the screening influence. The present results of resistivity are found in qualitative agreement with available experimental and theoretical whenever exists.*

PACS numbers: 72.10.-d, 71.15.Dx, 71.45.Gm, 72.15.Cz, 76.60.Cq, 81.05.Bx
Key words: pseudopotential, electrical resistivity, thermoelectric power, Knight Shift, PY theory, local field correction functions

1 Introduction

During the last several years there has been an increasing interest in the properties of non-crystalline conductors such as liquid metals and liquid metallic alloys. Such a liquid exhibits metallic as well as fluid-like behavior and hence can help to make a link between the theory of the liquid states and the theory of the electronic states in metals. And hence the study of electrical transport properties of liquid metals and their alloys remain one of the favourite quantities either experimentally or theoretically.[1−16] The physical properties of complex systems are a subject of considerable interest in both fundamental and applied physics. A large work of research has been focused on semiconductors in general Ge and Si in particular. This is because of its importance in technological applications such as electronic devices. Despite the rich accumulation of experimental studies, the atomistic approach to the problem of the liquid metals had been very slow in progress, until Ziman[4] proposed the theory of electrical resistivity of liquid metals.

Recently, the dc electrical resistivities of liquid Ga-Sb and In-Sb alloys have been reported by Aoki *et al.*[10] experimentally. Also, the electrical resistivity and the thermoelectric power of liquid Au-Si alloys have been measured by Tatsuya and Satoru[11] as a function of temperature using Fabcr–Ziman theory.[1−16] The electrical resistivity of liquid Rb-Pb and Cs-Pb alloys as a function of composition and temperature are reported by Meijer *et al.*[12] Mott[13] has studied electrical resistivity of some liquid metals and this alloys using model potential formalism. Grosdidier *et al.*[14] have studied the structure and electrical resistivity of liquid Ni-Ge alloys using neutron diffraction method. Schnyders and Zytveld[15] have very carefully measured the electrical resistivity and thermoelectric power of liquid Ge and Si using the Ziman formalism, with a recent pseudopotential and the experimental structure factor. They found that the thermoelectric power calculations are much more sensitive to the structure factor and evaluated this property using experimental structure factor but their results were very poor while the resistivity deviates about 38% for Ge and 11% for Si, from the experimental data. Bose *et al.*[16] have reported the transport properties of liquid Si and Ge semiconductors. Also, very recently we have reported electrical and magnetic transport properties of some liquid metals and liquid alloys.[7−9]

During the last several decades the concepts of pseudopotential have played an important role in the theory of liquid metals and their alloys.[1−16] Also, to the best of our knowledge after 1993, the transport properties of such type of the liquid metals of the different groups of the periodic table have been reported by researchers very rare in the literature. Keeping in mind the cardinal features of this developments, in the present article we are intended to report the transport properties viz. electrical resistivity ρ, the thermoelectric power (TEP) α, thermal conductivity σ, Knight-Shifts and temperature coefficient of the Knight-Shifts of liquid Si and Ge semiconductors based on the well known empty core model EMC potential of Ashcroft.[17] In the present work, the theoretical structure factors are computed from the well known Percus–Yevic PY hard sphere model with proper packing density.[18] Seven different types of the local field correction functions proposed by Taylor (T),[19] Ichimaru–Utsumi (IU),[20] Farid *et al.* (F)[21] and Sarkar *et al.* (S)[22] are employed for the first time to investigate the

---

*E-mail address: voraam@yahoo.com; Permanent address: Parmeshwari 165, Vijaynagar Area, Hospital Road, Bhuj–Kutch, 370 001, Gujarat, India

influence of exchange and correlation effects with reference to the static Hartree (H)[23] screening function in the present computations.

2 Theoretical Methodology

The Faber[4] approach of investigating electrical resistivity of liquid metals assumes the model of a gas of conduction electrons which interact with and are scattered by irregularly placed metal ions. As an external electric field drives the electron through the disordered medium, the scattering determines the electrical resistance, which can be calculated using perturbation theory: the transition rate from an initial state $|\boldsymbol{k}\rangle$ to the final state $|\boldsymbol{k}+\boldsymbol{q}\rangle$ on the Fermi level with the density of state is given by

$$P(\theta)=\frac{2\pi}{\hbar}|\langle \boldsymbol{k}+\boldsymbol{q}|\,W\,|\boldsymbol{k}\rangle|^2\,\frac{1}{2}\,N_{FE}(E_F)\,, \tag{1}$$

where θ is the angle between $\boldsymbol{k}$ and $\boldsymbol{k}+\boldsymbol{q}$, the factor 1/2 arises from the fact that electron spin does not change on scattering. Now the conductivity in the relaxation time approximation is given by

$$\sigma=\frac{1}{3}e^2v_F^2\tau N_{FE}(E_F)\,. \tag{2}$$

Here e is electronic charge, v_F velocity of the electrons at the Fermi level and τ the relaxation time. The relaxation time τ is given by

$$\frac{1}{\tau}=\int(1-\cos\theta)P(\theta)\,\mathrm{d}\Omega\,, \tag{3}$$

where θ is scattering angle, Ω is solid angle and $P(\theta)$ is probability for scattering through the angle θ.

Now assuming the free-electron distribution, an expression for the electrical resistivity of liquid metal in terms of the average of the product of the structure factor and pseudopotential matrix element can be written as[1−16]

$$\rho=\frac{3\,\pi\,m^2}{4e^2\hbar^3nk_F^6}\int_0^\infty S(q)|V(q)|^2\,q^3\,\mathrm{d}q\theta(2k_F-q)\,, \tag{4}$$

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

The expression of the thermoelectric power (TEP) α is given by[3,4]

$$\alpha=-\Big(\frac{\pi^2k_B^2T}{3|e|E}\,\chi\Big)_{E=E_F}\,, \tag{5}$$

with

$$\chi=3-\frac{2S(2k_F)V^2(2k_F)}{\langle S(q)\,|V(q)|^2\rangle}\,, \tag{6}$$

It is well known that if a temperature gradient is applied to a metal the conduction electrons will carry a heat current along it even though an electric current is prevented from flowing and that indeed they are responsible for the major part of the thermal conductivity. The expression of the thermal conductivity (σ) for the liquid metal can be written as[3,4]

$$\sigma=\Big(\frac{\pi^2k_B^2T}{3|e|^2\rho}\Big)\,. \tag{7}$$

Here, e E, E_F, T, k_B, and χ are the electronic charge, energy, Fermi energy, temperature (in K), the Boltzmann's constants and the term of dimensionless thermoelectric power.

In the free electron approximation the temperature dependence of the Knight-Shifts at a constant volume in the liquid phase is given by[9]

$$\frac{\partial\ln K}{\partial T}=\frac{-3Z}{4T_mE_Fk_F^2}\int_0^\infty a(q)W(q)\Big(\frac{q}{2k_F}\Big)\times\ln\Big|\frac{q+2k_F}{q-2k_F}\Big|\mathrm{d}\left(\frac{q}{2k_F}\right)\,, \tag{8}$$

and the Knight-Shift of a liquid metal is given by[5,9]

$$\frac{K_1}{K_O}=\frac{-3Z}{4E_Fk_F^2}\int_0^\infty a(q)W(q)\Big(\frac{q}{2k_F}\Big)\times\ln\Big|\frac{q+2k_F}{q-2k_F}\Big|\mathrm{d}\left(\frac{q}{2k_F}\right)\,. \tag{9}$$

Here $a(q)$ is the structure factor derived via the Percus–Yevic (PY) hard sphere model[18] and depends only on the packing fraction η, $W(q)$ the form factor, T_M the melting temperature, $E_F=(\hbar k_F^2/2m)$ the Fermi energy and $k_F=(3\pi^2Z/\Omega_O)^{1/3}$ the Fermi wave vector with Ω_O the atomic volume of the liquid metals.

In the present work, we have used Ashcroft's well known empty core (EMC) model potential[17] including seven different types of the local field correlation functions.[19−23] The form factor explored in the present investigation is of the form[17]

$$W(q)=\frac{-4\pi Ze^2}{\Omega_O\,q^2\,\varepsilon\,(q)}\,\cos(qr_C)\,, \tag{10}$$

where Z is the valence, Ω_O the atomic volume, r_C the parameter of the potential and $\varepsilon(q)$ the modified Hartree dielectric function.[23] The parameter of the potential, r_C may be set from appropriate experimental information (e.g., the Fermi surface or ionization energy). In this instance, it was determined by the known electrical resistivities of the liquid metals at the melting points.

3 Results and Discussion

The input parameters and constants viz. valance Z, atomic volume Ω_O, melting temperature T, packing fraction η, and potential parameter r_C of the liquid metals used in the present computations are narrated in Table 1. The input parameters are taken from the literature.[7−9]

The presently computed results of electrical transport properties viz. electrical resistivity ρ, the thermoelectric power (TEP) α, thermal conductivity σ and Knight-Shifts liquid Si and Ge semiconductors are narrated in Tables 2 and 3 with available experimental[15] or theoretical[15,16] data whenever exists in the literature.

Table 1 The input parameters and constants.

Metals	Z	Ω_O (au)^3	T (K)	η	r_C (au)
Si	4	121.48	1733	0.38	0.97
Ge	4	146.25	1253	0.38	1.007

The comparisons for the presently calculated electrical resistivity ρ of Si and Ge liquid metals with available experimental[15] or theoretical[15,16] yielding are narrated in Tables 2 and 3. From Tables 2 and 3 it is noticed that, the present results of the electrical resistivity ρ of the liquid metals are found in qualitative agreement with the experimental or theoretical findings. Also, it is noted that among the five employed local filed correction functions, the local field correction function due to H (without exchange and correlation) gives the minimum numerical value of the electrical resistivity, while the local field correction function due to F gives the maximum value. The present results of the electrical resistivity ρ obtained from S-local field correction function are found very close to the experimental or theoretical data. In comparison with the presently computed results of the electrical resistivity ρ from static H-function, the percentile influences for Si and Ge liquid metals of T, IU, F and S-functions are of the order of 36.71%–175.60% and 18.35%–69.42%, respectively. The calculated electrical resistivity ρ of Si and Ge liquid metals deviate in the range of 5.36%–52.86% and 1.15%–44.80% from the experimental data,[15] respectively.

Table 2 Various properties of Si.

Properties	Present results					Exp.[17]	Others[4,18]
	H	T	IU	F	S		
ρ (in $\mu\Omega\cdot$cm)	37.05	89.23	99.11	102.11	63.22	66.8, 80	41.2, 45.5, 55, 57.4, 66.2, 75.9
α (in μV$\cdot$K)	−13.82	−13.76	−14.06	−13.99	−13.89	−0.3	−1.4, −2.2, −3.5, −3.3, −6.4
σ (in watt/K$\cdot$cm)	0.21	0.09	0.08	0.08	0.12	–	–
K_1/K_O	0.10	0.12	0.10	0.10	0.10	–	–
$K\%$	0.141	0.167	0.146	0.146	0.147	–	–
$\frac{\partial \ln K}{\partial T}$ (in 10^{-4} K^{-1})	0.57	0.68	0.59	0.59	0.60	–	–

Table 3 Verius propertie of Ge.

Properties	Present results					Exp.[17]	Others[4,18]
	H	T	IU	F	S		
ρ (in $\mu\Omega\cdot$cm)	51.28	81.07	84.88	86.88	64.90	60, 75.2	46.3, 57, 66.6,57, 67.3, 69, 180
α (in μV$\cdot$K)	−15.00	−15.29	−15.67	−15.59	−15.29	−2.1	−1.1, −3.6, −10.1
σ (in watt/K$\cdot$cm)	1.06	0.67	0.64	0.63	0.84	–	–
K_1/K_O	−0.35	−0.43	−0.37	−0.37	−0.36	–	–
$K\%$	0.330	0.399	0.345	0.345	0.344	–	–
$\frac{\partial \ln K}{\partial T}$ (in 10^{-4} K^{-1})	1.68	1.90	2.02	2.03	1.76	–	–

The comparisons for the presently calculated thermoelectric power (TEP) α of Si and Ge liquid metals with experimental[15] or theoretical[15,16] yielding are narrated in Tables 2 and 3. From Tables 2 and 3 it is noticed that, the present results of the thermoelectric power (TEP) of liquid metals are found in qualitative agreement with the experimental or theoretical findings. Also, it is noted that, among the seven employed local filed correction functions, the local field correction function due to H (without exchange and correlation) gives the minimum numerical value of the thermoelectric power (TEP) α, while the local field correction function due to IU gives the maximum value. The computed data of the thermoelectric power (TEP) α are found higher than available experimental results. The percentile influences from static H-function on the thermoelectric power (TEP) α for Si and Ge liquid metals of various local field correction functions are found of the order of 0.43%–1.74% and 1.67%–4.47%, respectively. Large percentile deviation are found from the experimental data in the computed results of the thermoelectric power (TEP) α for Si and Ge liquid metals. The higher values of the computed TEP for liquid metals seems impossible to be predicted in terms of the usual pseudopotential formalism for simple metals, since the effect of the d-resonance above the Fermi level appears to give rise to the significant increase in the scattering amplitude in this metal.

The comparisons for the computed thermal conductivity σ of Si and Ge liquid metals are reported in Tables 2 and 3. From Tables 2 and 3 it is noticed that, among the five employed local filed correction functions, the local field correction function due to F gives the minimum numerical value of the thermal conductivity σ, while the local field correction function due to H (without exchange and correlation) gives the maximum value. The experimental or theoretical data of the thermal conductivity σ is not available in the literature for further comparisons. In comparison with the presently computed results of the thermal conductivity σ from static H-function, the percentile influences for Si and Ge liquid metals of various local field correction functions are of the order of 23.81%–61.90% and 15.09%–40.57%, respectively.

From Tables 2 and 3, it can be noted that among the five employed local field correction functions, the local field correction function due to H (without exchange and correlation) gives minimum value of the Knight-Shifts (K_1/K_O) of liquid metals at melting point while the local field correction function due to T gives maximum value. In comparison with the presently computed results of the Knight-Shifts (K_1/K_O) of various local field correction functions with respect to static H-function, the percentile influences for Si and Ge liquid metals are of the order of 5.06%–29.21% and 4.26%–29.79%, respectively. The experimental or theoretical data of the thermal conductivity σ is not available in the literature for further comparisons.

From Tables 2 and 3, it is noticed that among all the employed local field correction functions, the local field correction function due to H (without exchange and correlation) gives minimum value of the Knight-Shifts ($K\%$) of liquid metals at melting point while the local field correction function due to T gives maximum value. In comparison with the presently computed results of the temperature coefficients of Knight-Shift of various local field correction functions with respect to static H-function, the percentile influences for Si and Ge liquid metals are of the order of 4.69%–29.72% and 4.26%–18.44%, respectively. The experimental or theoretical data of the thermal conductivity σ is not available in the literature for further comparisons.

The temperature coefficients of the Knight-Shifts of liquid metals are narrated in Tables 2 and 3. From Tables 2 and 3, it is noticed that among all the employed local field correction functions, the local field correction function due to H (without exchange and correlation) gives minimum value of temperature coefficients Knight-Shifts of liquid metals at melting point while the local field correction function due to T gives maximum value. The experimental or theoretical data of the thermal conductivity σ is not available in the literature for further comparisons. In comparison with the presently computed results of the temperature coefficients of Knight-Shift of various local field correction functions with respect to static H-function, the percentile influences for Si and Ge liquid metals are of the order of 4.85%–29.48% and 5.26%–19.30%, respectively.

The numerical values of the transport properties viz. electrical resistivity ρ, the thermoelectric power (TEP) α, thermal conductivity σ, Knight-Shifts and temperature coefficient of the Knight-Shifts are found to be quite sensitive to the selection of the local field correction function and showing a significant variation with the change in the function. Thus, the calculations of the transport properties viz. electrical resistivity ρ, the thermoelectric power (TEP) α, thermal conductivity σ, Knight-Shifts and temperature coefficient of the Knight-Shifts are one of the sensitive tests for the proper assessment of the form factor of the model potential and in the absence of experimental information such calculations may be considered as one of the guidelines for further investigations either theoretical or experimental. This is very much essential for obtaining concrete conclusions.

It is apparent that for all liquid metals, using the resistivity model of Ziman,[4] better calculated agreement with experimental values was obtained by allowing variation in atomic volume. One could conclude from this information that structure information in resistivity models seems to be required. In the preset work it has been found that one can try a well known local EMC pseudopotential in the theory of the liquid metals. This EMC model potential is capable of giving satisfactory results for electrical transport properties of some liquid metals. But, it is absolutely necessary to examine the stability of the form factor against various local field correction functions before its application for the comprehensive study of metallic properties. This can give a unique combination of the bare-ion pseudopotential with a proper local field correction function and hence one can also decide the nature of screening in the particular metal.

The improvement in the present findings may be achieved either by incorporating other forms of exchange and correlation effects or by suggesting the modification in determining the parameter of the potential. As the structure factor plays an important role in determining these properties, one can also include one component plasma approximation,[24] charge hard sphere approximation,[24,25] soft sphere approximation[26] in the present calculations.

4 Conclusions

Lastly we concluded that, the transport properties viz. the electrical resistivity ρ, the thermoelectric power (TEP)

α, thermal conductivity σ, Knight-Shifts and temperature coefficient of the Knight-Shifts of Si and Ge liquid metals using EMC model potential and Percus–Yevic (PY) hard sphere model with five different types of local field correction functions is reported for the first time. The EMC model potential with more advanced IU, F, and S-local field correction functions generate consistent results regarding the transport properties. Hence, the EMC model potential is found suitable for studying the transport properties of liquid metals. Also, the present investigation predicts that the present study of the transport properties is sensitive to the selection of the proper local field correction function.

References

[1] P.L. Rossiter, *The Electrical Resistivity of Metal and Alloys*, Cambridge University Press, London (1987).

[2] Y. Waseda, *The Structure of Non-crystalline Materials Liquid and Amorphous Solids*, McGraw-Hill, New York (1980).

[3] M. Shimoji, *Liquid Metals*, Academic Press, London (1977).

[4] T.E. Faber, *An Introduction to the Theory of Liquid Metals*, Cambridge University Press, London (1972).

[5] R.K. Willardson and A.C. Beer, *Semiconductors and Semimetals*, Vol. 33, Academic, Boston (1991).

[6] N.E. Cusack, *The Physics of Structurally Disordered Matter*, Institute of Physics, Adam Hilger, England (1986).

[7] A.M. Vora, M.H. Patel, B.Y. Thakore, *et al.*, Solid State Phys. **45** (2002) 427.

[8] Aditya M. Vora, Russian Phys. J. **49** (2006) 834; Optoelec. Adv. Mater.-Rap. Commun. **1** (2007) 227; Phys. Chem. Liq. **46** (2008) 223.

[9] Aditya M. Vora, Phys. Chem. Liq. **46** (2008) 442; Turkish J. Phys. **31** (2007) 341; Chinese J. Phys. **46** (2008) 426; J. Ovonic Research **3** (2007) 57, 83, 129.

[10] H. Aoki, K. Hotoduka, and T. Itami, J. Non-Cryst. Sol. **312-314** (2002) 222.

[11] O. Tatsuya and O. Satoru, J. Phys. Soc. Jpn. **72** (2003) 352.

[12] J.A. Meijer, G.J.B. Vinke, and W. van der Lugt, J. Phys. F: Met. Phys. **16** (1986) 845.

[13] N.F. Mott, Phil. Mag. **26** (1972) 1249.

[14] B. Grosdidier, J.P. Lutz, S. Saadeddine, and J.G. Gasser, J. Non-cryst. Sol. **205-207** (1996) 393.

[15] H.S. Schnyders and J.B. Van Zytveld, J. Phys : Condens Mat. **8** (1996) 10875.

[16] G. Bose, H.C. Gupta, and B.B. Tripathi, J. Phys. Chem. Sol. **35** (1974) 595.

[17] N.W. Ashcroft, J. Phys. C: Solid State Phys. **1** (1968) 232.

[18] J.K. Percus and G.J. Yevick, Phys. Rev. **110** (1958) 1.

[19] R. Taylor, J. Phys. F: Met. Phys. **8** (1978) 1699.

[20] S. Ichimaru and K. Utsumi, Phys. Rev. B **24** (1981) 7385.

[21] B. Farid, V. Heine, G. Engel, and I.J. Robertson, Phys. Rev. B **48** (1993) 11602.

[22] A. Sarkar, D.S. Sen, S. Haldar, and D. Roy, Mod. Phys. Lett. B **12** (1998) 639.

[23] W.A. Harrison, in *Elementary Electronic Structure*, World Scientific, Singapore (1999).

[24] S. Ono and I. Yokoyama, J. Phys. F.: Met. Phys. **14** (1984) 2909.

[25] O. Akinlade, Phys. Stat. Sol. (b) **169** (1992) 23.

[26] Aditya M. Vora, Optoelec. Adv. Mater.-Rap. Commun. **1** (2007) 639.