Journal of Materials Science Research and Reviews

Volume 6, Issue 4, Page 730-736, 2023; Article no.JMSRR.106412

Determination of Electronic Quality Factor, Universal Electrical Conductivity, Effective Mass and Mobility of Charge Carriers of Alloy N-Si_XGe_{1-X}

Karlo Barbakadze [a], Giorgi Kakhniashvili [b], Zurab Adamia [c,d] and Irakli Nakhutsrishvili [b*]

[a] Sukhumi Institute of Physics and Technology, Georgia.
[b] Institute of Cybernetics of Georgian Technical University, Georgia.
[c] Tbilisi State University, Georgia.
[d] University of Georgia, Georgia.

Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

Article Information

Open Peer Review History:
This journal follows the Advanced Open Peer Review policy. Identity of the Reviewers, Editor(s) and additional Reviewers, peer review comments, different versions of the manuscript, comments of the editors, etc are available here: https://www.sdiarticle5.com/review-history/106412

Original Research Article

Received: 14/07/2023
Accepted: 19/09/2023
Published: 25/09/2023

ABSTRACT

The temperature dependences of the electronic quality factor and the universal electrical conductivity of n-type Si_xGe_{1-x}, as well as the dependences of the Seebeck coefficient on the specific and the universal conductivities, are studied. The effective masses and mobilities of charge carriers are calculated for different temperatures, temperature dependences of the eleqtronic quality factor and the thermoelectric figure of merit are studied. Based on the investigated n-Si_xGe_{1-x} (x=0.83) together with p-$Si_{0.83}Ge_{0.17}$, a thermoelectric module was manufactured and its energetic characteristics were studied.

**Corresponding author: Email: iraklinakhutsrishvili52@gmail.com;*

Keywords: Thermoelectric sige; electronic quality factor; universal electrical conductivity.

1. INTRODUCTION

Crystalline and amorphous SiGe composites are wiedly used in thermogenerators, coolers, sensors [1,2], thin-film transistors [3], batteries [4], solar cells [5,6], photodetectors [7,8] and others. These alloys are good high-temperature materials for the temperature range up to 1200℃ and is being intensively studied at the present time [9-11]. For the study, we chose an $Si_x Ge_{1-x}$ alloy of n-type conductivity, since in some cases this type has advantages over the p-type. For example, the maximum of figure of merit ZT is about 2.5 times greater for n-type $Si_{0.7}Ge_{0.3}$ than for p-type (at the same values of x and concentration of charge carriers n= $3.2 \cdot 10^{26}$ m^{-3}). This follows from the fact that the specific electrical conductivity is 2.5-3 times higher, Seebeck coefficient is 1.4-2 times larger (accordingly, the power factor σS^2 is ~2 orders of magnitude greater), and thermal conductivity coefficient is 1.1-1.3 times smaller at the same temperatures. Also with neutron fluences $\geq 10^{19}$ and irradiation temperatures $\geq$ 600 ℃ n-type Si_xGe_{1-x} is more radiation resistant [12].

In Ref.[13], the concept of universal electrical conductivity of thermoelectrics was introduced, which we denote by σ': $\sigma' = \frac{\sigma}{B_E}\left(\frac{q_e}{k_B}\right)^2$. Here $B_E=\sigma S^2/B_S$ is the electronic quality factor, and B_S is a dimensionless quantity depending on S (σ – specific electroconductivity, S – Seebeck coefficient, q_e – elementary charge, k_B – Boltzmann's constant) (*). B_E and σ' are important characteristics of thermoelectric materials. In particular, factor B_E performs scaling of thermoelectric quantities.

2. METHODOLOGY

In the experiments, we used samples in the form of rectangular parallelepipeds with dimensions of 10x10x20 mm, prepared by hot pressing of powders obtained from zone-melted ingots. For n-type conductivity, phosphorus was used as a dopant. The values of x in $Si_x Ge_{1-x}$ were 0.7 and 0.83. The concentration of charge carriers was n= $3.2 \cdot 10^{26}$ m^{-3}. The study was carried out at 50-1180℃. The upper limit was limited by the melting point of the alloy. The measurement error of S was 3% , and of specific resistivity $\rho(=\sigma^{-1})$ 5% . The thermal conductivity coefficients (χ) were also measured with an error of no more than 7% .

3. RESULTS AND DISCUSSION

Fig. 1. shows B_E - t dependences for n-$Si_x Ge_{1-x}$, which repeat the shape of the schematic curve from [13], which illustrates the presence of additional effects. (For an ideal thermoelectric, the electronic qualitry factor is independent of temperature.)

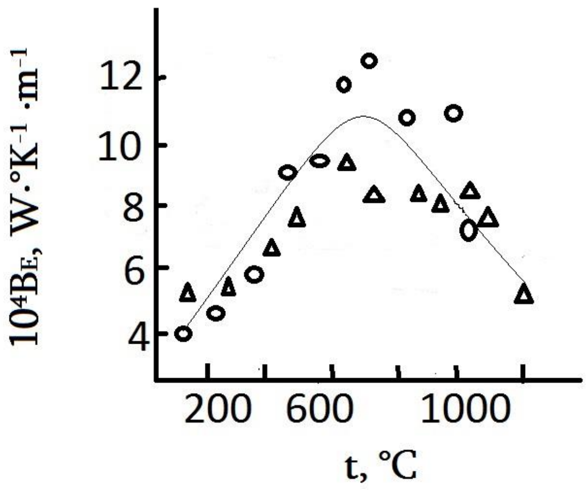

Fig. 1. Temperature dependences of electronic quality factor for $Si_{0.7} Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ)

First consider the temperature dependences of universal electrical conductuvuty in $Si_{0.7}$ $Ge_{0.3}$ and $Si_{0.83}Ge_{0.17}$. This is shown in Fig. 2. As can be seen from this figure, the experimental points form almost a single set, i.e. there is a scaling of the specific electrical conductivity.

Consider the dependence S - σ for Si_xGe_{1-x}. It turned out that it can be determined in a very simple way, without resorting to the Pisarenko formula [14] - a study of the dependence σS^2 (power factor) - S showed their rectilinearity (Fig. 3): $\sigma S^2 = kS + b$, where k is the slope of the straight lines, b - the ordinate of the point of their intersection with the axis σS^2 when extrapolating these lines to S→0. The numerical values of the constants were: k≅7.5, b≈0 for x=0.7 and k≅10, b≅$5 \cdot 10^{-4}$ for x=0.83. From the last equation we get:

$$S = \frac{k}{2\sigma} + \left[\left(\frac{k}{2\sigma}\right)^2 + \frac{b}{\sigma}\right]^{1/2} \quad (1)$$

The plot of Eq.(1) is generally a higher-order curve, but due to the relatively narrow range of variables, almost straight lines are obtained (Fig. 4). For dependence S - σ' we will have:

$$S = 6.73 \cdot 10^7 \frac{k}{B_E\sigma'} + \left[4.53 \cdot 10^{15}\left(\frac{k}{B_E\sigma'}\right)^2 + 1.35 \cdot 10^8 \frac{b}{B_E\sigma'}\right]^{1/2} \quad (2)$$

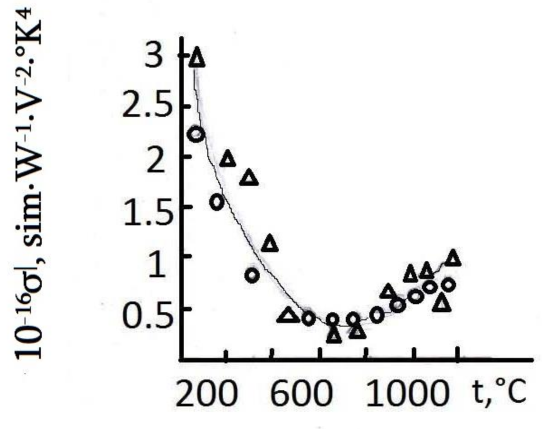

Fig. 2. Temperature dependences of universal electrical conductivity in $Si_{0.7}$ $Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ)

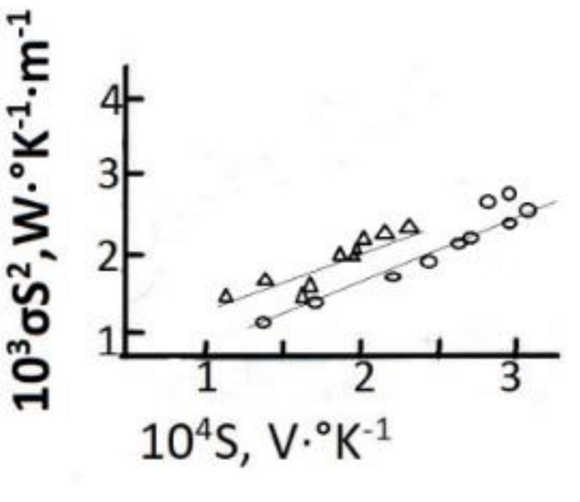

Fig. 3. Dependences σS^2 - S for $Si_{0.7}$ $Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ)

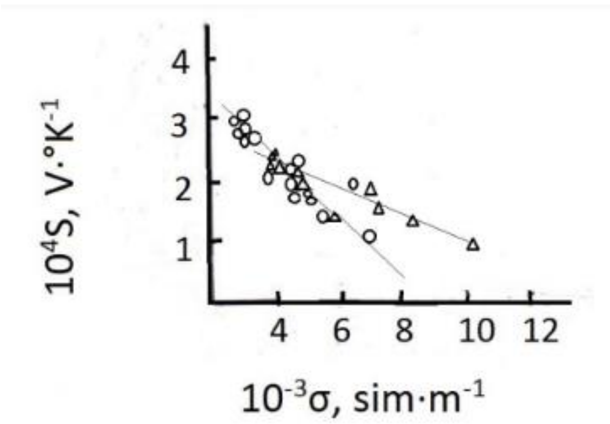

Fig. 4. Dependences S – σ for $Si_{0.7}Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ)

On Fig. 5 is presented S - σ' dependence. As can be seen, the experimental points form almost a single set, regardless of the meaning of x in Si_xGe_{1-x} (i.e. electronic quality factor scales specific electroconductivity). This dependence is described by the empirical expression $S \cong 226.67(\sigma')^{-0.38}$.

The above results are similar to the data for p-SiGe [15] and $Bi_2Sr_2Co_{1.8}O_y$ thermoelectrics [16]. We calculated the effective masses (m^*) of charge carriers for Si_xGe_{1-x} at some temperatures. The following formula are used for the calculation [17]:

$$m^* \cong \frac{h^2}{2k_BT}\left[\frac{3n}{16\sqrt{\pi}}\left(e^{S_r-2} - 0.17\right)\right]^{2/3}. \qquad (3)^{(**)}$$

Values m^*/m_0 (m_0 - rest mass) calculated from Eq.(3) for different temperatures are shown in the table.

The obtained values of m^*/m_0 are approximate to the corresponding values for some thermoelectrics [18,19].

We also calculated the mobilities (μ) of charge carriers. μ is related to m^*/m_0 by the following formula [20]:

$$\mu = \left(\frac{m^*}{m_0}\right)^{-3/2} \mu_W \, , \qquad (4)$$

Where

μ_W is the weighted mobility:

$$\mu_W = \frac{3.31\cdot 10^{-7}}{\rho}\left(\frac{T}{300}\right)^{-3/2}\left[\frac{e^{S_r-2}}{1+e^{-5(S_r-1)}} + \frac{\frac{3}{\pi^2}S_r}{1+e^{5(S_r-1)}}\right] \qquad (5)$$

(ρ – specific resistivity, T – absolute temperature). By combining Eqs (3-5), as well as replacing ρ with σ and $\left[\frac{e^{S_r-2}}{1+e^{-5(S_r-1)}} + \frac{\frac{3}{\pi^2}S_r}{1+e^{5(S_r-1)}}\right] \equiv B_S^{'}$, we finally get:

$$\mu = 3.31 \cdot 10^{-7}\sigma\left(\frac{T}{300}\right)^{-3/2} B_S^{'}\left(\frac{m^*}{m_e}\right)^{-3/2}. \qquad (6)$$

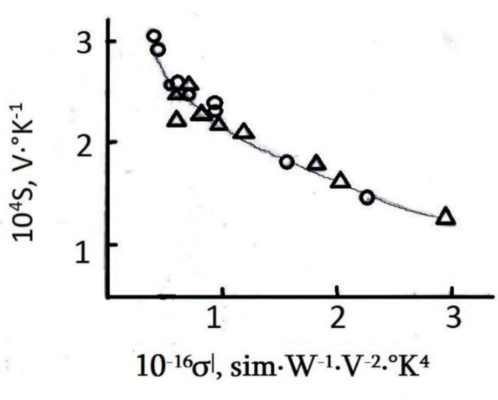

Fig. 5. Dependences S – σ' for $Si_{0.7}Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ)

The values of mobility calculated by the equation (6) turned out to be on average 1 order higher than for Si or Ge (0.145 and 0.39 $m^2/V\cdot sec$, respectively [21]. These results should be considered overestimated. Therefore, we carried out experimental verification. Were obtained values of μ in the range of (0.54-0.65) $m^2/V\cdot sec$, which can be considered acceptable (they are approaching data for SiGe alloy at 300ºK with the same type of conductivity and concentration of charge carriers [22].

Fig. 6. shows the temperature dependences of the thermoelectric figure of merit ZT ($Z=\sigma S^2/\chi$). As can be seen from this figure, $Si_{0.7}Ge_{0.3}$ and $Si_{0.83}Ge_{0.17}$ have almost the same temperature dependence of ZT. For both alloys, the maximum of figure of merit is $ZT\sim 0.8$ ($\cong 0.84$ at 870℃ for $Si_{0.7}Ge_{0.3}$ and $\cong 0.76$ at 900℃ for $Si_{0.83}Ge_{0.17}$)(***)

Based on the investigated n-Si_xGe_{1-x} (x=0.83) together with p-$Si_{0.83}Ge_{0.17}$, a thermoelectric module was manufactured (Fig. 7). The power factor calculated with the values of the Seebeck coefficient and specific electrical conductivity was $PF=2.3\cdot 10^{-5} W/K^2m$; and coefficient of performance η=9.1%.

Table 1. Values of m^*/m_0 in Si_xGe_{1-x} for different temperatures

	m^*/m_0	
t,℃	$Si_{0.7}Ge_{0.3}$	$Si_{0.83}Ge_{0.17}$
80	-	2.6
155	2.98	-
200	-	3.13
280	-	3
300	3.73	-
390	-	3.5
445	3.06	-
490	-	3.55
550	3.8	-
645	4.56	-
650	-	3.85
735	-	3.45
740	4.59	-
855	3.76	-
885	-	2.73
940	4.16	-
990	2.82	2.5
1055	2.45	-
1085	-	1.28
1125	-	1.8
1130	1.79	-
1180	-	1.7

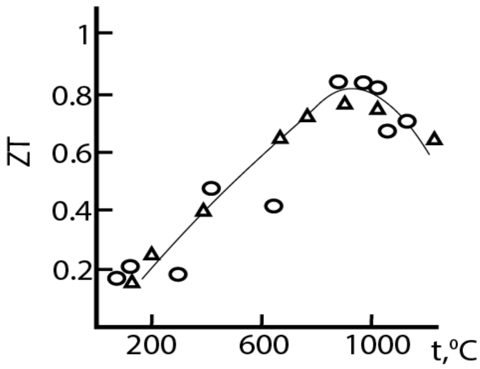

Fig. 6. Temperature dependences of ZT in $Si_{0.7}Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ)

a b

Fig. 7. a - thermoelectric module connected to water cooler, b - thermoelectric module testing.

4. CONCLUSION

In n-type conductivity Si_xGe_{1-x}, (x=0.7 and 0.83) the dependence of the power factor on the Seebeck coefficient is rctilinear: $\sigma S^2 = kS + b$. We will have $S = \frac{k}{2\sigma} + \left[\left(\frac{k}{2\sigma}\right)^2 + \frac{b}{\sigma}\right]^{1/2}$ for S - σ dependences, and for S - σ' dependences: $S = 6.73 \cdot 10^7 \frac{k}{B_E \sigma'} + \left[4.53 \cdot 10^{15} \left(\frac{k}{B_E \sigma'}\right)^2 + 1.35 \cdot 10^8 \frac{b}{B_E \sigma'}\right]^{1/2}$. The study of the temperature dependence of the electronic quality factor shows the presence of additional effects (band convergence etc.). The obtained values of m^*/m_0 are approximate to the corresponding values for some thermoelectrics. The experimentally determined values of μ in Si_xGe_{1-x} were (0.54-0.65) m^2/V·sec. For both $Si_{0.7}Ge_{0.3}$ and $Si_{0.83}Ge_{0.17}$ the thermoelectric figure of merit ZT is ~ 0.8. A noticeable difference in alloys Si_xGe_{1-x} with x=0.7 and 0.83 is observed for almost all thermoelectric characteristics. The exception is the value σ' (scaled specific electrical conductivity σ), which are scaled by the electronic quality factor B_E. Based on the investigated n-Si_xGe_{1-x} (x=0.83) together with p-$Si_{0.83}Ge_{0.17}$, a thermoelectricmodule was manufactured and its energetic characteristics were studied. The power factor was 2.3·10-5W/K2m, and coefficient of performance 9.1%.

Footnote belows:

(*) $B_S = \frac{q}{k_B}\left[\frac{\frac{qS}{k_B} e^{2-\frac{qS}{k_B}}}{1+e^{-5\left(\frac{qS}{k_B}-1\right)}} + \frac{3.29S}{1+e^{5\left(\frac{qS}{k_B}-1\right)}}\right]$ - the scaled power factor ($B_S = \frac{\sigma S^2}{B_E}$) [13].

(**) Formula (3) is fair when |S|>$0.75 \cdot 10^{-4}$V/°K. In our case S=(1.08÷3.07)·10^{-4}V/°K.

(***)For p-Si_xGe_{1-x} (0.7≤x≤0.8, n= $3.2 \cdot 10^{26}$ m^{-3}), $(ZT)_{max}$ ≅0.5-0.65 at 800℃. (preliminary data)

ACKNOWLEDGEMENT

This article is dedicated to the memory of Guram Bokuchava, director of the Sukhumi Institute of Physics and Technology.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Schwinge C. et al. Optimization of LPCVD phosphorous-doped Si Ge thin films for CMOS-compatible thermoelectric applications. Appl Phys Lett. 2022;120 :art.# 031903.
2. Big-Alabo A. Finite element modelling and optimization of Ge/Si Ge super lattice based thermoelectric generators. Appl Sci. 2021;3:art.#189.
3. Jang K. et al. Electrical and structural characteristics of excimer laser-crystallized polycrystalline $Si_{1-x}Ge_x$ thin-film transistors. Materials. 2019;12:art.#1739.
4. Murata H. et al. $Si_{1-x}Ge_x$ anode synthesis on plastic films for flexible rechargeable batteries. Sci Report. 2022;12:13779.
5. Idda A, Ayat L, Dahbi N. Improving the performance of hydrogenated amorphous silicon solar cell using a-SiGe:H Alloy. Ovonic Res. 2019;15:271–278.
6. Singh AK. et al. Heterostructure silicon and germanium alloy based thin film solar cell efficiency analysis. Engin and Manufacturing. 2020;2:29–40.
7. Zimmerman H. SiGe photodetectors, chapt. in Silicon optoelectronic integrated circuits. 2004: 95-99.
8. Aberl J. et al. SiGe quantum well infrared photo detectors on strained-silicon-on-insulator. Opt Express. 2019;27:32009–32018.
9. Duhan N, Mishra BK, Singh IV. XFEM simulation of dislocation in Si_xGe_{1-x} alloy under thermal loads. Proc. Structural Integrity. 2022;42:863-870.
10. Cardenas IA, Siu TC, Shimono MG, Thai S. Installing quaternary germanium centers in sila- diamondoid cores via skeletal isomerization. Inorg. Chem; 2023. DOI: 10.26434/chemrxiv-2023-dk558.
11. G.Bokuchava, I.Nakhutsrishvili, K.Barbakadze. Monolithic module based on $Si_{0.7}Ge_{0.3}$ alloy for thermoelectric generator. AJ Sci. and Technology. 2023;14: is in print.
12. Bokuchava G. Physical-mechanical and electrophysical properties of polycrystalline silicon-germanium alloys. Thesis, Tbilisi. 2008:135.
13. Zhang X et al. Electronic quality factor for thermoelectrics. Sci.Advances. 2020;6:art.# eabc0726.
14. Snyder GJ, Toberer E. Complex thermoelectric materials. Nature Materials. 2008;7:105-114.

15. Bokuchava G, Nakhutsrishvili I, Barbakhadze K. Some thermoelectric parameters of alloy p-SiGe. Bull. Georg. Acad. Sci. 2023;17: is in print.
16. Nakhutsrishvili I et al. Dependence of the Seebeck coefficient on specific and universal elecyrical conductivities of $Bi_2Sr_2Co_{1.8}O_y$ thermoelectric doped with strontium borate and graphene. Materials Sci. Res. and Rev. 2023;6:670-675.
17. Zevalkink A et al. A practical field guide to thermoelectrics. Appl. Phys. Rev. 2018;5: 021303.
18. Namiki H et al. Relationship between the density of states effective mass and carrier concentration of thermoelectric phosphide $Ag_6Ge_{10}P_{12}$ with strong mechanical robustness. Materials Today Sustain. 2022;18: art.#100116.
19. Hong, M, Li, M. et al.,Advances in versatile GeTe thermoelectrics from materials to devices. Adv. Materials. 2022;35:art.# 2208272.
20. Snyder GJ et al. Weighted mobility. Sci. Advances. 2020;25:art.# 2001537.
21. Schäffer F. Silicon-Germanium (Si_xGe_{1-x}). chapt. in Properties of Advanced Semiconductor Materials. 2001:1, Heavily 49-188.
22. Dismukes JD et al. Thermal and electrical properties of heavily doped Ge-Si alloys up to 1300ºK. Appl. Phys. 1964;35:2899–2907.

Peer-review history:
The peer review history for this paper can be accessed here:
https://www.sdiarticle5.com/review-history/106412