Short communication

MAXIMIZATION OF THE FIGURE OF MERIT OF ALLOY Si_xGe_{1-x}

ABSTRACT

The dependence of maximums of figure of merit ($(ZT)_{max}$) on thermoelectric quality factor (B) for thermoelectric Si_xGe_{1-x} of n- and p-type conductivity with a charge carrier concentration of $3.2\cdot10^{26}m^{-3}$ has been considered. The values of x are: 0.7, 0.72, 0.76, 0.8 and 0.83. For all samples, $(ZT)_{max}$ appears at about 900°C. The $(ZT)_{max}$– σ' (universal electrical conductivity) dependence allows us to assume with sufficient accuracy the mentioned maxima for other values of σ' (that is, for Si_xGe_{1-x} with other relative compositions as well. Thus, σ' can be used to predict of $(ZT)_{max}$. With this approach, (is not required) a coefficient of thermal conductivity (k_L) is not required. $\sigma'S^2 - S$ dependence is also considered (S – Seebeck coefficient). Experimental points and the averaged curve for a large number of samples calculated from the data of literature match well. The middle part of this dependence ($1\cdot10^{-4}\leq S\leq2.5\cdot10^{-4}$ $V\cdot K^{-1}$) is well described by the parabolic empirical expression. And in the range $0\leq S\leq6\cdot10^{-4}V\cdot K^{-1}$ the equation of exponential type should be used. Experimental points in coordinates $\sigma' - B_S/S^2$ ($B_S=\sigma S^2/B_E$, σ - specific electrical conductivity, B_E – electronic quality factor) are well located on a straight line for all x in n- and p-Si_xGe_{1-x} ,except (of) for some points for p-$Si_{0.7}Ge_{0.3}$. The dependence $\sigma' - B_S/S^2$ have the form of a straight line with a slope of $1.347\cdot10^8$ $Sim\cdot W^{-1}\cdot K^{-2}$.

Keywords: Thermoelectric SiGe; maximums of figure of merit; electrical conductivity.

1. INTRODUCTION

Si_xGe_{1-x} composites are widely used in thermogenerators, coolers, sensors [1,2], thin-film transistors-MOSFETs [3,4], batteries [5], solar cells [6,7], photodetectors [8,9] and others.This article discusses the maximization of the figure of meritof thermoelectric Si_xGe_{1-x}. This problem is the key to thermoelectric energy conversion. The 2023 Special Conference [10] featured numerous papers covering thermoelectric generators, sensors, and energy harvesting in general.

The dependence of the maximum value of the figure of merit of thermoelectric materials on a number of parameters was studied both before and recently [11-15]. In [16] is considered the thermoelectric quality factor $B=B_ET/k_L=ZT/B_S^{(*)}$. In this work, the dependence of the maximum value of the figure of merit $ZT=\sigma S^2T/k_L$ on B, which is regular for different thermoelectrics, is given.

In [17,18], we studied some thermoelectric characteristics of the SiGe alloy. This article discusses the electrical quality factor and universal electrical conductivity of Si_xGe_{1-x} (concentration of charge carriers$3.2\cdot10^{26}m^{-3}$). The quality factor is calculated. Data on the dependences $(ZT)_{max}$ – B, $(ZT)_{max}$ – x, σ' – x and $(ZT)_{max}$ – σ' are presented. The values of B_E, σ', kL and ZT are calculated based on the temperature dependences of electrical conductivity (σ=1/ρ, ρ is electrical resistivity), thermal conductivity and Seebeck coefficients according to data from [19]. For all samples $(ZT)_{max}$ appears at about 900°C.

2. DISCUSSION

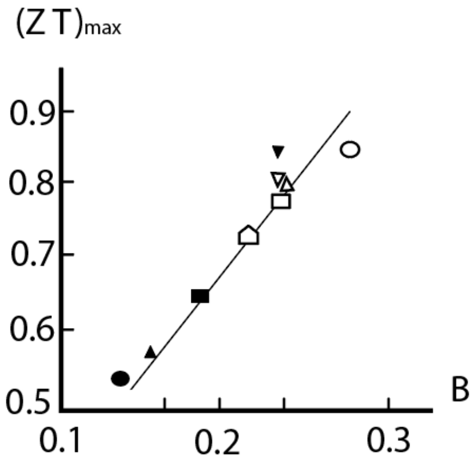


Fig.1. Dependence $(ZT)_{max}$ – B in Si_xGe_{1-x} : ○ - x=0.7, Δ - x=0.72, □ - x=0.76, ∇ - x=0.8, ⌂ - x=0.83 (n-type); ● - x=0.7, ▲ - x=0.76, ■ - x=0.8 (p-type);▼- from [20].

Figure 1 shows the dependence $(ZT)_{max}$ – B, it can be described by the expression $(ZT)_{max}\cong3.2B+0.05$. Values of $(ZT)_{max}$ can also be estimated indirectly: consider the dependence of $(ZT)_{max}$ on the universal electrical conductivity (σ') given by expression $\sigma'=(q/k_B)^2\sigma/B_E =(q/k_B)^2B_S/S^2$. Let's (bring) also depict the dependences $(ZT)_{max}$ – x and σ' – x (Figs.2 and 3). As can be seen from the Fig.2, for the n-type, $(ZT)_{max}$ decreases with increasing x ($(ZT)_{max}\cong -0.81x+1.42$), and for the p-type, it increases ($(ZT)_{max}\cong0.39x+0.28$).

In [20] among various thermoelectric materials, data on $Si_{0.9}Ge_{0.1}$ are given: $(ZT)_{max}\cong0.87$ at a temperature of about 900°C. With this value and the Lorentz number, the corresponding Seebeck coefficient can be calculated: $S\cong1.47\cdot10^{-4}V\cdot K^{-1}$. From the latter: $B_S\cong3.96$ and $B\cong0.23$. This point is shown in Fig.1.

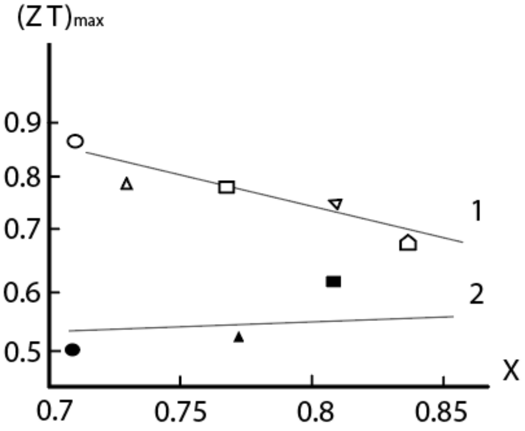


Fig.2. Dependence $(ZT)_{max}$ – x in Si_xGe_{1-x}: 1 - n-type, 2 - p-type. ○, ● - x=0.7, Δ - x=0.72, □, ▲ - x=0.76,∇, ■ - x=0.8, ⌂ - x=0.83.

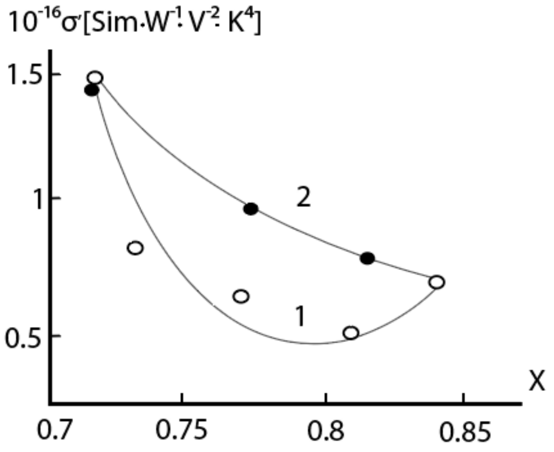


Fig.3. Dependence σ' – x in Si_xGe_{1-x} (σ' for $(ZT)_{max}$) $^{(**)}$: 1 - n-type, 2 - p-type.

By combining the dependences $(ZT)_{max}$ – x and σ' – x, we will get the $(ZT)_{max}$ – σ' dependence (Fig.4). This dependence gives: $\lg(ZT)_{max} \cong -0.4\lg\sigma' + 6.2$. This allows us to predict with sufficient accuracy the mentioned maximum for other values of σ', i.e. for Si_xGe_{1-x} with other relative compositions. Thus the universal electrical conductivity can be used to predict $(ZT)_{max}$. With this approach, no thermal conductivity coefficient is required. It should be noted that the points calculated from data for some other thermoelectrics also fit satisfactorily on this straight line (see figure). Also it should be noted that there is no regularity in the dependence of $(ZT)_{max}$ with other parameters (including $\sigma' S^2$).

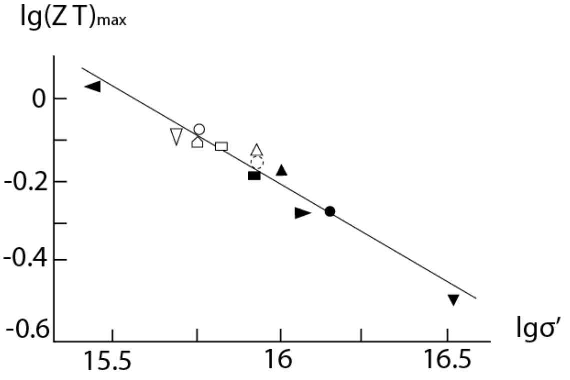


Fig.4. Dependence $\lg(ZT)_{max}$ – lgσ' for Si_xGe_{1-x} (σ' for $(ZT)_{max}$) $^{(**)}$: ○ - x=0.7, Δ - x=0.72, □ - x=0.76, ∇ -x=0.8, ⌂ - x=0.83 (n-type); ● - x=0.7, ▲ - x=0.76, ■ - x=0.8 (p-type); ◄ and ▼ - for $NaCo_{0.9}Cr_{0.1}O_2$ and $NaCoO_2$ [21], ◌ and ► - for $Cu_{1.98}S_{0.9}Se_{0.1}$ and $Cu_{1.98}S_{0.8}Se_{0.2}$ [22].

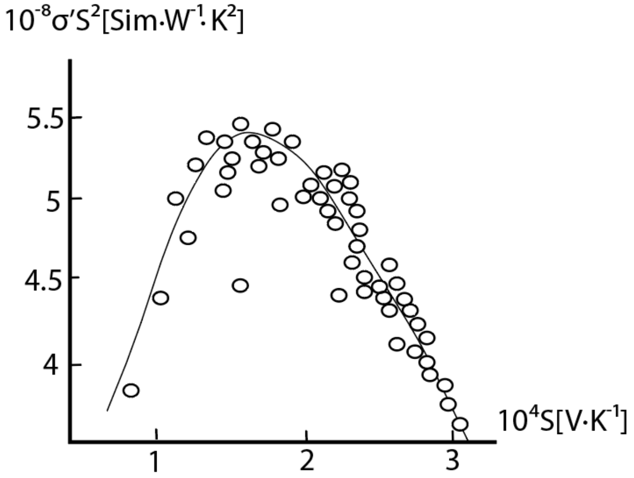


Fig.5. Dependence σ'S^2 – S. The points correspond to all x values in n- and p-Si_xGe_{1-x}.

The product of the universal electrical conductivity and the square of the Seebeck coefficient we will conditionally call the "universal power factor". Fig.5 shows σ'S^2 – S dependence and the averaged curve for a large number of samples calculated from the data of [16] (solid line). On this graph, the points obtained by formula $\sigma' S^2 = (q/k_B)^2 B_S \cong 1.347\cdot 10^8 B_S$ and obtained experimentally are very close to each other (sometimes they coincide).

The middle part of this dependence ($1\cdot 10^{-4} \le S \le 2.5\cdot 10^{-4}$ V·K^{-1}) is well described by the expression $\sigma' S^2 \cong -1.63\cdot 10^{16} S^2 + 5.72\cdot 10^{12} S + 5\cdot 10^7$. And in the range $0 \le S \le 6\cdot 10^{-4}$V·$K^{-1}$ the equation of type $\sigma' S^2 = aS^b e^{cS}$ should be used, where a, b and c are constants.

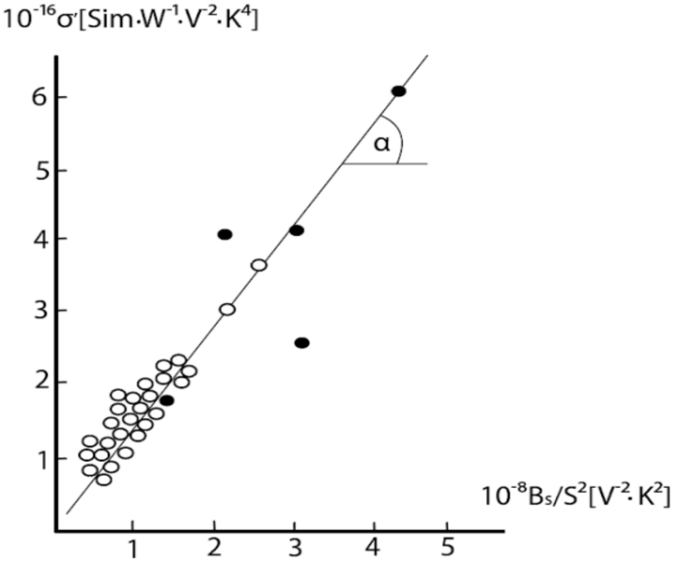


Fig.6. Dependence $\sigma' - B_S/S^2$ for Si_xGe_{1-x} : (○) - all examined values of x in n- and p-type Si_xGe_{1-x} , except for p-$Si_{0.7}Ge_{0.3}$ (●); $tg\alpha=1.347\cdot10^8$.

Experimental points in coordinates $\sigma' - B_S/S^2$ are well located on a straight line for all x in n- and p-Si_xGe_{1-x},except of some points for p-$Si_{0.7}Ge_{0.3}$ (Fig.6). (Obviously, the dependence $\sigma' - B_S/S^2$ will have the same form for any thermoelectric – the form of a straight line with a slope of $1.347\cdot10^8$ $\mathrm{Sim\cdot W^{-1}\cdot K^{-2}}$.)

3. CONCLUSSION

The alloy Si_xGe_{1-x} of n- and p-type conductivity has been considered for different values of x. The dependence of maximums of figure of merit on thermoelectric quality factor for this alloy is rectilinear: $(ZT)_{max} \cong 3.2B+0.05$. Dependence $(ZT)_{max}$ on universal electrical conductivity is: $\lg(ZT)_{max} \cong -0.4\lg\sigma'+6.2$. This allows us to assume the mentioned maxima for other values of σ' (that is, for Si_xGe_{1-x} with other relative compositions as well. Thus, σ' can be used to predict of $(ZT)_{max}$.

Footnote belows:

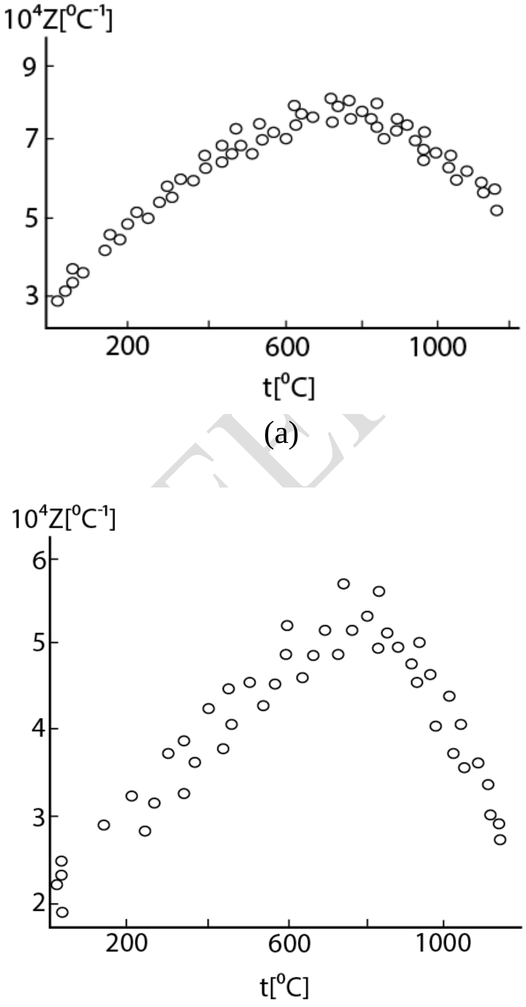
$$^{(*)}B_S=\sigma S^2/B_E=\left[\frac{\left(\frac{q_eS}{k_B}\right)^2 e^{2-\frac{q_eS}{k_B}}}{1+e^{-5\left(\frac{q_eS}{k_B}-1\right)}}+\frac{3.29S}{1+e^{5\left(\frac{q_eS}{k_B}-1\right)}}\right]$$ - the scaled power factor.

(**) $(ZT)_{max}$ corresponds to σ'_{min} .

APPENDIX

We also studied the temperature dependence of thermoelectrical efficiency $Z=\sigma S^2/k_L$, included in the expression of figure of merit. Figure 7 shows these dependences for all n- and p-Si_xGe_{1-x} samples. It can be seen that they have a regular character and exhibit a maximum at about 800°C. (As mentioned above, the maximums of the figure of merit itself shift to 900°C.)

Figure 8 shows the temperature dependence of Z_{max} for SiGe and some other thermoelectrics (literature data compiled in [20]). This regular dependence can be described by the empirical expression $\lg Z_{max} \cong -1.040 \lg T + 0.136$.



(a)

(b)

Fig.7. Temperature dependences of Z: (a) n-Si_xGe_{1-x}; (b) p-Si_xGe_{1-x} .
The points belong to all values of x in Si_xGe_{1-x}.

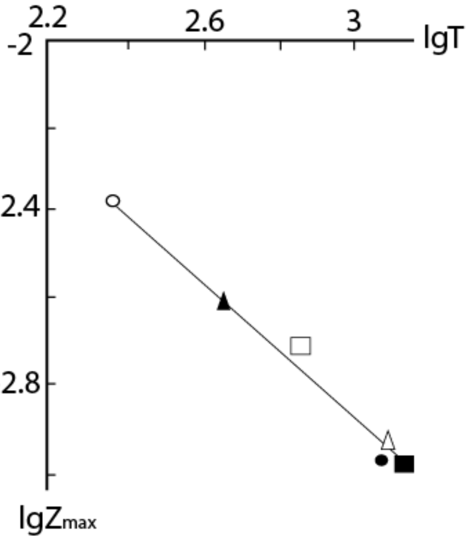


Fig.8. Dependence Z_{max} – T: o –$CsBi_4Te_6$, Δ - $Si_{0.9}Ge_{0.1}$, □ - PbTe, ● - n-Si_xGe_{1-x}, ▲ - Bi_2Te_3, ■ - p-Si_xGe_{1-x}.

REFERENCES

1. Schwinge C, Kühnel K et al. Optimization of LPCVD phosphorous-doped SiGe thin films for CMOS-compatible thermoelectric applications. Appl. Phys. Lett. 2022; 120: 031903.
2. Big-Alabo A. Finite element modelling and optimization of Ge/Si Ge super lattice based thermoelectric generators. Appl. Sci. 2021; 3: 189.
3. Jang K, Kim Y et al. Electrical and structural characteristics of excimer laser-crystallized polycrystalline $Si_{1-x}Ge_x$ thin-film transistors. Materials. 2019; 12: 1739.
4. Murata, H., Nozawa, K., Suzuki et al.Si_{1-x} Ge_x anode synthesis on plastic films for flexible rechargeable batteries. Sci. Report. 2022; 12: 13779.*Sci.*
5. Breeden M, Fang Z, Chang et al. $Al_2O_3/Si_{0.7}Ge_{0.3}$ (001) & $HfO_2/Si_{0.7}Ge_{0.3}$(001) interface trap state reduction via in-situ N_2/H_2 RF downstream plasma passivation. Appl. Surf. Sci. 2019; 478: 1065-1073.
6. 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.
7. Singh AK, Kumar M, Kumar D et al. Heterostructure silicon and germanium alloy based thin film solar cell efficiency analysis. Engin. and Manufacturing 2020; 2: 29–40.

8. Zimmerman H. SiGe photodetectors, inSilicon Optoelectronic Integrated Circuits, eds. Chun K, Itoh et al. Vienna, Austria, 2018, 1-435.
9. Aberl J, Brehm M, Fromherz T et al. Opt. Express. 2019; 27: 32009–32018.
10. Proc. 19th European Conference on Thermoelectrics, Prague, Czech Rep., Sept.17-21, 2023.
11. Simon R. Maximum figure of merit of thermoelectric materials. Adv. Energy Conversion. 1981; 1: 81-92.
12. Mahan GD. Figure of merit for hermoelectrics. Appl. Phys. 1989; 65: 1578-1583.
13. Wang H, Pei Y, LaLonde AD et al. Material design considerations based on thermoelectric quality factor. Thermoelect. Nanomater. 2013; 182: 3-32.
14. Sun Y, LiuY, Li R et al.Strategies to improve the thermoelectric figure of merit in thermoelectric functional materials. Front. Chem. 2022; 10: 865281.
15. Feng L, Guo A,LiuK et al.Highly deformable $Ag_2Te_{1-x}Se_x$-based thermoelectric compounds. Materials Today Phys. 2023; 33: 101051.
16. Zhang X, Bu Z, Shi X et al. Electronic quality factor for thermoelectrics. Sci. Advances. 2020; 6: eabc0726.
17. Bokuchava G, Barbakadze K,Nakhutsrishvili I. On the thermoelectric alloy n-Si_xGe_{1-x}. Material Sci. & Engin. 2023; 7: 54-57.
18. Bokuchava G, Barbakadze,Nakhutsrishvili I. Some thermoelectric parameters of alloy p-SiGe. Bull. Georg. Acad. Sci. 2023;17: 33-37.
19. Barbakadze K, Bokuchava G, IsakadzeZ et al.High temperature thermoelectric generator based on SiGe alloys.Sci. Journal of LEPL – Agmashenebeli Nat. Defence Acad. of Georgia. 2022; 47-51.
20. Tritt TM. Thermoelectric materials, phenomena, and applications: A bird's eye view. MRS Bull. 2006;31: 188-196.
21. Krasutskaya NS, Klyndyuk A. Thermoelectric ceramics based on the layered sodium cobaltite.Proc. X Int. Conf. Materials and Structures of Modern Electronics.2022: 122-127.
22. Zhao L, Fei FY, Wang J et al. Improvement of thermoelectric properties and their correlations with electron effective mass in $Cu_{1.98}S_xSe_{1-x}$. Sci. Rep. 2017; 7: 40436.