



# **Optimizing Power Factor in SixGe<sub>1-x</sub> Alloys and Some Other Thermoelectric Materials: Insights and Empirical Relationships**

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## **Authors' contributions**

*This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.*

## **Article Information**

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**Received: 23/02/2024**

**Accepted: 27/04/2024**

**Published: 01/05/2024**

**Short Communication**

## **ABSTRACT**

In this article, the issue of determining the power factor maximums of Si<sub>x</sub>Ge<sub>1-x</sub> alloy with different compositions is investigated. This issue is discussed also for other thermoelectrics based on literature data. It is shown that for the values of the Seebeck coefficient in the interval (1-4)10<sup>-4</sup>V/K, (PF)<sub>max</sub> corresponds to the minimum of the specific electrical conductivity. The interdependence of these thermoelectric parameters has a regular character. The dependences lg(σS<sup>2</sup>)<sub>max</sub> – lgσ<sub>min</sub> for various thermoelectrics based on literature and our data in the corresponding interval of changes of variables are described by a single empirical expression lg(σS<sup>2</sup>)<sub>max</sub> ≅ 0.583(lgσ<sub>min</sub>)<sup>2</sup> - 3.332lgσ<sub>min</sub>. The temperature dependence of the Seebeck coefficient described by the equation  $S = \frac{3}{2} \frac{k_B}{q_e} \ln T + C$ , where C depends on the concentration and effective mass of charge carriers, as well as on the Debye temperature. This dependence has the same character as dependence σS<sup>2</sup> – T and have maximum around 1100K.

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Additionally, the dependences of power factor on specific electrical conductivity were studied. For different thermoelectrics they are described by empirical expressions such as  $\sigma S^2 \cong (a/\sigma)^b$  or  $\sigma S^2 \cong c\sigma^d$ , where constants a, b, c and  $d > 0$ . For a number of thermoelectrics, the dependences  $\sigma S^2$  on the Seebeck coefficient are rectilinear, while for another series they are power-law. And this is a more general case. The temperature dependences of  $\sigma S^2$  and of scaled power factor ( $B_s$ ) are also studied. Both are described by a quadratic equation. It has been established that the maximum power factor corresponds to the minimum  $B_s$ . Thus, in this case to estimate  $(\sigma S^2)_{\max}$  can be used as  $\sigma_{\min}$ , and  $(B_s)_{\min}$ .

**Keywords:** Thermoelectrics; power factor; electrical conductivity.

## 1. INTRODUCTION

Since the seventies of the last century, the  $\text{Si}_x\text{Ge}_{1-x}$  alloy has been used in thermoelectric generators in spacecraft for long-distance flights with a long service life [1-3]. This alloy is also used in many branches of science and technology [4-15].

N-type  $\text{Si}_x\text{Ge}_{1-x}$  has a number of advantages over the P-type: the maximum of figure of merit (ZT) is about 2.5 times greater for N-type than for P-type (at concentration of charge carriers  $n = 3.2 \cdot 10^{26} \text{m}^{-3}$  and at the same compositions). 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 is ~2 orders of magnitude greater), and thermal conductivity coefficient is 1.1-1.3 times smaller at the same temperatures. Also with neutron fluencies  $\geq 10^{19}$  and irradiation temperatures  $\geq 600^\circ\text{C}$  N-type  $\text{Si}_x\text{Ge}_{1-x}$  is more radiation resistant [16].

This article is a continuation of work [17], where the maximization of the figure of merit of thermoelectric material SiGe is considered. Together with ZT, power factor (PF) is an important energy characteristic of thermoelectrics, which is included in the expression of the ZT:  $\text{PF} \cong \sigma S^2$ , where  $\sigma$  is the specific electrical conductivity, S - Seebeck coefficient. Here we consider N- $\text{Si}_x\text{Ge}_{1-x}$  alloy ( $x=0.7, 0.72, 0.76, 0.8$  and  $0.83$ ) based on experimental data of [18]. Since the remaining thermoelectric materials are also taken from the literature, the experimental section is not included.

## 2. DISCUSSION

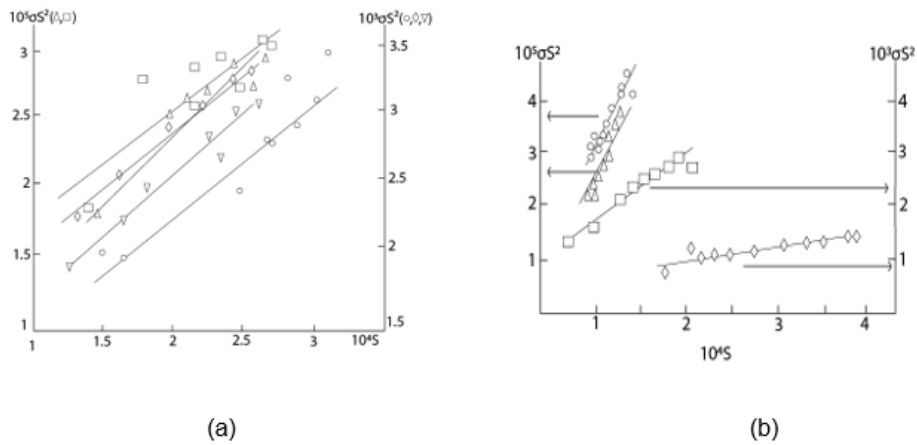
According to a fairly large number of works, the range of changes of the Seebeck coefficient is  $(1-4)10^{-4} \text{V/K}$ . With such a relatively narrow

range, the  $\sigma S^2 - S$  dependence is almost rectilinear:  $\sigma S^2 = kS + b$ , where k is the slope of the straight lines, and b is the ordinate of the point of their intersection with the axis  $\sigma S^2$  when extrapolating these lines to  $S \rightarrow 0$ . From the last equation we get:  $S = \frac{k}{2\sigma} + \left[ \left( \frac{k}{2\sigma} \right)^2 + \frac{b}{\sigma} \right]^{1/2}$ . After simple transformations we will have:  $\sigma S^2 = \frac{k}{2\sigma} + b$ , that is, in this case  $(\text{PF})_{\max}$  will correspond to  $\sigma_{\min}$ .

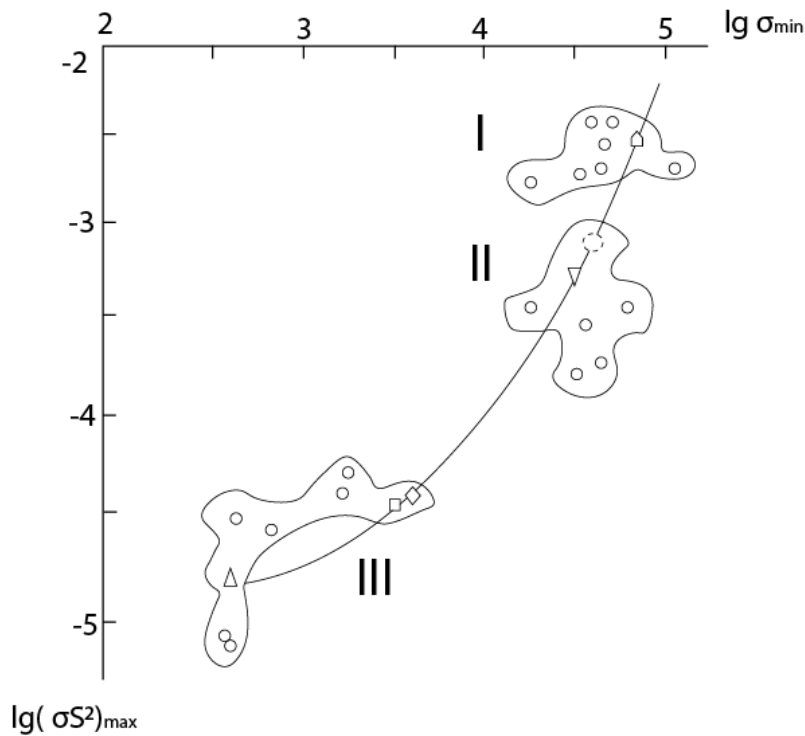
Fig 1 shows  $\sigma S^2 - S$  dependencies for different thermoelectric materials, namely for a, b and c. These dependencies are constructed based on experimental data from the following works: [18] (SiGe), [19]  $(\text{Bi}_2\text{Sr}_{1.925}[\text{Sr}(\text{BO}_2)_2]_{0.075}\text{Co}_{1.8}\text{O}_y)$ ,  $\text{Bi}_2\text{Sr}_2\text{Co}_{1.8}\text{O}_y$ , [20]  $(\text{SiGeMo}_{0.2})$ , and [21]  $(\text{Sb}_{1.7}\text{Bi}_{0.4}\text{Te}_3)$ .

Fig 2 shows  $\lg(\sigma S^2)_{\max} - \lg\sigma_{\min}$  dependences for different thermoelectrics using literature and our data. In the obtained intervals of change of variables, these dependencies can be described as a whole by the empirical expression  $\lg(\sigma S^2)_{\max} \cong 0.583(\lg\sigma_{\min})^2 - 3.332\lg\sigma_{\min}$  (solid line in Fig.2). The entire dependence is divided into three areas: (I)  $10^{-2} < (\text{PF})_{\max} < 10^{-3}$ , (II)  $10^{-3} < (\text{PF})_{\max} < 10^{-4}$  and (III)  $10^{-4} < (\text{PF})_{\max} < 10^{-5} \text{W/K}^2\text{m}$ . By means of this approximate relationship, it will be possible to predict the order of  $(\text{PF})_{\max}$  according to  $\sigma_{\min}$ . The scatter of points around the averaged line is apparently due to the non-strict rectilinearity of the corresponding  $\sigma S^2 - S$  dependences. When these dependencies are practically rectilinear, then the points fit well on the curve (compare Figs.1 and 2).

Fig 3 shows the temperature dependences of  $\sigma S^2 - T$  and  $S - \ln T$  for  $\text{Si}_{0.72}\text{Ge}_{0.28}$  and  $\text{Si}_{0.76}\text{Ge}_{0.24}$  (dependencies for other compositions have the same form). From this figure it is clear that these dependences have a maximum at the same temperature ( $\sim 1100\text{K}$ ).



**Fig. 1. Typical dependences  $\sigma S^2 - S$ : (a)  $\text{Si}_x\text{Ge}_{1-x}$ ,  $x=0.7$  (o),  $0.72$  ( $\Delta$ ),  $0.76$  ( $\square$ ),  $0.8$  ( $\diamond$ ) and  $0.83$  ( $\nabla$ ); (b) (o)  $\text{Bi}_2\text{Sr}_{1.925}[\text{Sr}(\text{BO}_2)_2]_{0.075}\text{Co}_{1.8}\text{O}_y$ , ( $\Delta$ )  $\text{Bi}_2\text{Sr}_2\text{Co}_{1.8}\text{O}_y$ ,  $\square$  -  $\text{SiGeMo}_{0.2}$ , and ( $\diamond$ )  $\text{Sb}_{1.7}\text{Bi}_{0.4}\text{Te}_3$ .  $[\sigma S^2]=\text{W}/\text{K}^2\text{m}$ ,  $[S]=\text{V}/\text{K}$**



**Fig. 2. Dependences  $\lg(\sigma S^2)_{\max} - \lg\sigma_{\min}$ . The coordinates of the points are calculated according to the data of following works: sect.I - [18] ( $\text{Si}_{0.7}\text{Ge}_{0.3}$ ), [20] ( $\text{SiGe}$ ,  $\text{SiGeMo}_{0.2}$ ),  $\text{PbTe}$  [22]; sect.II - [21] ( $\text{Sb}_{1.7}\text{Bi}_{0.4}\text{Te}_3$ ), [23]  $\text{Bi}_2\text{Te}_3$ , ( $\text{Bi}_{0.98}\text{Sn}_{0.02}$ ) $_2\text{Te}_{2.7}\text{Se}_{0.3}$ ), [24]  $\text{Si}_{0.68}\text{Ge}_{0.32}\text{Ga}$ , [25]  $\text{Ni}_2\text{CuCrFe}$ ; sect.III - [19]  $\text{Bi}_2\text{Sr}_2\text{Co}_{1.8}\text{O}_y$ ,  $\text{Bi}_2\text{Sr}_{1.9}[\text{Sr}(\text{BO}_2)_2]_{0.1}\text{Co}_{1.8}\text{O}_y$  (and the same thermoelectrics with different composition of components). Figurative points correspond to Fig.1:  $\Delta$  -  $\text{Bi}_2\text{Sr}_2\text{Co}_{1.8}\text{O}_y$ ,  $\square$  -  $\text{Si}_{0.72}\text{Ge}_{0.28}$ ,  $\diamond$  -  $\text{Bi}_2\text{Te}_3$ ,  $\nabla$ ,  $\circ$  -  $\text{SiGeGa}$ ,  $\triangle$  -  $\text{SiGeMo}_{0.2}$**

It should be noted that for practically all other thermoelectrics considered above (and also for  $\text{P-Si}_x\text{Ge}_{1-x}$ ), a rectilinear dependence of the Seebeck coefficient on the natural logarithm of

temperature was observed (Fig.3). Therefore, for them the following formula was used [25,26]:

$$S = \frac{3}{2} \frac{k_B}{q_e} \ln T + C, \quad (1)$$

where C depends on the concentration and effective mass of charge carriers, as well as on the Debye temperature ( $k_B$  - Boltzmann's constant,  $q_e$  - elementary charge,  $T$  - absolute temperature)<sup>(\*)</sup>. Fig 3(b) shows these dependences for  $Sb_{1.7}Bi_{0.4}Te_3$ ,  $Tl_9Sb_{0.99}Sn_{0.1}Te_6$  [27] and  $SiGeMo_{0.2}$ . From Fig.4(a) it is clear that the experimental points form a

practically single set with an average overall slope  $K \equiv tg\alpha \cong 1.122 \cdot 10^{-4}$ . The slopes of the lines presented in Fig.3(b) are  $tg\alpha \cong 1.324$ ,  $1.475$  and  $1.050 \cdot 10^{-4}$ , respectively. These slopes which approach to  $K = \frac{3 k_B}{2 q_e} \cong 1.293 \cdot 10^{-4}$  with more or less accuracy.

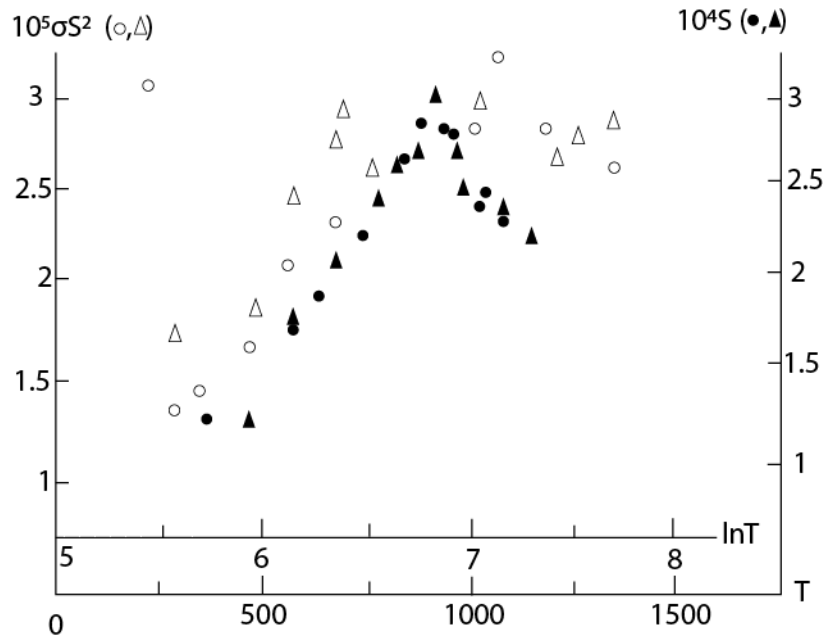


Fig. 3. Dependencies  $\sigma S^2 - T$  and  $S - \ln T$  for  $Si_{0.72}Ge_{0.28}$  (o,  $\Delta$ ) and  $Si_{0.76}Ge_{0.24}$  (•,  $\blacktriangle$ ). ( $\ln 1100 \cong 7$ , the scales are different on the abscissa axes) [ $\sigma S^2$ ]=W/K<sup>2</sup>m, [S]=V/K, [T]=K

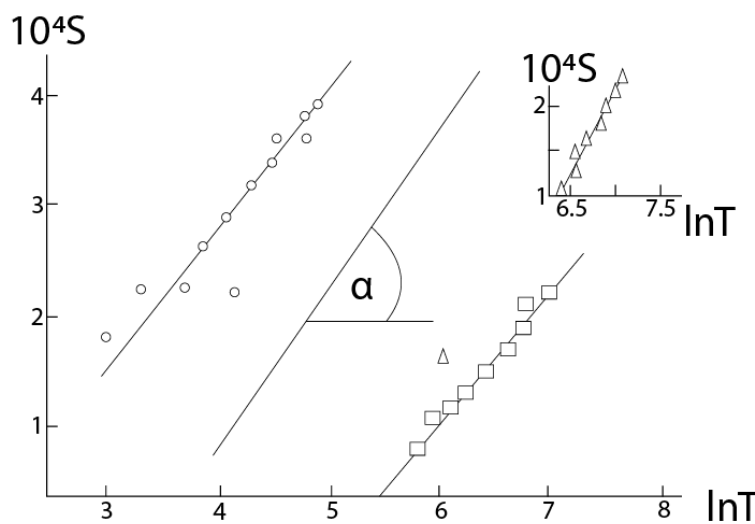


Fig. 4. Dependences  $S - \ln T$  for  $Sb_{1.7}Bi_{0.4}Te_3$  (o),  $Tl_9Sb_{0.99}Sn_{0.1}Te_6$  ( $\Delta$ ) and  $SiGeMo_{0.2}$  ( $\square$ ). A straight line without points was constructed at  $tg\alpha \cong 1.293 \cdot 10^{-4}$  with arbitrarily taken  $b = -4.4$ . [S]=V/K, [T]=K

Since the values of  $K$  do not coincide exactly with  $\frac{3k_B}{2q_e}$ , it is difficult to estimate the corresponding values of the constant  $A$  (see Footnote below) from the values of  $C$  calculated below. However, according to as yet unpublished data for  $P\text{-Si}_{0.7}\text{Ge}_{0.3}$ , the temperature dependence of mobility is described by the expression  $\mu \cong \frac{1}{2} T^{-3/2}$ , which indicates phonon scattering of charge carriers [28].

#### NOTE

(\*)  $C = \frac{k_B}{q_e} \left[ A + \ln \frac{2(2\pi m^* k_B)^{3/2}}{(2\pi h^3)^{3n}} \right]$ , where  $A$  depends on the scattering mechanism and takes values from 2 to 4 ( $m^*$  and  $n$  – effective mass and concentration of charge carriers).

### 3. CONCLUSION

A method is proposed for determining the maximum power factor of  $\text{Si}_x\text{Ge}_{1-x}$  alloys of different compositions and different conductivities. Other thermoelectrics are also considered based on literature data.

The dependences  $\lg(\sigma S^2)_{\max} - \lg\sigma_{\min}$  for various thermoelectrics based on literature and our data in the corresponding interval of changes of variables are described by a one empirical expression  $\lg(\sigma S^2)_{\max} \cong 0.583(\lg\sigma_{\min})^2 - 3.332\lg\sigma_{\min}$ .

The temperature dependence of the Seebeck coefficient described by the equation  $S = \frac{3k_B}{2q_e} \ln T + C$ . This dependence has the same character as dependence  $\sigma S^2 - T$  and have maximums around 1100K.

#### COMPETING INTERESTS

Authors have declared that no competing interests exist.

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