Minireview Article

The Power Factor Maximums of Alloy Si_xGe_{1-x} and Some Other Thermoelectric

ABSTRACT

In this article, the issue of determining the power factor maximums of Si_xGe_{1-x} 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 $(1\text{-}4)10^{-4}$V/K, $(PF)_{max}$ corresponds to the minimum of the specific electrical conductivity. The interdependence of these thermoelectric parameters has a regular character. 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 single empirical expression $lg(\sigma \mathbf{S}^2)_{max} \cong 0.583(lg\sigma_{min})^2\text{-}3.332lg\sigma_{min}$. The temperature dependence of the Seebeck coefficient described by the equation $S=\frac{3}{2}\frac{k_B}{q_e}lnT+C$, where C depends on the concentration and effective bmass of charge carriers, as well as on the Debye temperature. This dependence has the same character as dependence $\sigma S^2 - T$ and have maximum around 1100K.
Additionally, the dependences of power factor on specific electrical conductivity were studied. For different thermoelectrics they are described by empirical expressions such as $\sigma S^2 \cong (a/\sigma)\text{-}b$ or $\sigma S^2 \cong c\sigma^{-d}$, where constants a, b, c and $d>0$. For a number of thermoelectrics, the dependences σS^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 σS^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 σ_{min}, and $(B_S)_{min}$.

Keywords:SiGe thermoelectric; power factor; electrical conductivity.

1. INTRODUCTION

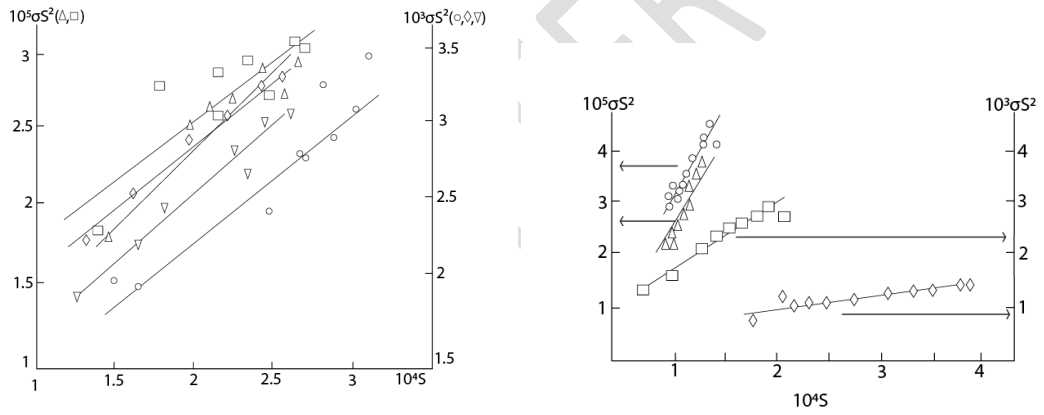
Since the seventies of the last century, the Si_xGe_{1-x} alloy has been used in thermoelectric generators in spacecraft for long-distance flights with a long service life [1-3]. This alloy is also used in many branches of science and technology [4-15].

N-type Si_xGe_{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 $n= 3.2\cdot10^{26}m^{-3}$ 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 $\geq10^{19}$and irradiation temperatures $\geq$600°C N-type Si_xGe_{1-x} is more radiation resistant [16].

This article is a continuation of work [17], where the maximization of the figure of meritof 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: PF≡ σS^2, where σ is the specific electrical conductivity, S - Seebeck coefficient. Here was studied N-Si_xGe_{1-x} alloy at x=0.7, 0.72, 0.76, 0.8 and 0.83. Experimental data taken from [18].Since the remaining thermoelectric materials are also taken from the literature, the experimental section is not included.

Seebeck coefficient

According to a fairly large number of works, the range of changes of the Seebeck coefficient is (1-4)10^{-4}V/K. With such a relatively narrow range, the σS^2 - S dependence is almost rectilinear: σS^2=kS+b, where k is the slope of the straight lines, and bis the ordinate of the point of their intersection with the axis σS^2 when extrapolating these lines to S→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 $(PF)_{max}$ will correspond to σ_{min}.



(a) (b)

Fig. 1. Typical dependences σS^2- S: (a) Si_xGe_{1-x}, x=0.7 (o), 0.72 (Δ), 0.76 (□), 0.8 (◊) and 0.83 (∇); (b) (o) $Bi_2Sr_{1.925}[Sr(BO_2)_2]_{0.075}Co_{1.8}O_y$ [18], (Δ) $Bi_2Sr_2Co_{1.8}O_y$ [18], □ - $SiGeMo_{0.2}$ [19], and (◊) $Sb_{1.7}Bi_{0.4}Te_3$ [20].[σS^2]=W/K^2m, [S]=V/K.

Thermoelectrics

Figure 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 describedas a whole by the empirical expression $lg(\sigma \mathbf{S}^2)_{max} \cong 0.583(lg\sigma_{min})^2 - 3.332lg\sigma_{min}$ (solid line in Fig.2). The entire dependence is divided into three areas: (I) $10^{-2} < (PF)_{max} < 10^{-3}$, (II) $10^{-3} < (PF)_{max} < 10^{-4}$ and (III) $10^{-4} < (PF)_{max} < 10^{-}$

^{5}W/K^{2}m.By means of this approximate relationship, it will be possible to predict the order of $(PF)_{max}$ according to σ_{min}. The scatter of points around the averaged line is apparently due to the non-strict rectilinearity of the corresponding σS^2 - S dependences. When these dependencies are practicalli rectilinear, then the points fit well on the curve (compare Figs.1 and 2).

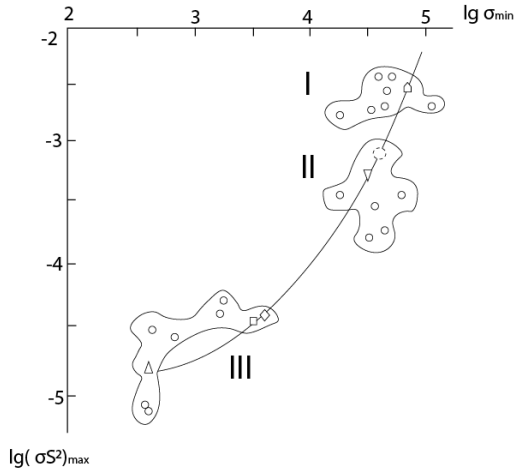


Fig. 2. Dependences $lg(\sigma S^2)_{max} - lg\sigma_{min}$. The coordinates of the points are calculated according to the data of following works: (sect.I) $Si_{0.7}Ge_{0.3}$ [17], SiGe, $SiGeMo_{0.2}$ [19], PbTe [21]; (sect.II) $Sb_{1.7}Bi_{0.4}Te_3$ [20], Bi_2Te_3, $(Bi_{0.98}Sn_{0.02})_2Te_{2.7}Se_{0.3}$ [22], $Si_{0.68}Ge_{0.32}Ga$ [23],$Ni_2CuCrFe$ [24];(sect.III)$Bi_2Sr_2Co_{1.8}O_y$, $Bi_2Sr_{1.9}[Sr(BO_2)_2]_{0.1}Co_{1.8}O_y$ [18] (and the same thermoelectrics with different composition of components). Figurative points correspondto Fig.1: Δ - [19], □ - $Si_{0.72}Ge_{0.28}$, ◊ - [23] ,∇ - [24], ○ - [24], ⌂ - [19].

Figure 3 shows the temperature dependencesof σS^2 – T and S – lnTfor $Si_{0.72}Ge_{0.28}$ and $Si_{0.76}Ge_{0.24}$ (dependencies for other compositions have the same form). From this figure it is clear that these dependences have a maximum at the same temperature (~1100K).

It should be noted that for practically all otherthermoelectrics considered above (and also for P-Si_xGe_{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]:

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

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)$^{(*)}$. Figure 4(a) shows these dependences forP-Si_xGe_{1-x}, and Figure 4(b) - 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≡tgα≅1.122·10^{-4}. The slopes of the lines presented in Fig.4(b) are tgα ≅1.324, 1.475 and 1.050·10^{-4}, respectively. These slopes which approach to K=$\frac{3}{2}\frac{k_B}{q_e}$ ≅1.293·10^{-4} with more or less accuracy.

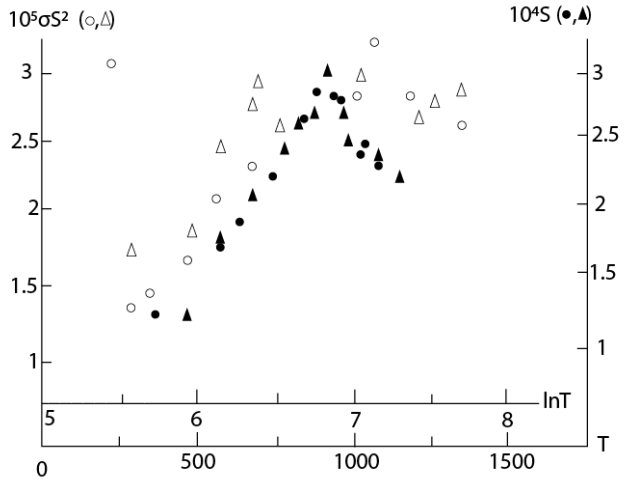
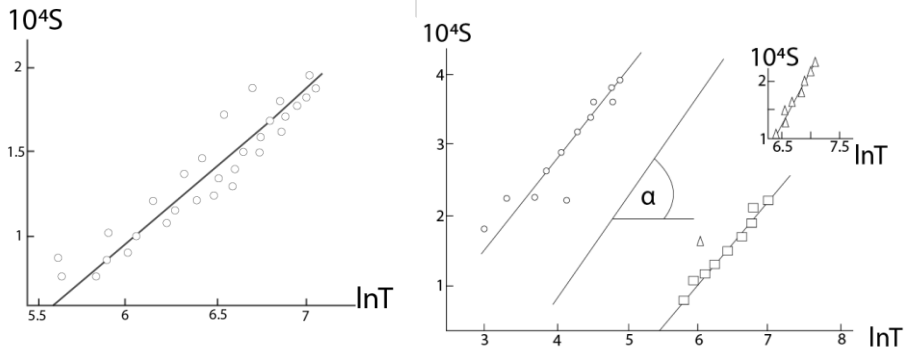


Fig. 3. DependenciesσS^2 – T and S – lnTfor $Si_{0.72}Ge_{0.28}$(o, Δ**)** and $Si_{0.76}Ge_{0.24}$ **(●, ▲)**.
(ln1100≅7, the scales are different on the abscissa axes).
[σS^2]=W/K^{2}m, [S]=V/K, [T]=K.



(a)(b)

Fig.4. Dependencies S - lnT: (a) P-Si_xGe_{1-x} - x=0.72, 0.76, 0.8 at $n=3.2\cdot10^{26}m^{-3}$ and P-$Si_{0.7}Ge_{0.3}$ at $n=2\cdot10^{26}m^{-3}$.The points belong to all values of x in Si_xGe_{1-x} (in most cases, the points for different x overlap each other);

(b) $Sb_{1.7}Bi_{0.4}Te_3$ (o), $Tl_9Sb_{0.99}Sn_{0.1}Te_6$ (Δ) and $SiGeMo_{0.2}$ (□). A straight line without points was constructed at $tg\alpha\cong1.293\cdot10^{-4}$ with arbitrarily taken b=-4.4. [S]=V/K.

Since the values of K do not coincide exactly with $\frac{3}{2}\frac{k_B}{q_e}$, it is difficult to estimate the corresponding values of the constant A (see Footnote below) from the values of Ccalculated below.However, according to as yet unpublished data for P-$Si_{0.7}Ge_{0.3}$, 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].
Figure 5 presents σS^2 – σ dependences for $Si_{0.7}Ge_{0.3}$ and $Tl_8Sn_2Te_6$ [29]. The first is described by the empirical expression $\sigma S^2\cong(108/\sigma)-1\cdot10^{-4}$, and the second: $\sigma S^2\cong(37.5/\sigma)-4.5\cdot10^{-4}$. It should be noted that the second one is better described by the expression $\sigma S^2\cong6.728\sigma^{-1.993}$. This is due to the fact that the σS^2 – S dependence for $Tl_8Sn_2Te_6$ is power law type and not rectilinear. And this is a more general case.

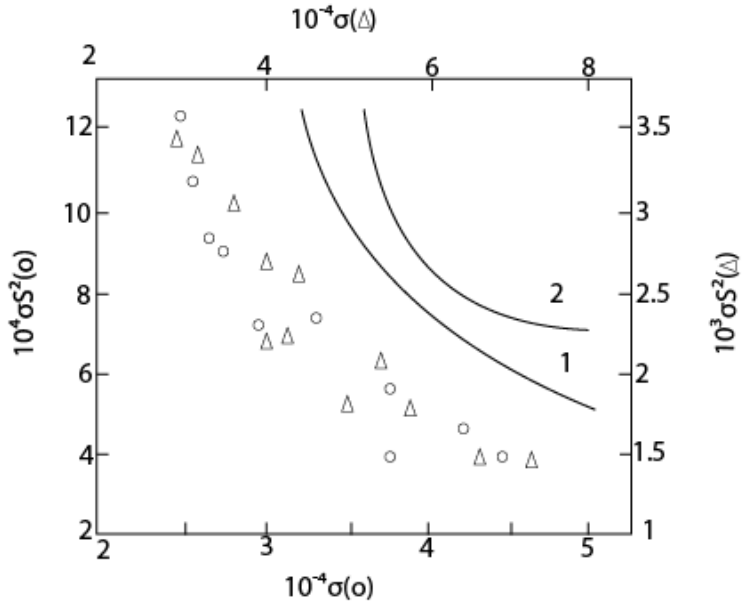
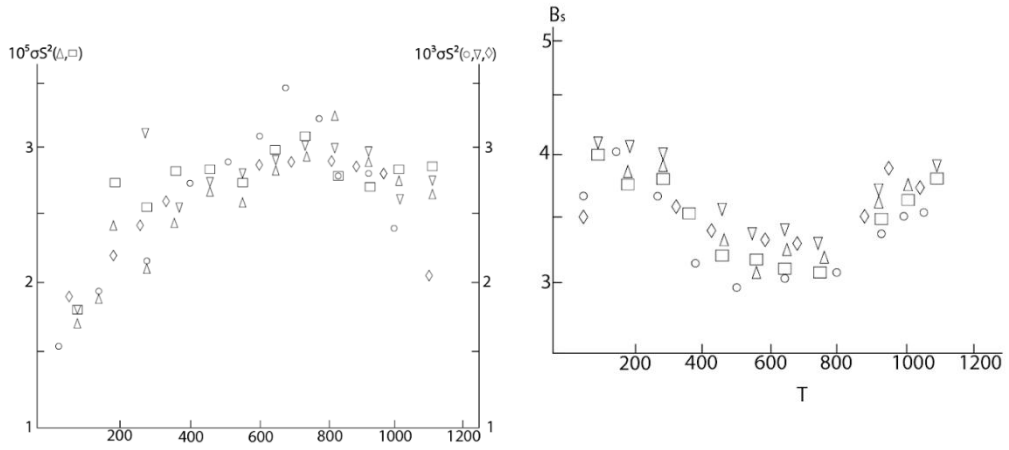


Fig. 5. Dependences σS^2 – σ: (o) - $Tl_8Sn_2Te_6$, (Δ) -$Si_{0.7}Ge_{0.3}$; lines without points- shematic graphs of functions $y=x^{-1/3}$ (1) and $y=ax^{-b}$, $b\neq-1/3$ (2). [σ]=Sim/m, $[\sigma S^2]=W/K^2$.

Temperature dependences of the power factor

Figure 6a shows the temperature dependences of the power factor for allsamplesN-Si_xGe_{1-x}, having the shape of a parabola with a negative coefficient at T^2. Calculation of the scaled power factor ($B_S=\sigma S^2/B_E$, where B_E is the electronic quality factor [30]) showed that its temperature dependence also has the shape of a parabola (but with a positive coefficient at T^2 (Fig.6b). Presented in Fig.5 dependencies can be described by empirical expressions $\sigma S^2=-1.67210^{-n-6}T^2+3.421\cdot10^{-n-3}T+1.15\cdot10^{-n}$, where n=3 for $Si_{0.7}Ge_{0.3}$, $Si_{0.8}Ge_{0.22}$, $Si_{0.83}Ge_{0.17}$and n=5 for $Si_{0.72}Ge_{0.28}$, $Si0_{.76}Ge_{0.24}$; $B_S=2.067\cdot10^{-6}T^2-3.905\cdot10^{-3}T+4.9$. Both dependences exhibit extremums at approximately the same temperature (1000-1100K). Since B_S depends

only on the Seebeck coefficient (it is given by the expression $B_S=\left[\frac{e^{S_r-2}}{1+e^{-5(S_r-1)}}+\frac{\frac{3}{\pi^2}S_r}{1+e^{5(S_r-1)}}\right]$, where $S_r=\frac{q_e}{k_B}S$ is the reducedSeebeck coefficient), to estimate $(\sigma S^2)_{max}$ can be used as σ_{min}, and $(B_S)_{min}$ (if the themperature dependencies of σS^2 and $B_S$are described by a quadratic equations).



(a)(b)

Fig. 6. Temperature dependences of σS^2 (a) and B_S (b) in Si_xGe_{1-x}: x=0.7 (o), 0.72 (Δ), 0.76 (□), 0.8 (◊) and 0.83 (∇).

$[\sigma S^2]=W/K^2m$, [T]=K.

Footnote:

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

2. CONCLUSION

A method is proposed for determining the maximum power factor of Si_xGe1_{-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 single empirical expression$lg(\sigma \mathbf{S}^2)_{max}\cong 0.583(lg\sigma_{min})^2-3.332lg\sigma_{min}$.

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

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