

THE MAXIMUMS OF FIGURE OF MERIT OF ALLOY $\text{Si}_x\text{Ge}_{1-x}$

ABSTRACT

The dependence of maximums of figure of merit ($(ZT)_{\max}$) on thermoelectric quality factor (B) for thermoelectric $\text{Si}_x\text{Ge}_{1-x}$ of n- and p-type conductivity with a charge carrier concentration of $3.2 \cdot 10^{26} \text{m}^{-3}$ has been considered. The values of x are: 0.7, 0.72, 0.76, 0.8 and 0.83. For all samples, $(ZT)_{\max}$ appear 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 $\text{Si}_x\text{Ge}_{1-x}$ with other relative compositions as well. Thus, σ' can be used to predict of $(ZT)_{\max}$. With this approach, is not required coefficient of thermal conductivity (k_L). $\sigma'S^2$ – 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 ($1 \cdot 10^{-4} \leq S \leq 2.5 \cdot 10^{-4} \text{V} \cdot \text{K}^{-1}$) is well described by the parabolic empirical expression. And in the range $0 \leq S \leq 6 \cdot 10^{-4} \text{V} \cdot \text{K}^{-1}$ the equation of exponential type should be used. Experimental points in coordinates σ' – 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- $\text{Si}_x\text{Ge}_{1-x}$, except of some points for p- $\text{Si}_{0.7}\text{Ge}_{0.3}$. The dependence σ' – B_S/S^2 have the form of a straight line with a slope of $1.347 \cdot 10^8 \text{Sim} \cdot \text{W}^{-1} \cdot \text{K}^{-2}$.

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

1. INTRODUCTION

$\text{Si}_x\text{Ge}_{1-x}$ 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 merit of thermoelectric $\text{Si}_x\text{Ge}_{1-x}$. This problem is the key to thermoelectric energy conversion.

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 [10-14]. In [15] is considered the thermoelectric quality factor $B = B_E T / k_L = ZT / B_S^{(*)}$. In this work, the dependence of the maximum value of the figure of merit $ZT = \sigma S^2 T / k_L$ on B , which is regular for different thermoelectrics, is given.

In [16,17], we studied some thermoelectric characteristics of the SiGe alloy. This article discusses the electrical quality factor and universal electrical conductivity of $\text{Si}_x\text{Ge}_{1-x}$ (concentration of charge carriers $3.2 \cdot 10^{26} \text{m}^{-3}$). The quality factor is calculated. Data on the dependences $(ZT)_{\text{max}} - B$, $(ZT)_{\text{max}} - x$, $\sigma' - x$ and $(ZT)_{\text{max}} - \sigma'$ are presented. The values of BE , σ' , kL and ZT are calculated based on the temperature dependences of electrical conductivity ($\sigma=1/\rho$, ρ is electrical resistivity), thermal conductivity and Seebeck coefficients according to data from [18]. For all samples $(ZT)_{\text{max}}$ appears at about 900°C .

2. DISCUSSION

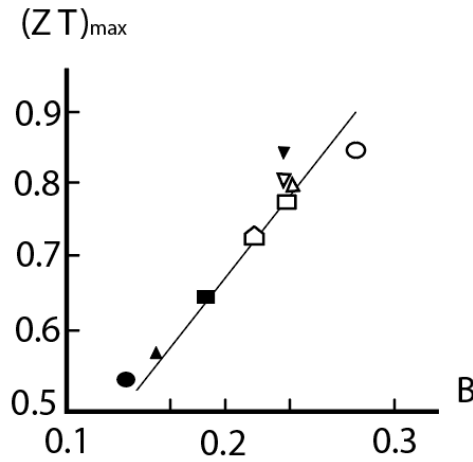


Fig.1. Dependence $(ZT)_{\text{max}} - B$ in $\text{Si}_x\text{Ge}_{1-x}$: \circ - $x=0.7$, Δ - $x=0.72$, \square - $x=0.76$, ∇ - $x=0.8$, \triangle - $x=0.83$ (n-type); \bullet - $x=0.7$, \blacktriangle - $x=0.76$, \blacksquare - $x=0.8$ (p-type); \blacktriangledown - from [19].

Figure 1 shows the dependence $(ZT)_{\text{max}} - B$, it can be described by the expression $(ZT)_{\text{max}} \cong 3.2B + 0.05$. Values of $(ZT)_{\text{max}}$ can also be estimated indirectly: consider the dependence of $(ZT)_{\text{max}}$ on the universal electrical conductivity (σ') given by expression $\sigma' = (q/k_B)^2 \sigma / B_E = (q/k_B)^2 B_S / S^2$. Let's bring also the dependences $(ZT)_{\text{max}} - x$ and $\sigma' - x$ (Figs.2 and 3). As can be seen from the Fig.2, for the n-type, $(ZT)_{\text{max}}$ decreases with increasing x ($(ZT)_{\text{max}} \cong -0.81x + 1.42$), and for the p-type, it increases ($(ZT)_{\text{max}} \cong 0.39x + 0.28$).

In [19] among various thermoelectric materials, data on $\text{Si}_{0.9}\text{Ge}_{0.1}$ are given: $(ZT)_{\text{max}} \cong 0.87$ at a temperature of about 900°C . With this value and the Lorentz number, the corresponding Seebeck coefficient can be calculated: $S \cong 1.47 \cdot 10^{-4} \text{V} \cdot \text{K}^{-1}$. From the latter: $B_S \cong 3.96$ and $B \cong 0.23$. This point is shown in Fig.1.

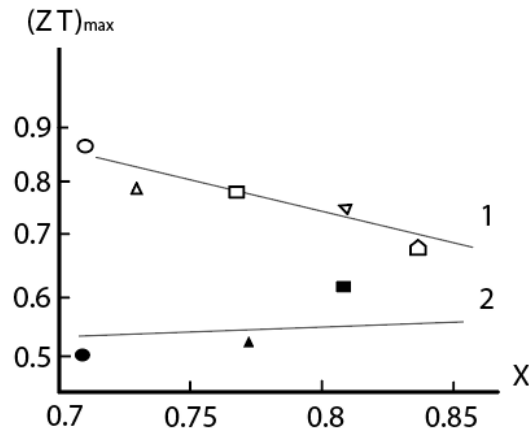


Fig.2. Dependence $(ZT)_{\max} - x$ in $\text{Si}_x\text{Ge}_{1-x}$: 1 - n-type, 2 - p-type. \circ, \bullet - $x=0.7$, Δ - $x=0.72$, \square, \blacktriangle - $x=0.76$, ∇, \blacksquare - $x=0.8$, $\triangleleft, \blacktriangleleft$ - $x=0.83$.

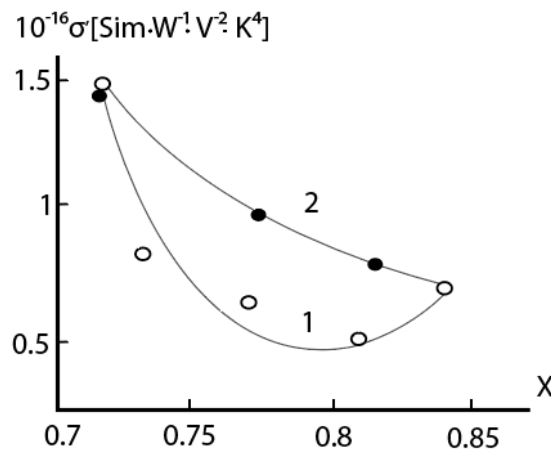


Fig.3. Dependence $\sigma' - x$ in $\text{Si}_x\text{Ge}_{1-x}$ (σ' for $(ZT)_{\max}$)^(**): 1 - n-type, 2 - p-type.

By combining the dependences $(ZT)_{\max} - x$ and $\sigma' - x$, we will get the $(ZT)_{\max} - \sigma'$ dependence (Fig.4). This dependence gives: $\lg(ZT)_{\max} \cong -0.41\lg\sigma' + 6.2$. This allows us to predict with sufficient accuracy the mentioned maximum for other values of σ' , i.e. for $\text{Si}_x\text{Ge}_{1-x}$ 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 $\sigma'S^2$).

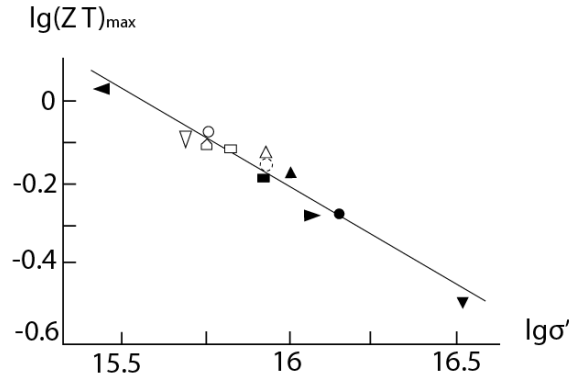


Fig.4. Dependence $\lg(ZT)_{\max} - \lg\sigma'$ for $\text{Si}_x\text{Ge}_{1-x}$ (σ' for $(ZT)_{\max}$) (**): \circ - $x=0.7$, Δ - $x=0.72$, \square - $x=0.76$, ∇ - $x=0.8$, \triangleleft - $x=0.83$ (n-type); \bullet - $x=0.7$, \blacktriangle - $x=0.76$, \blacksquare - $x=0.8$ (p-type); \blacktriangleleft and \blacktriangledown - for $\text{NaCo}_{0.9}\text{Cr}_{0.1}\text{O}_2$ and NaCoO_2 [20], \circ and \blacktriangleright - for $\text{Cu}_{1.98}\text{S}_{0.9}\text{Se}_{0.1}$ and $\text{Cu}_{1.98}\text{S}_{0.8}\text{Se}_{0.2}$ [21].

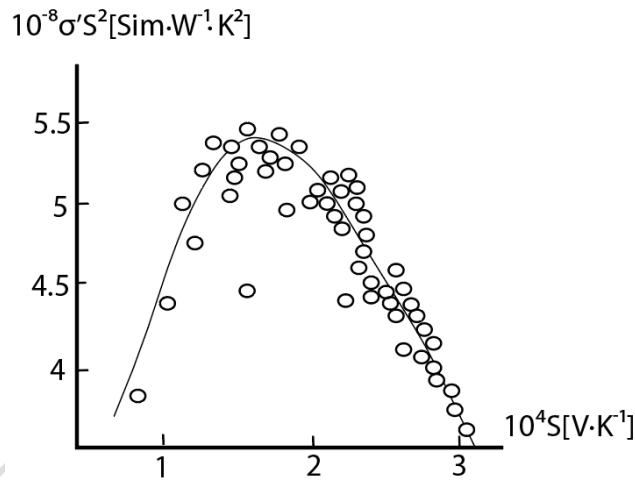


Fig.5. Dependence $\sigma'S^2 - S$. The points correspond to all x values in n- and p- $\text{Si}_x\text{Ge}_{1-x}$.

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 $\sigma'S^2 - S$ dependence and the averaged curve for a large number of samples calculated from the data of [15] (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 ($1 \cdot 10^{-4} \leq S \leq 2.5 \cdot 10^{-4} \text{ V} \cdot \text{K}^{-1}$) 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 $0 \leq S \leq 6 \cdot 10^{-4} \text{ V} \cdot \text{K}^{-1}$ the equation of type $\sigma'S^2 = aS^b e^{cS}$ should be used, where a , b and c are constants.

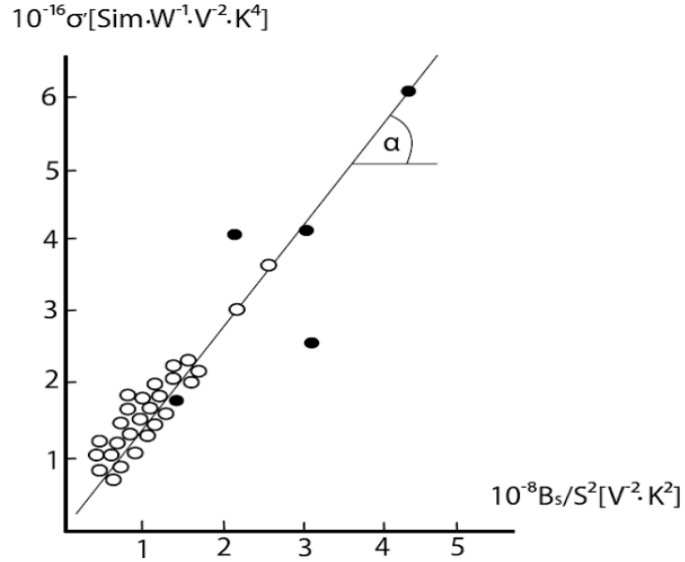


Fig.6. Dependence $\sigma' - B_S/S^2$ for $\text{Si}_x\text{Ge}_{1-x}$: (○) - all examined values of x in n- and p-type $\text{Si}_x\text{Ge}_{1-x}$, except for p- $\text{Si}_{0.7}\text{Ge}_{0.3}$ (●); $\text{tg}\alpha=1.347 \cdot 10^8$.

Experimental points in coordinates $\sigma' - B_S/S^2$ are well located on a straight line for all x in n- and p- $\text{Si}_x\text{Ge}_{1-x}$, except of some points for p- $\text{Si}_{0.7}\text{Ge}_{0.3}$ (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 $1.347 \cdot 10^8 \text{ Sim} \cdot \text{W}^{-1} \cdot \text{K}^{-2}$.)

3. CONCLUSION

The alloy $\text{Si}_x\text{Ge}_{1-x}$ 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: $(ZT)_{\text{max}} \cong 3.2B + 0.05$. Dependence $(ZT)_{\text{max}}$ on universal electrical conductivity is: $\lg(ZT)_{\text{max}} \cong -0.4 \lg \sigma' + 6.2$. This allows us to assume the mentioned maxima for other values of σ' (that is, for $\text{Si}_x\text{Ge}_{1-x}$ with other relative compositions as well. Thus, σ' can be used to predict of $(ZT)_{\text{max}}$.

Footnote belows:

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

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

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