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# METHOD FOR DETERMINING THE MAXIMUM OF POWER FACTOR OF N-TYPE SIGE THERMOELECTRIC

(short communication)

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**Abstract.** The article discusses a method for estimating the maximum value of the power factor of the SiGe alloy.  $(PF)_{max}$  can be determined from  $(B_S)_{min}$ , where  $B_S$  is the scaled power factor.

Keywords: SiGe alloy, Maximum of power factor, Scaled power factor

### Itroduction

Thermoelectric materials convert thermal energy into electrical energy. They are used to supply electricity to spacecraft and in many fields of science and technology. Power factor (PF= $\sigma$ S<sup>2</sup>,  $\sigma$  - specific electrical conductivity, S - Seebeck coefficient) is an important energy characteristic of thermoelectric. It is included in the expression of the figure of merit: ZT=  $\sigma$ S<sup>2</sup>T/ $\lambda$  (T - absolute temperature,  $\lambda$  - thermal conductivity). For different thermoelectrics the power factor ranges from hundred thousandths to units W/K<sup>2</sup>m [1-3]<sup>(1)</sup>.

This communication is a continuation of works [4,5], where the maximization of the figure of merit and power factor of thermoelectric material SiGe are considered. In particular, it has been established that the maximum of the PF corresponds to the minimum of  $\sigma$ . Their interdependence for various thermoelectrics (according to the literature and our data) is described by one empirical expression  $lg(\sigma S^2)_{max} \cong 0.583(lg\sigma_{min})^2$ -3.332lg $\sigma_{min}$ .

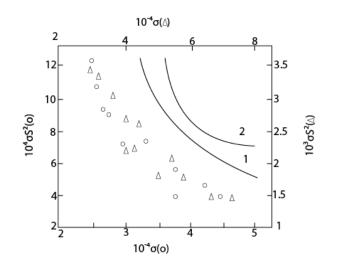


Figure 1. Dependences  $\sigma S^2 - \sigma$ : ( $\Delta$ ) - Si<sub>0.7</sub>Ge<sub>0.3</sub>, (o) - Tl<sub>8</sub>Sn<sub>2</sub>Te<sub>6</sub>; lines without points - shematic graphs of functions y=x<sup>-1/3</sup> (1) and y=ax<sup>-b</sup>, b $\neq$ -1/3 (2). [ $\sigma$ ]=Sim/m, [ $\sigma S^2$ ]=W/K<sup>2</sup>m. Figure 1 presents  $\sigma S^2 - \sigma$  dependence for  $Si_{0.7}Ge_{0.3}$ . There is also a graph for  $Tl_8Sn_2Te_6$  [6] for comparison. The first is described by the empirical expression  $\sigma S^2 \cong (108/\sigma) - 1 \cdot 10^{-4}$ , and the second:  $\sigma S^2 \cong (37.5/\sigma) - 4.5 \cdot 10^{-4}$ . It should be noted that the second one is better described by the expression  $\sigma S^2 \cong 6.728\sigma^{-1.993}$ . This is due to the fact that the  $\sigma S^2 - S$  dependence for  $Tl_8Sn_2Te_6$  is power law type and not rectilinear.<sup>(2)</sup> And this is a more general case.

In this communication another method is considered: to estimate  $(PF)_{max}$ , you can also use  $(B_S)_{min}$ ,

where B<sub>S</sub> is the scaled power factor. It is given by the expression [7] B<sub>S</sub> =  $\left[\frac{e^{S_r-2}}{1+e^{-5(S_r-1)}} + \frac{\frac{\pi^2}{3}S_r}{1+e^{5(S_r-1)}}\right]$ ,

where  $S_r = \frac{q_e}{k_B} S$  is the reduced Seebeck coefficient.

# Experimental

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<sub>x</sub> Ge<sub>1-x</sub> were 0.7, 0.72, 0.76, 0.8 and 0.83. The concentration of charge carriers was  $n=3.2 \cdot 10^{26} \text{ m}^{-3}$ . The study was carried out at 50-1180°C. The upper limit was limited by the melting point of the alloy. The measurement error of Seebeck coefficient was 3% and of specific electrical conductivity 5%.

### Discussion

Figure 2a shows the temperature dependences of the power factor for all samples  $Si_xGe_{1-x}$ , having the shape of a parabola with a negative coefficient at T<sup>2</sup>. Calculation of the scaled power factor showed that its temperature dependence also has the shape of a parabola (but with a positive coefficient at T<sup>2</sup> (Fig.2b). Presented dependencies can be described by empirical expressions  $\sigma S^2$ =-1.67210<sup>-n-6</sup>t<sup>2</sup>+3.421·10<sup>-n-3</sup>t+1.15·10<sup>-n</sup>, where n=3 for Si<sub>0.7</sub>Ge<sub>0.3</sub>, Si<sub>0.8</sub>Ge<sub>0.22</sub>, Si<sub>0.83</sub>Ge<sub>0.17</sub> and n=5 for Si<sub>0.72</sub>Ge<sub>0.28</sub>, Si<sub>0.76</sub>Ge<sub>0.24</sub>; B<sub>S</sub>=2.067·10<sup>-6</sup>t<sup>2</sup>-3.905·10<sup>-3</sup>t+4.9. All dependences exhibit extremums at approximately the same temperature: (700-800)°C. Since B<sub>S</sub> depends only on the Seebeck coefficient, to estimate ( $\sigma S^2$ )<sub>max</sub> can be used (B<sub>S</sub>)<sub>min</sub> (if the themperature dependencies of  $\sigma S^2$  and B<sub>S</sub> are described by a quadratic equations).

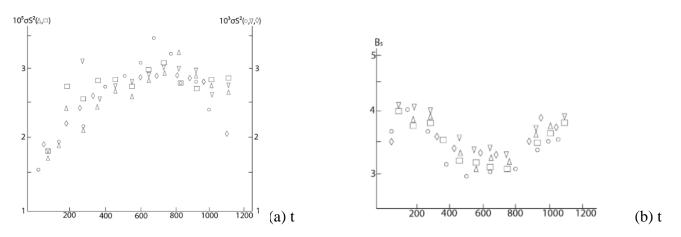


Figure 2. Temperature dependences of  $\sigma S^2$  (a) and  $B_S$  (b) in  $Si_xGe_{1-x}$ : x=0.7 (o), 0.72 ( $\Delta$ ), 0.76 ( $\Box$ ), 0.8 ( $\Diamond$ ) and 0.83 ( $\nabla$ ). [ $\sigma S^2$ ]=W/K<sup>2</sup>m, [t]=°C.

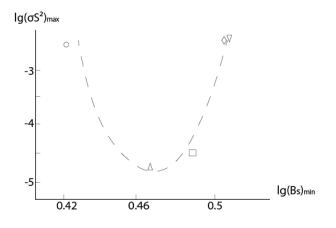


Figure 3. Dependence  $\lg(\sigma S^2)_{max}$  -  $\lg(B_S)_{min}$  in Si<sub>x</sub>Ge<sub>1-x</sub>: x=0.7 (o), 0.72 ( $\Delta$ ), 0.76 ( $\Box$ ), 0.8 ( $\diamond$ ) and 0.83 ( $\nabla$ ).

Figure 3 shows points in coordinates  $\lg(\sigma S^2)_{max}$  -  $\lg(B_S)_{min}$ . The dependence is not quite clear-cùt in order to predict the PF according to  $B_S$  for  $Si_xGe_{1-x}$  alloy with other compositions. However, if we take this dependence as a parabola, its extremum will correspond to the value  $(B_S)_{min}$  (respectively, to the T), as in Figures 2a,b.

Footnotes:

<sup>(1)</sup>For relatively small PFs, the ZT can take on high values depending on  $\lambda$ .

<sup>(2)</sup>For SiGe, the  $\sigma S^2$  - S dependences are almost rectilinear [8]:  $\sigma S^2 = kS + b$ , 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. After simple transformations we will have:  $\sigma S^2 = \frac{k}{2\sigma} + b$ . This indicates that the maximum value of the power factor will correspond to the minimum value of specific electrical conductivity.

# Conclusion

A method for estimating the maximum value of the power factor of the SiGe alloy is discussed.  $(PF)_{max}$  can be determined from  $(B_S)_{min}$ , where  $B_S$  is the scaled power factor. All presented dependences have extrema at approximately the same temperatures:  $(700-800)^{\circ}C$ .

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