Original Research Article

DETERMINATION OF ELECTRONIC QUALITY FACTOR, UNIVERSAL ELECTRICAL CONDUCTIVITY, EFFECTIVE MASS ANDMOBILITY OF CHARGE CARRIERS OF ALLOY n-Si_xGe_{1-x}

ABSTRACT

The temperature dependences of the electronic quality factor and the universal electrical conductivity of n-type $Si_x\,Ge_{1-x}$, as well as the dependences of the Seebeck coefficient on the specific and the universal conductivities, are studied. The effective masses and mobilities of charge carriers are calculated for different temperatures, temperature dependences of the eleqtronic quality factor and the thermoelectric figure of merit are studied.

Keywords: thermoelectric SiGe; electronic quality factor; universal electrical conductivity

1. INTRODUCTION

Crystalline and amorphous SiGe composites are wiedly used in thermogenerators, coolers, sensors [1, 2], thin-film transistors [3], batteries [4], solar cells [5,6], photodetectors [7,8] and others. These alloys are good high-temperature materials for the temperature range up to 1200℃. For the study, we chose an Si_xGe_{1-x} alloy of n-type conductivity, since in some cases this type has advantages over the p-type. For example, the maximum of figure of merit ZT is about 2.5 times greater for n-type$Si_{0.7}Ge_{0.3}$ than for p-type (at the same values of x and concentration of charge carriers $n= 3.2\cdot10^{26}\ m^{-3}$). Thisfollows 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 σS^2 is ~2 orders of magnitude greater), and thermal conductivity coefficient is 1.1-1.3 times smaller at the same temperatures. Also with neutron fluences $\geq10^{19}$ and irradiation temperatures ≥600℃ n-type $Si_xGe_{1-x}$is more radiation resistant [9].

In Ref.[10], the concept of universal electrical conductivity of thermoelectrics was introduced, whichwe denote by σ': $\sigma'=\frac{\sigma}{B_E}\left(\frac{q_e}{k_B}\right)^2$. Here $B_E=\sigma S^2/B_S$ is the electronic quality factor, and B_S is a dimensionless quantity depending on S(σ – specific electroconductivity, S – Seebeck coefficient, q_e – elementary charge, k_B – Boltzmann's constant)$^{(*)}$. $B_E$andσ'are important characteristics of thermoelectric materials. In particular, factor B_E performs scaling of thermoelectric quantities.

2. 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_xGe_{1-x}were 0.7 and 0.83.The concentration of charge carriers was $n= 3.2 \cdot 10^{26}$ m^{-3}. The study was carried out at 50-1180℃. The upper limit was limited by the melting point of the alloy. The measurement error of S was 3% , and of specific resistivity $\rho(=\sigma^{-1})$ 5% . The thermal conductivity coefficients (χ) were also measured with an error of no more than 7% .

3. RESULTS AND DISCUSSION

Fig.1 shows B_E - t dependences for n-$Si_x Ge_{1-x}$, which repeat the shape of the schematic curve from [10], which illustrates the presence of additional effects. (For an ideal thermoelectric, the electronic qualitry factor is independent of temperature.)

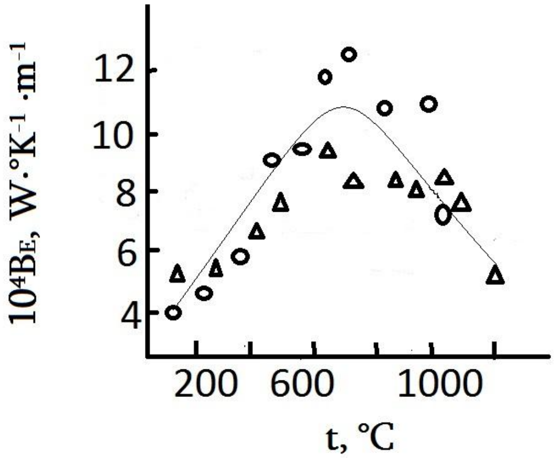

Fig.1. Temperature dependences of electronic quality factor for $Si_{0.7}Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ).

First consider the temperature dependences of universal electrical conductuvuty in $Si_{0.7}Ge_{0.3}$ and $Si_{0.83}Ge_{0.17}$. This is shown in Fig.2. As can be seen from this figure, the experimental points form almost a single set, i.e. there is a scaling of the specific electrical conductivity.

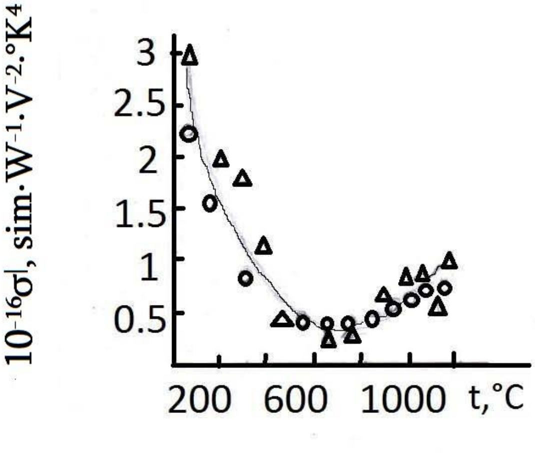

Fig.2. Temperature dependences of universal electrical conductivity in $Si_{0.7}$ $Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ).

Consider the dependence S- σ forSi_xGe_{1-x}. It turned out that it can be determined in a very simple way, without resorting to the Pisarenko formula [11] - a study of the dependence σS^2(power factor) - S showed their rectilinearity (Fig.3): $\sigma S^2=kS + b$, where k is the slope of the straight lines, b- the ordinate of the point of their intersection with the axis σS^2 when extrapolating these lines to$S\to 0$. The numerical values of the constants were: k≅7.5, b≈0 for x=0.7and k≅10, $b\cong 5\cdot 10^{-4}$ for x=0.83. From the last equation we get:

$$S = \frac{k}{2\sigma} + \left[\left(\frac{k}{2\sigma}\right)^2 + \frac{b}{\sigma}\right]^{1/2} \quad (1)$$

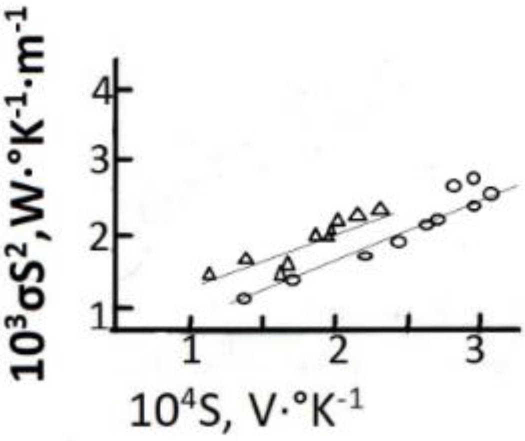

Fig.3. DependencesσS^2-S for$Si_{0.7}Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ).

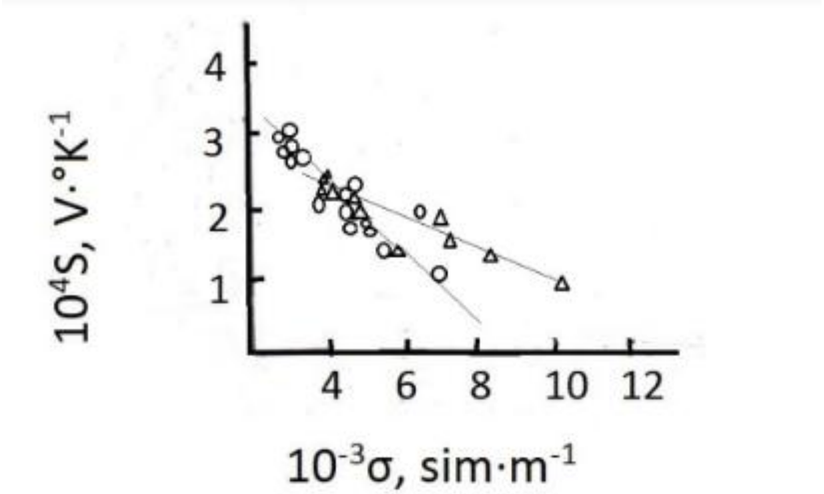

Fig.4. DependencesS – σ for$Si_{0.7}Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ).

The plot of Eq.(1) is generally a higher-order curve, but due to the relatively narrow range of variables, almost straight lines are obtained (Fig.4). For dependence S-σ' we will have:

$$S = 6.73 \cdot 10^7 \frac{k}{B_E \sigma'} + \left[4.53 \cdot 10^{15} \left(\frac{k}{B_E \sigma'}\right)^2 + 1.35 \cdot 10^8 \frac{b}{B_E \sigma'}\right]^{1/2} \qquad (2)$$

On Fig.5is presented S - σ' dependence.As can be seen, the experimental points form almost a single set, regardless of the meaning of x in Si_xGe_{1-x}(i.e. electronic quality factor scales specific electroconductivity). This dependence is described by the empirical expression $S \cong 226.67(\sigma')^{-0.38}$.

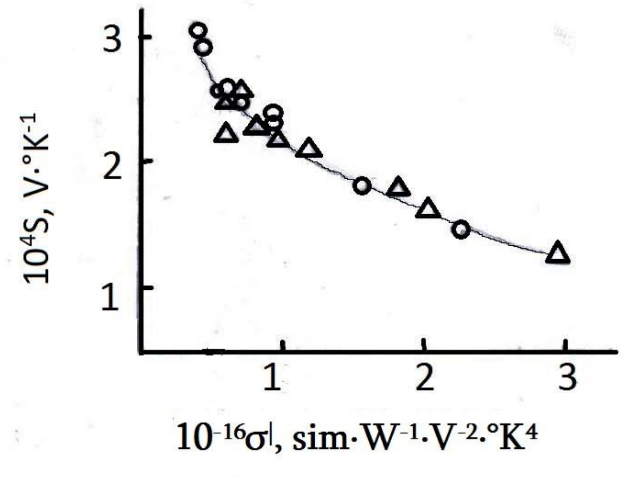

Fig.5. Dependences $S - \sigma'$ for $Si_{0.7}Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ).

The above results are similar to the data for p-SiGe [12] and $Bi_2Sr_2Co_{1.8}O_y$thermoelectrics[13].

We calculated the effective masses (m^*) of charge carriers for Si_xGe_{1-x}at some temperatures. The following formula are used for the calculation [14]:

$$m^* \cong \frac{h^2}{2k_B T}\left[\frac{3n}{16\sqrt{\pi}}\left(e^{S_r-2} - 0.17\right)\right]^{2/3}. \ (3)^{(**)}$$

Values m^*/m_0(m_0 - rest mass) calculated from Eq.(3) for different temperatures are shown in the table.

Table 1

Values of m^*/m_0 in Si_xGe_{1-x} for different temperatures

t,℃	m^*/m_0	
	$Si_{0.7}Ge_{0.3}$	$Si_{0.83}Ge_{0.17}$
80	-	2.6
155	2.98	-
200	-	3.13
280	-	3
300	3.73	-
390	-	3.5
445	3.06	-
490	-	3.55
550	3.8	-
645	4.56	-
650	-	3.85
735	-	3.45
740	4.59	-
855	3.76	-
885	-	2.73
940	4.16	-
990	2.82	2.5
1055	2.45	-
1085	-	1.28
1125	-	1.8
1130	1.79	-
1180	-	1.7

The obtained values of m^*/m_0 are approximate to the corresponding values for some thermoelectrics [15,16].

We also calculated the mobilities (μ) of charge carriers. μ is related to m^*/m_0 by the following formula [17]:

$$\mu = \left(\frac{m^*}{m_0}\right)^{-3/2} \mu_W \ , \tag{4}$$

where μ_W is the weighted mobility:

$$\mu_W = \frac{3.31 \cdot 10^{-7}}{\rho} \left(\frac{T}{300}\right)^{-3/2} \left[\frac{e^{S_r - 2}}{1 + e^{-5(S_r - 1)}} + \frac{\frac{3}{\pi^2} S_r}{1 + e^{5(S_r - 1)}}\right] \tag{5}$$

(ρ − specific resistivity, T − absolute temperature). By combining Eqs (3-5), as well as replacing ρ withσ and $\left[\frac{e^{S_r - 2}}{1 + e^{-5(S_r - 1)}} + \frac{\frac{3}{\pi^2} S_r}{1 + e^{5(S_r - 1)}}\right] \equiv B_S'$, we finally get:

$$\mu = 3.31 \cdot 10^{-7} \sigma \left(\frac{T}{300}\right)^{-3/2} B_S' \left(\frac{m^*}{m_e}\right)^{-3/2} . \tag{6}$$

The values of mobility calculated by the equation (6) turned out to be on average 1 order higher than for Si or Ge (0.145 and0.39m^2/V·sec, respectively [18]).These results should be considered overestimated. Therefore, we carried out experimental verification. Were obtained values of μ in the range of (0.54-0.65) m^2/V·sec, which can be considered acceptable (they are approaching data forSiGe alloy at 300°K with the same type of conductivity and concentration of charge carriers [19]).

Figure 6 shows the temperature dependences of the thermoelectric figure of merit ZT ($Z = \sigma S^2/\chi$). As can be seen from this figure, $Si_{0.7}Ge_{0.3}$ and $Si_{0.83}Ge_{0.17}$ have almost the same temperature dependence of ZT. For both alloys, the maximum of figure of merit is ZT~0.8 ($\cong$ 0.84 at 870°C for $Si_{0.7}Ge_{0.3}$and $\cong$ 0.76 at 900°C for $Si_{0.83}Ge_{0.17}$)$^{(***)}$

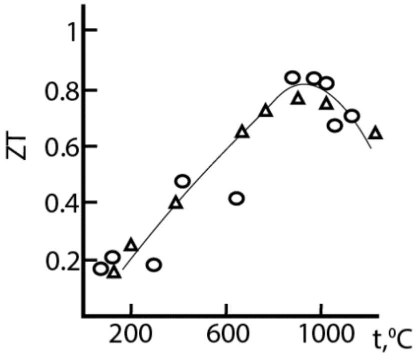

Fig.6. Temperature dependences of ZT in $Si_{0.7}Ge_{0.3}$ (o) and $Si_{0.83}Ge_{0.17}$ (Δ).

4. CONCLUSION

In n-type conductivity Si_xGe_{1-x}, (x=0.7 and 0.83) the dependence of the power factor on the Seebeck coefficient is rctilinear:$\sigma S^2=kS+b$. We will have $S=\frac{k}{2\sigma}+\left[\left(\frac{k}{2\sigma}\right)^2+\frac{b}{\sigma}\right]^{1/2}$ for S -σ dependences, and for S -σ' dependences:$S=6.73\cdot10^7\frac{k}{B_E\sigma'}+\left[4.53\cdot10^{15}\left(\frac{k}{B_E\sigma'}\right)^2+1.35\cdot10^8\frac{b}{B_E\sigma'}\right]^{1/2}$. The study of the temperature dependence of the electronic quality factor shows the presence of additional effects (band convergence etc.).The obtained values of m^*/m_0 are approximate to the corresponding values for some thermoelectrics. The experimentally determined values of μ in Si_xGe_{1-x} were (0.54-0.65) m^2/V·sec. For both $Si_{0.7}Ge_{0.3}$ and$Si_{0.83}Ge_{0.17}$ the thermoelectric figure of merit ZTis ~0.8. A noticeable difference in alloys Si_xGe_{1-x} with x=0.7 and 0.83 is observed for almost all thermoelectric characteristics. The exception is the value σ' (scaled specific electrical conductivityσ), which are scaled by the electronic quality factor B_E.

Footnote belows:

(*) $B_S=\frac{q}{k_B}\left[\frac{\frac{qS}{k_B}e^{2-\frac{qS}{k_B}}}{1+e^{-5\left(\frac{qS}{k_B}-1\right)}}+\frac{3.29S}{1+e^{5\left(\frac{qS}{k_B}-1\right)}}\right]$- the scaled power factor $(B_S=\frac{\sigma S^2}{B_E})$[10].

(**)Formula (3) is fair when $|S|>0.75\cdot10^{-4}$V/°K. In our case $S=(1.08\div3.07)\cdot10^{-4}$V/°K.

(***)For p-Si_xGe_{1-x} ($0.7\leq x\leq0.8$,n= $3.2\cdot10^{26}$ m^{-3}),$(ZT)_{max}\cong$0.5-0.65 at 800°C.(preliminary data)

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