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On the thermoelectric alloy n-Si_xGe_{1-x}

Abstract

The temperature dependences of the electronic quality factor and universal electrical conductivity of the n-type Si_xGe_{1-x} alloy, as well as the dependence of the Seebeck coefficient on the specific and universal electrical conductivities are studied. Based on the measured thermoelectric parameters (Seebeck and thermal conductivity coefficients, specific resistance) the values of thermoelectric efficiency Z are calculated.

The temperature dependences of universal electrical conductivity shows that the experimental points form almost a single set. This is due to the fact that changes of σ and B_E compensate each other. And, in general, the electronic quality factor BE performs scaling of thermoelectric quantities.

The temperature dependences of thermoelectric efficiency shown that all Si_xGe_{1-x} samples have a fairly high efficiency ($\geq 7\cdot10^{-4}$ $grad^{-1}$), the maximum of which is reached at about 700^0C. The studied alloy were used as an element of a monolithic thermoelectric module.

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

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Introduction

Si_xGe_{1-x} 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 1200^0C.[9,10] They occupy an important place next to other well-known thermoelectric materials: Bi_2Te_3,[5] GeSbInTe,[6] Mg_2Si,[7] PbTe[8] etc.

In Ref.[11] the concept of electronic quality factor (B_E) of thermoelectric was introduced: $B_E=(\hbar N_V C_l/3\pi^2 m^* \xi^2)(k_B/q)^2$, where ħ is reduced Planck's constant, C_l is a combination of elastic constants, ξ - deformation potential coefficient , m* - electron rest mass, N_V - band degeneracy, k_B - Boltzmann's constant, q - elementary charge. To calculate B_E , based on experimental data (Seebeck coefficient - S, specific electrical conductivity - σ), the formula is used:

$$B_E = \sigma S^2/B_S\,, \qquad (1)$$

where $B_s = \frac{q}{k_B}\left[\frac{\frac{qS}{k_B}e^{2-\frac{qS}{k_B}}}{1+e^{-5\left(\frac{qS}{k_B}-1\right)}} + \frac{\frac{\delta^2}{3}S}{1+e^{5\left(\frac{qS}{k_B}-1\right)}}\right]$ is scaled power factor (q – elementary charge, kB - Boltzmann's constant). Universal electrical conductivity (σ') is connected to specific conductivity as:

$$\sigma' = \left(\frac{q_e}{k_B}\right)^2 \frac{\delta}{B_E}\,. \qquad (2)$$

B_E and σ' are important characteristics of thermoelectric materials. In particular, factor B_E performs scaling of thermoelectric quantities.

In this paper, we investigate the n-type of Si_xGe_{1-x} alloy at x=0.72, 0.76 and 0.8. The temperature dependences of electronic quaility factor (B_E) and universal electrical conductivity (σ') have been studied; also the dependence of the Seebeck coefficient on specific and universal electrical conductivities. The obtained results are compared with the previously obtained data for n-type $Si_{0.7}Ge_{0.3}$ and $Si_{0.83}Ge_{0.17}$,[12] as well as for Si_xGe_{1-x} of p-type conductivity.[13]

Experimental

We made SiGe alloys with n-type conductivity. The method of joint grinding of the components and vacuum hot pressing of the obtained ultradisperse powder was used. The alloying element for n-type conduction was phosphorus (0.5 wt.%). The concentration of charge carriers was $3.2\cdot10^{20}cm^{-3}$. It was defined by measuring the Hall constant at room temperature.

The grain sizes of the powder were evaluated with an optical microscope "Nicon" and an X-ray diffractometer DRON-3M. Ultradisperse powder consisted mainly of 60–80 nanometer Si and Ge grains.

The temperature dependences of specific electrical resistivity (ρ), Seebeck and thermal conductivity coefficients (respectively S and χ) were used according to the data of[9] On this basis, we built the temperature dependences of specific electrical conductivity (σ=1/ρ), which is shown in Figure 1. They have a parabolic shape.

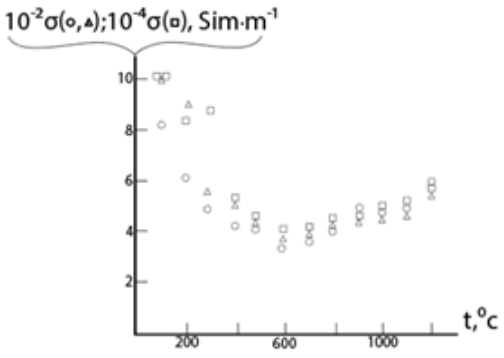

Figure 1 Temperature dependences of σ: x=0.72 (o), 0.76 (Δ) and 0.8 (□) in Si_xGe_{1-x}.

Results and discussions

Figure 2 shows the (σ – S) dependences. They are built by comparing of (σ – t) and (S– t) dependencies. It can be seen from this figure that (σ – S) dependences for compositions of Si_xGe_{1-x} alloy at x=0.72 and 0.76 is practically the same. And for x=0.8, the values of σ are two orders of magnitude greater at the same temperatures (same as for dependence (σ – t)).

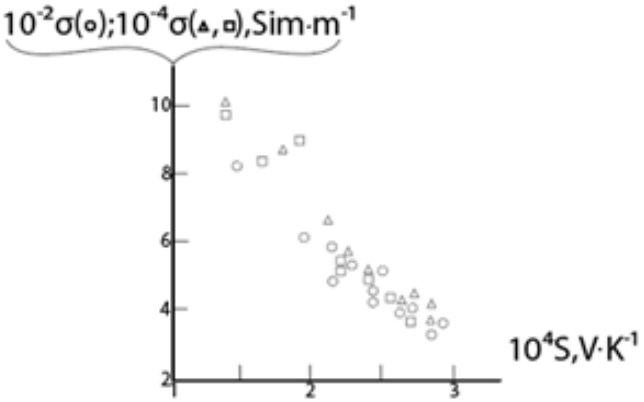

Figure 2 Dependences (σ – S): x=0.72 (o), 0.76 (Δ) and 0.8 (□) in Si_xGe_{1-x}.

Figure 3 shows the temperature dependences of B_E. Their appearance indicates the presence of additional effects (band convergence, bipolar effects, additional scattering).[11] As can be seen, the temperature behavior of B_E is the same for all samples. However, for $Si_{0.8}Ge_{0.2}$ values B_E are two orders of magnitude greater than for $Si_{0.72}Ge_{0.28}$ and $Si_{0.76}Ge_{0.24}$ at the same temperatures.

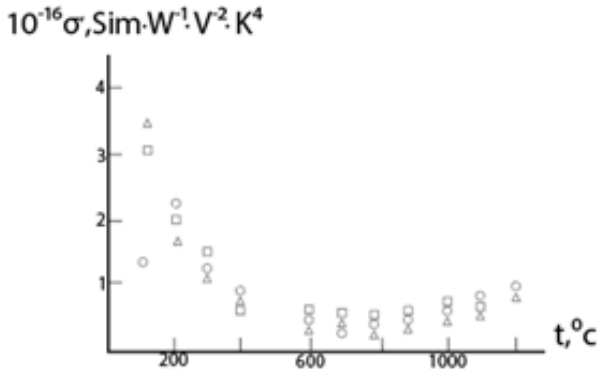

Figure 3 Temperature dependences of B_E: x=0.72 (o), 0.76 (Δ) and 0.8 (□) in Si_xGe_{1-x}.

The temperature dependences of σ' are shown in Figure 4. The figure shows that the experimental points form almost a single set. This is due to the fact that changes of σ and B_E compensate each other (see above). And, in general, the electronic quality factor B_E performs scaling of thermoelectric quantities. (σ' – t) dependences also have the shape of a parabola. In particular, the middle of this set (region 200-1100□) is well described by the empirical equation $\sigma' = 1.274 \cdot 10^{11} t^2 - 1.714 \cdot 10^{14} t + 6.510^{16}$.

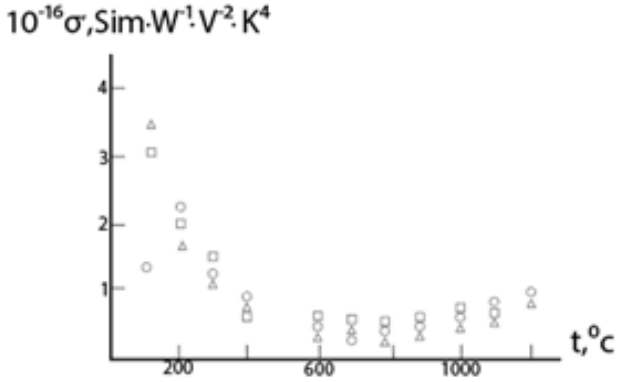

Figure 4 Temperature dependences of σ': x=0.72 (o), 0.76 (Δ) and 0.8 (□) in Si_xGe_{1-x}.

Figure 5 shows the dependences of (σ'– S): the experimental points form almost a single set. This set is described by the empirical expression $\sigma' = 3.095 \cdot 10^{11} S^{-1.259}$.

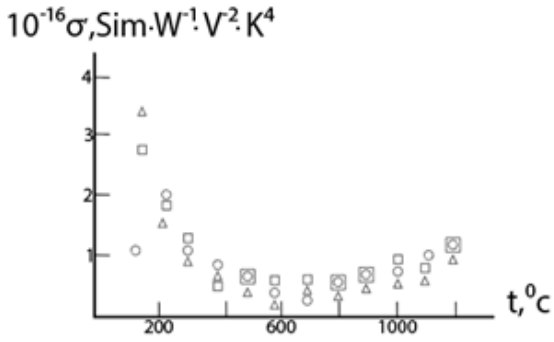

Figure 5 Dependences (σ' – S): x=0.72 (o), 0.76 (Δ) and 0.8 (□) in Si_xGe_{1-x}.

From Figure 1 & 2 show a large difference between the (σ – t) and (σ – S) dependences for x=0.72, 0.76 in SixGe1-x and for x=0.8. And in Figure 6 experimental points form a common set for all samples. This is due to the fact that changes in σ and B_E compensate each other.

When considering the dependence (σ - σ'), turned out to be are practically rectilinear (Figure 5). Based on the rectiliearity of the dependencies (σ - σ') and Eq.(2), one could assume that B_E=const. However, this is on the ideal case. Under real conditions, additional effects leads to a complex change of B_E (see above), which depends both on the specific electrical conductivity and on the Seebeck coefficient. These dependencies are shown in Figures 6 & 7. The dependences B_E – S are described by the empirical expression of type $B_E = aS^b + c$, where a, b and c are constants. It can be concluded that the indicated straightness is due to the comparative narrowness of the range of variables.

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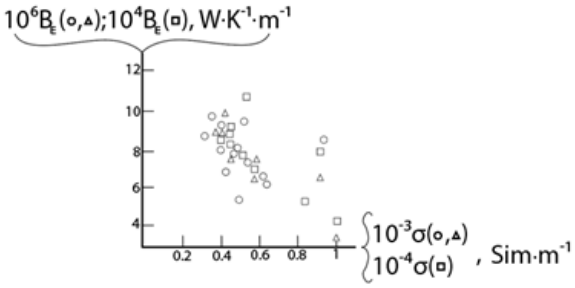

Figure 6 Dependences (B_E – σ): x=0.72 (o), 0.76 (Δ) and 0.8 (□) in Si_xGe_{1-x}.

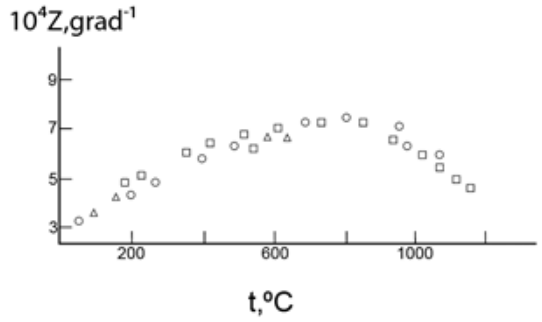

Figure 7 Dependences (B_E – S): x=0.72 (o), 0.76 (Δ) and 0.8 (□) in Si_xGe_{1-x}.

Consider the temperature dependences of thermoelectric efficiency Z= σS2/χ (Figure 8). It can be seen that all Si_xGe_{1-x} samples have a fairly high efficiency ($Z_{max} \cong 7 \cdot 10^{-4}$ grad^{-1}) the maximum of which is reached at about 700^{0}C. The studied alloy were used as an element of a monolithic thermoelectric module.[14]

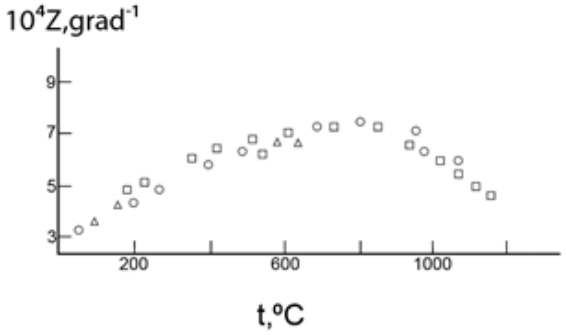

Figure 8 Temperature dependences of Z: x=0.72 (o), 0.76 (Δ) and 0.8 (□) in Si_xGe_{1-x}.

Comparing the above results with the previously obtained data for n-Si_xGe_{1-x} at x=0.7 and 0.83, we will see a qualitative identity. As for p-SixGe1-x, thermoelectric parameters are some what different. Eg. the power factor is ~2 orders of magnitude smaller at the same values of x and concentration of charge carriers (n= $3.2 \cdot 10^{26}$ m^{-3}). This follows from the fact that the specific electrical conductivity is 2.5-3 times -, and Seebeck coefficient is 1.4-2 times smaller at the same temperatures.

Conclusion

The study of the n-type alloy SixGe1-x (x=0.72, 0.76 and 0.8) showed that:

I. (σ – S) and (σ –t) dependences for compositions of Si_xGe_{1-x} alloy at x=0.72 and 0.76 is practically the same. And for x=0.8, the values of σ are two orders of magnitude greater at the same temperatures.

II. The appearance of the temperature dependences of B_E indicates the presence of additional effects (band convergence, bipolar effects, additional scattering). The temperature behavior of B_E is the same for all samples. However, for $Si_{0.8}Ge_{0.2}$ values B_E are two orders of magnitude greater than for $Si_{0.72}Ge_{0.28}$ and $Si_{0.76}Ge_{0.24}$ at the same temperatures.

III. The temperature dependences of σ' shows that the experimental points form almost a single set. This is due to the fact that changes of σ and B_E compensate each other. In general, the electronic quality factor B_E performs scaling of thermoelectric quantities.

IV. (σ' – t) dependences have the shape of a parabola: the middle of this set (region 200-1100^{0}C) is well described by the empirical equation $\sigma' = 1.274 \cdot 10^{11}t^2 - 1.714 \cdot 10^{14}t + 6.510^{16}$.

V. The dependences B_E – S are described by the empirical expression of type $B_E = aS^b + c$, where a and b are constants.

VI. Dependence (σ - σ') is rectilinear: $\sigma = k'\sigma' + b'$, where k′ is the slope of the lines, and b′ is the ordinate of the point of intersection of these lines with the σ axis during their extrapolation. Based on this rectiliearity and formula $\sigma' \cong 7.424 \cdot 10^{-9} B_E \sigma$, one could assume that B_E=const. However, this is on the ideal case. Under real conditions, additional effects leads to a complex change of B_E.

VII. All Si_xGe_{1-x} samples have a fairly high efficiency (≥7.10^{-4} grad^{-1}), the maximum of which is reached at about 700^{0}C.

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Conflicts of interest

There are no conflicts of interest.

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