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Determination of the Seebeck Coefficient and Other Thermoelectric Parametersusing Specific Resistivity and Concentration of Charge Carriers of N-$Si_{0.96}Ge_{0.04}$ Alloy Irradiated by ^{60}Co γ-photons

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

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ABSTRACT

The thermoelectric alloy N-$Si_{0.96}Ge_{0.04}$-P irradiated by ^{60}Co gamma-photons is been studied. The temperature dependences of the Seebeck coefficient, power and electronic quality factors, as well as the universal electrical conductivity and effective masses of electrons in the interval (250÷400)°C are calculated. All these dependences are different from the results previously

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obtained for Si_xGe_{1-x} with other compositions (except for effective mass). This should be associated with a significant difference in specific resistivities and concentrations of charge carriers.

Keywords: SiGe alloy; seebeck coefficient; γ-radiation.

1. INTRODUCTION

Si_xGe_{1-x} alloys are materials widely used in many fields of science and technology [1-15]. Nuclear radiation detectors, pressure sensors, thermistors, thermal neutron monochromators and X-ray diffractometry devices are also created on their basis [16-19].(1) In work [20] N-type $Si_{0.96}Ge_{0.04}$-P was irradiated with ^{60}Co gamma photons and the electrical resistance, concentration, and mobility of charge carriers were measured. According to this work, at temperatures ≥150°C, electrical characteristics undergo non-monotonic changes.

Since the main purpose of [20] was to study N-P conversion, dissociation of phosphor-vacanci (PV) centers and formation of vacancy-oxygen (VO) centers, no emphasis was placed on the Seebeck coefficient and other thermoelectric characteristics.

2. MATERIALS AND METHODS

In the present work, the temperature dependences of the Seebeck coefficient, power and electronic quality factors, as well as the universal electrical conductivity in the interval (250 ÷ 400)°C for N-$Si_{0.96}Ge_{0.04}$-P have been studied. Values of resistivity and charge carrier concentration are used from [20]. In this work is shown that in the monocrystalline N-Si+0.4at.%Ge irradiated with ^{60}Co gamma photons non-monotonic changes in electrical resistance, charge carriers concentration and mobility were detected by isochron alannealing at a temperature range of (20-400)°C. The contribution of current transformations in the structure of radiation defects to the temperature changes of electrical characteristics is analyzed. N-P conversion was detected atthe critical temperature (~100°C) of isochron alannealing. Dissociation of PV centers and formation of electrically active VO centers were detected in the (120-150)°C range. As a result, the concentration of current carriers increases. At elevated temperatures (>150°C) non-monotonic changes in electrical characteristics are observed. The paper [20] analyzes the contribution of germanium to the anomalous temperature changes of the electrophysical characteristics of the N-type SiGe alloy.

3. DISCUSSION

Combining formulas known from the literature relating concentration (n), specific resistivity (ρ), Seebeck coefficient (S), mobility (μ),effective mass (m*) and absolute temperature (T), we obtain a transcendental equation for S:

$$\frac{e^{11605S-2}}{S[1+e^{-5(11605S-1)}]}+\frac{3527.5}{1+e^{5(11605S-1)}} \cong 1.087\cdot10^{-9}(\rho n)^{2/3}, \quad (1)$$

in which there is no longer mobility, effective mass and temperature, and ρ and n are determined from the experimental temperature dependences of these parameters.

The dependence of the Seebeck coefficient on temperature of isochron alannealing calculated using Eq.(1) for a given n and ρ is shown in Fig. 1(a) (we used the values of concentration and resistivity at a given temperature). As can be seen from the figure, this dependence has a parabolic form, in contrast to the data for Si_xGe_{1-x} with other compositions (without irradiation), which have the form of straight lines [21-23].

In the Fig. 1(b) is presented the dependence of the power factor on temperature of isochron alannealing: PF≡ σS^2 ($\sigma=1/\rho$ - specific electrical conductivity). After determining the Seebeck coefficient and PF, the electronic quality factor (B_E) can be calculated: $B_E=PF/B_S$, where B_S is the scaled power factor(2) (Fig. 2(a)). Its increase (change) with temperature indicates the presence of additional effects [29]. However, the temperature variation of this dependence does not allow us to identify a specific scattering mechanism.

The dependence of the scaled power factor on the Seebeck coefficient is shown in Fig. 3. The experimental points fit well on the averaged curve presented in [24] for a large number (more than 3500) samples.

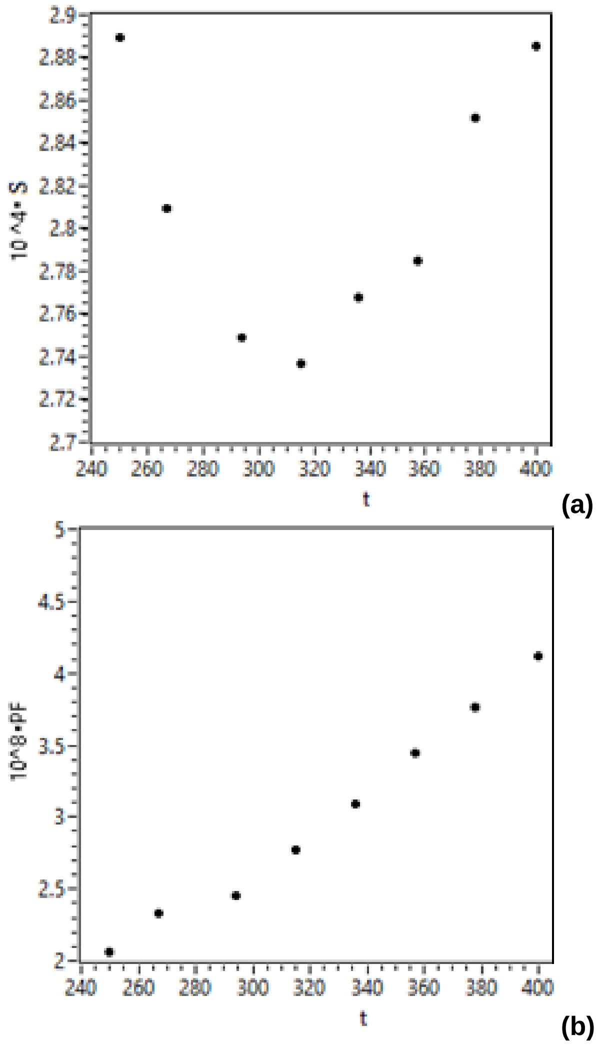

Fig. 1. Dependences of Seebeck coefficient (a) and power factor (b) on temperature of isochron alannealing

[S]=V/K, [PF]=W/K²·m, [t]=ºC

The determination of the electrical quality factor allows one to calculate the universal electrical conductivity, which is given by the following expression: $\sigma'=(q_e/k_B)^2(\sigma/B_E)\cong1.347\cdot10^8(\sigma/B_E)$. Its dependence on temperature of isochron alannealing is shown in Fig. 2(b).

It should be noted that the obtained values of PF are two orders of magnitude lower than for P-Si_xGe_{1-x} alloys and four orders of magnitude less than for N-$Si_xGe_{1-x}$with other compositions [27-29]. This should be associated with a significant difference in specific resistivities and concentrations of charge carriers.(3) It should not be concluded from this that radiation worsens the thermoelectric characteristics of the alloy: before irradiation of N-$Si_{0.6}Ge_{0.4}$, the value of power factor was $1.44\cdot10^{-7}$W/K^{2}m (i.e. in radiation, on the contrary, the power factor increases with temperature).

Determining the Seebeck coefficient allows you to calculateals the effective mass of charge carriers. For this purpose the following formula are used [25]:

$$\frac{m^*}{m_0} \cong 1.059\cdot10^{-15}\left(\frac{n^{2/3}}{T}\right)\left\{\frac{3\left[e^{(S_r-2)}-0.17\right]^{2/3}}{1+e^{-5(S_r-S_r^{-1})}}+\frac{S_r}{1+e^{5(S_r-S_r^{-1})}}\right\} \cong \frac{6.608\cdot10^{-15}}{T}\left[ne^{(S_r-2)}\right]^{\frac{2}{3}} \qquad (2)$$

(m_0 - electron rest mass). Fig. 4 shows the dependence of m^*/m_0 on temperature of isochron alannealing calculated from Eq.(2). This dependence can be approximately described by the empirical expression $m^*/m_0 \cong 6.918\cdot10^{-11}t^{3.373}-5.625\cdot10^{-3}$. The obtained values of the ratio of effective mass to rest mass are of the same order as for than for Si_xGe_{1-x} with other compositions.

In conclusion, we note that the temperature dependence of electron mobility given in [25] approaches a straight line at t≅(75÷430)ºC. But it can be more accurately described by the expression:

$$\frac{1}{\mu} \cong 8.116\cdot10^{3}t^{-3/2}+11.221\cdot10^{-3}t^{3/2}. \qquad (3)$$

Eq.(3) means that simultaneous scattering by impurities and thermal vibrations of the lattice takes place.

Footnote belows:

(1)The effects of Si, Ge and SiGe irradiation have been studied in a fairly large number of works [26-30].

(2)$B_S=\left[\frac{S_r^2e^{2-S_r}}{1+e^{-5(S_r-1)}}+\frac{\frac{\pi^2}{3}S_r}{1+e^{5(S_r-1)}}\right]$ and $S_r=\frac{q_e}{k_B}S \cong 1.1605\cdot10^4S$ is the reduced Seebeck coefficient (q_e - elementary charge, k_B - Boltzmann's constant). For relatively high values of S, the formula $B_S \cong S_r^2e^{(2-S_r)}$ can be used with sufficient accuracy.

(3)The samples studied in [21-23] had the following characteristics: $\rho \cong (0.15 \div 3)\cdot10^{-4}\Omega\cdot m$, $n \cong (2\div3.2)\cdot10^{26}m^{-3}$ and $m^*/m_0 \cong 1\div5$.

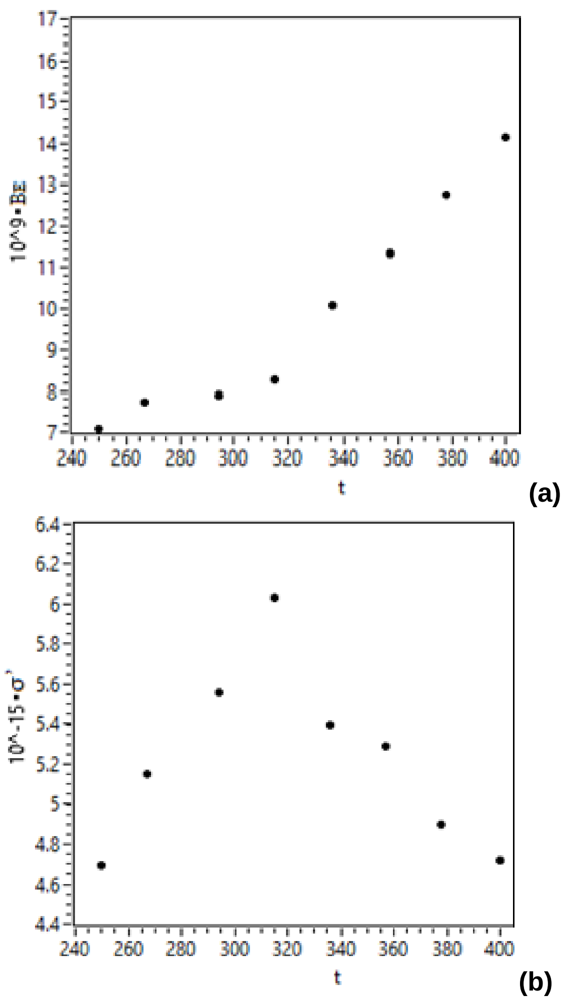

Fig. 2. Dependences of electronic quality factor (a) and universal electrical conductivity (b) on temperature of isochron alannealing

[B_E]=W/K²·m, [σ']=Sim·K⁴/W·V², [t]=ºC

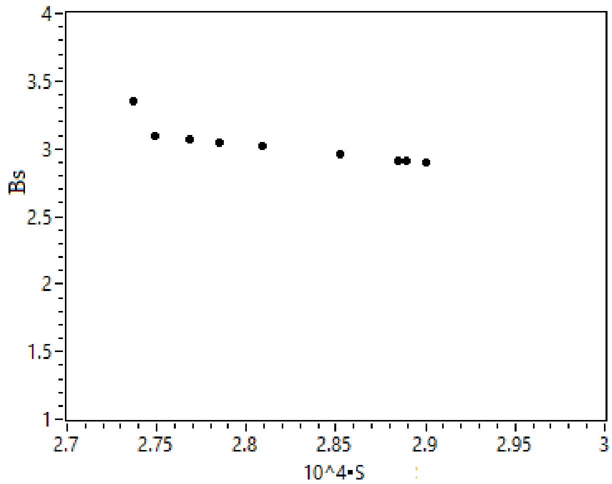

Fig. 3. Dependence of scaled power factor on the Seebeck coefficient
[S]=V/K, B_S – dimensionless

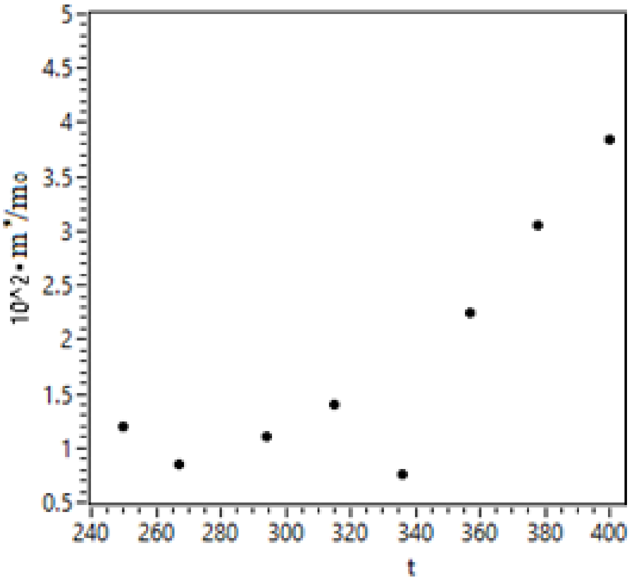

Fig. 4. Dependence of m^*/m_0 on temperature of isochron alannealing
[t]=^oC, m^*/m_0 – dimensionless

4. CONCLUSION

A formula has been obtained by means of which the Seebeck coefficient can be calculated depending on the resistance and the concentration of charge carriers. After determining the Seebeck coefficient, the power factor, electronic quality factor, universal electrical conductivity and effective mass are calculated. All these dependences are different from the results previously obtained for Si_xGe_{1-x} with other compositions (except for effective mass). This should be associated with a significant difference in specific resistivities and concentrations of charge carriers.

Competing interests

Authors have declared that no competing interests exist.

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