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Physics

Thermoelectric Parameters of Alloy p-$Si_{0.7}Ge_{0.3}$

Guram Bokuchava[*,†], Karlo Barbakadze[*], Irakli Nakhutsrishvili[**]

[*]*Ilia Vekua Sukhumi Institute of Physics and Technology, Tbilisi, Georgia*
[**]*Vladimer Chavchanidze Institute of Cybernetics, Georgian Technical University, Tbilisi, Georgia*

(Presented by Academy Member Anzor Khelashvili)

In this work, the temperature dependences of the electronic quality factor and the universal electrical conductivity of the p-type $Si_{0.7}Ge_{0.3}$, as well as the dependences of the Seebeck coefficient on the specific and universal conductivity are studied. The measured values of thermoelectric quantities (Seebeck and thermal conductivity coefficients, specific electrical resistivity) were used to calculate the dimensionless figure of merit ZT. The values of ZT were up to 0.6 for the concentration of charge carriers $n = 2 \cdot 10^{26} m^{-3}$ (optimum concentration) and 0.34 for the concentration $n = 3.2 \cdot 10^{26} m^{-3}$. It turned out that the dependence of the Seebeck coefficient on electrical conductivity can be determined in a very simple way, without resorting to the Pisarenko formula. A study of the dependence of the power factor on the Seebeck coefficient showed its straight forwardness. This fact allows us to describe the dependence of the Seebeck coefficient on electrical conductivity without taking into account the quantities included in the Pisarenko formula and using simple formula. The definition of the electron quality factor (B_E) makes it possible to evaluate temperature-dependent electron transport properties for thermoelectrics. The temperature dependence of B_E has form that, according to the literature data, indicates the presence of additional effects, such as: band convergence; bipolar effects and additional scattering. The dependence of the electronic quality factor on the universal electrical conductivity was also studied. Electronic quality factor makes scaling of electrical conductivity. *© 2023 Bull. Georg. Natl. Acad. Sci.*

thermoelectric *SiGe*, electronic quality factor, Seebeck coefficient

The thermoelectric material based on the *SiGe* alloy has been used for several decades as the main element of TEG in space flights [1]. Recently, μTEGs have also been created on the basis of *SiGe* [2]. This thermoelectric is characterized by high efficiency (i.e. figure of merit, ZT~1) [3]. The electronic quality factor (B_E) and universal electrical conductivity (σ') are important characteristics of thermoelectric materials [4]. In particular, BE performs scaling of thermoelectric quantities.

In this work, the temperature dependences of the electronic quality factor and the universal electrical conductivity of p-type $Si_{0.7}Ge_{0.3}$, as well as the dependences of the Seebeck coefficient (S) on the specific electrical conductivity (σ) and σ', are studied.

Dependence S - σ is given by the Pisarenko formula [5-7]: $S = \frac{8\pi^2 k_B^2}{3qh^2} m^* T \left(\frac{\pi}{3n}\right)^{2/3}$, where n is the concentration charge carriers, m^* is the effective mass, q is the elementary charge, T is the absolute temperature, k_B and h are the Boltzmann and Planck constants. Next, we can describe the dependence of the Seebeck coefficient on electrical conductivity without taking into account the quantities included in the Pisarenko formula and using a simple formula.

Experimental

In the experiments we used samples in the form of rectangular parallelepipeds with dimensions of 10 x 10 x 20 mm, prepared by hot pressing of powders obtained from zone-melted ingots. For p-type conductivity, phosphorus was used as a dopant. The concentration of charge carriers was 2 and $3.2 \cdot 10^{26} m^{-3}$. The study was carried out at 30-1150°C (the upper limit was limited by the melting point of the alloy). The measurement error of S was 3%, and of specific resistivity $\rho\left(=\sigma^{-1}\right)$ 5%. The thermal conductivity coefficients (λ) were also measured with an error of no more than 7%.

Results and Discussion

The electronic quality factor is related to the power factor $\left(\sigma S^2\right)$ by the expression $B_E = \sigma S^2 / B_S$, where $B_S = S_r \left[\frac{S_r \exp(S_r - 2)}{1 + \exp\left[-5(S_r - 1)\right]} + \frac{3.29}{1 + \exp\left[5(S_r - 1)\right]} \right]$ and $S_r = (q_e / k_B) S$ [4].

Fig. 1 shows the temperature dependence of B_E for $Si_{0.7}Ge_{0.3}$. For an ideal thermoelectric, the electron quality factor does not depend on temperature, and any deviation indicates the presence of additional effects [4, 8]. As can be seen from Fig. 1, these effects are also manifested in $Si_{0.7}Ge_{0.3}$ according to [4].

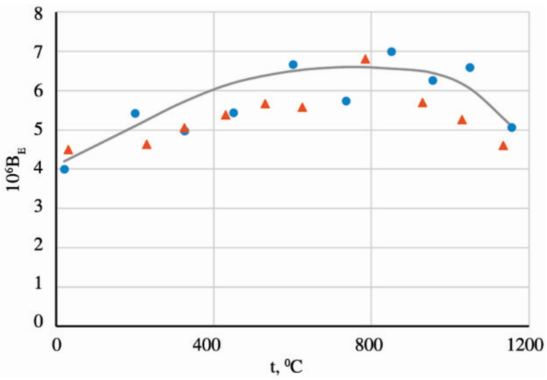


Fig. 1. B_E – t dependences in $Si_{0.7}Ge_{0.3}$. Here and below o - $n = 3.2 \cdot 10^{26}$, Δ - $3.2 \cdot 10^{26} m^{-3}$. $[B_E] = V \cdot K^{-2} \cdot m^{-1}$.

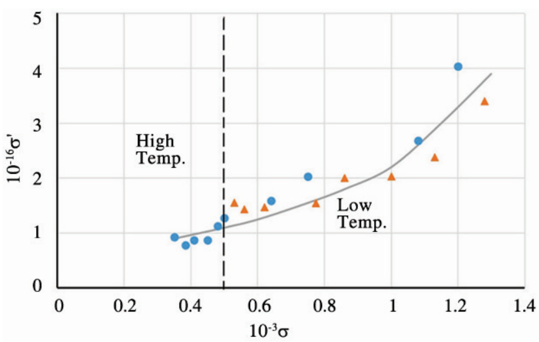


Fig. 2. Dependence $\sigma' - \sigma$. $[\sigma] = Sim \cdot m^{-1}$, $[\sigma'] = Sim \cdot W^{-1} \cdot V^{-2} \cdot K^4$.

Universal electrical conductivity is given by $\sigma' = \left(q_e / k_B\right)^2 \left(\sigma / B_E\right)$, i.e. scaling of the specific conductivity occurs. This can be seen from Fig. 2 – the experimental points form almost a single set. The figure shows an almost rectilinear arrangement of the experimental points. But this contradicts the data in Fig. 1.

Let us implement the following approach – from Fig. 1 it can be seen that BE first increases, reaches a maximum at about 740°C, then decreases. The dependence shown in Fig. 2 is divided into "low" (30-740°C) and high (740-1150°C) – temperature ranges (an increase in temperature corresponds to a decrease in σ and σ'). In the first one, σ' should increase with a decrease of $d\sigma'/d\sigma$, in the second – with its increase. This is clearly expressed for low-temperature region, but for high-temperature region, the location of the experimental points does not allow clear conclusion to be drawn.

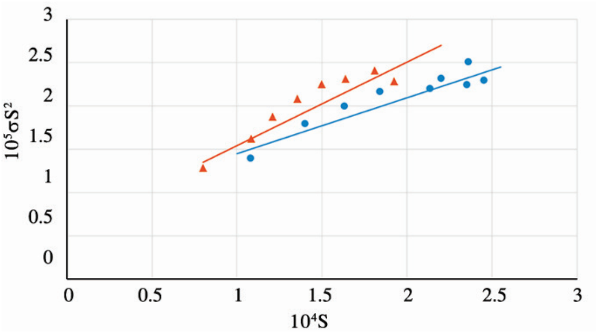


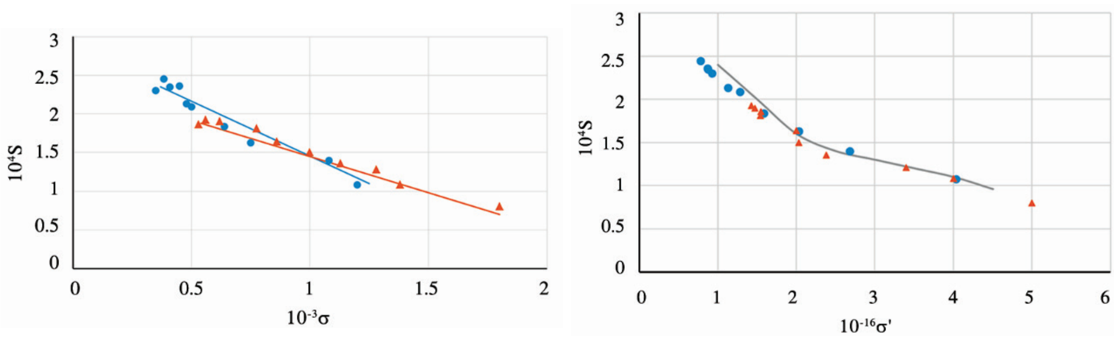
Fig. 3. Dependence $\sigma S^2 - S$. $[S] = V \cdot K^{-1}$, $[\sigma] = Sim \cdot m^{-1}$.

Consider the dependence $S - \sigma$ in $Si_{0.7}Ge_{0.3}$. It turned out that it can be determined in a very simple way, without resorting to the Pisarenko formula – study of the dependence $\sigma S^2 - S$ 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: $k = 0.075$, $b = 6.9 \cdot 10^{-6}$ for $n = 2 \cdot 10^{26} m^{-3}$ and $k = 0.1$, $b = 5 \cdot 10^{-6}$ for $n = 3.2 \cdot 10^{26}$. From the last equation we get:

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

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(a)). For dependence $S - \sigma'$ we have:

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



(a) (b)

Fig. 4. Dependencies (a) $S - \sigma$ and (b) $S - \sigma'$. $[\sigma] = Sim \cdot m^{-1}$, $[\sigma'] = Sim \cdot W^{-1} \cdot V^{-2} \cdot K^4$, $[S] = V \cdot K^{-1}$.

It can be seen from Fig. 4(b) that the experimental points form a regular set regardless of the value of n. This confirms the fact that the BE factor scales the thermoelectric quantities.

Conclusion

In the $Si_{0.7}Ge_{0.3}$ alloy of p-type conductivity, the temperature dependences of the electronic quality factor and universal electrical conductivity, as well as the dependences of the Seebeck coefficient on σ and σ', were studied. Based on the measured *S*, σ and λ values the $ZT = \sigma S^2 T / \lambda$ values were up to 0.6 for $n = 2 \cdot 10^{26} m^{-3}$ (optimal concentration) and 0.34 for $n = 3.2 \cdot 10^{26}$.

ფიზიკა

p-$Si_{0.7}Ge_{0.3}$ შენადნობის თერმოელექტრული პარამეტრები

გ. ბოკუჩავა*,†, კ. ბარბაქაძე*, ი. ნახუცრიშვილი**

** ილია ვეკუას სოხუმის ფიზიკისა და ტექნოლოგიის ინსტიტუტი, თბილისი, საქართველო*
*** საქართველოს ტექნიკური უნივერსიტეტი, ვლადიმერ ჭავჭანიძის კიბერნეტიკის ინსტიტუტი, თბილისი, საქართველო*

(წარმოდგენილია აკადემიის წევრის ა.ხელაშვილის მიერ)

ნაშრომში შესწავლილია p-ტიპის გამტარობის $Si_{0.7}Ge_{0.3}$ შენადნობის ელექტრონული ვარგისიანობის ფაქტორისა და უნივერსალური ელექტროგამტარობის ტემპერატურული დამოკიდებულებები, აგრეთვე ზეებეკის კოეფიციენტის დამოკიდებულება ხვედრით და უნივერსალურ ელექტროგამტარობებზე. გაზომილი თერმოელექტრული პარამეტრების საფუძველზე (ზეებეკისა და თბოგამტარობის კოეფიციენტები, ხვედრითი წინაღობა), ZT-ის მნიშვნელობებმა შეადგინა 0.6-მდე $n = 2 \cdot 10^{26} m^{-3}$-თვის (ოპტიმალური კონცენტრაცია) და 0.34-მდე $n = 3.2 \cdot 10^{26} m^{-3}$-თვის.

REFERENCES

1. Barbakadze K. (2022) Thermoelectric SiGe alloys. In: creation of a unified monolithic thermoelectric module based on SiGe alloys to create thermoelectric generators of different electrical power, 21 p. Tbilisi.
2. Li Y., Wahg G., Akbari-Saatlu M., Procek M., Radamson H.H. (2021) Si and SiGe nanowire for micro-thermoelectric generator: a review of the current state of the art. *Front. Materials,* **8**, 611078.
3. Ascencio-Hurtado R., Torres A. et al. (2022) N-type amorphous silicon-germanium thin films with embedded nanocrystals as a novel thermoelectric material of elevated ZT. *Alloys Comp.,* **890,** 161843.
4. Zhang X., Bu Z. et al. (2020) Electronic quality factor for thermoelectrics. *Sci. Advances,* **6,** eabc0726.
5. Snyder G., Toberer E. (2008) Complex thermoelectric materials. *Nature Materials,* **7**: 105–114.
6. Zhao L., Fey F.Y. et al. (2017) Improvement of thermoelectric properties and their correlations with electron effective mass in Cu1.98S x Se1−x . *Sci. Reports,* **7,** 40436.
7. Li M., Sun Q. et al. (2021) Optimizing electronic quality factor toward high-performance $Ge_{1-x-y}Ta_xSb_yTe$ thermoelectrics: the role of transition metal doping. *Adv. Materials,* **33,** 2102575.
8. Pey Y., Shi X.A. et al. (2011) Convergence of electronic bands for high performance bulk thermoelectrics. *Nature,* **473**: 66–69.

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