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I. Nakhutsrishvili (https://orcid.org/0000-0002-7961-3437)

Institute of Cybernetics of Georgian Technical University,
6 Anjaparidze str., 0186 Tbilisi

Corresponding author: I. Nakhutsrishvili, e-mail: *iraklinakhutsrishvili52@gmail.com*

The Maximums of the Power Factor of Thermoelectrics: Mathematical Approach and Practice

The goal of this article is to assess of the maximum values of the important thermoelectric parameter of materials – the power factor. Based on the formulas known from the literature that interconnect the thermoelectric parameters (effective mass and mobility of charge carriers, the Seebeck coefficient, temperature), the function of the specified coefficient is obtained. Its processing allows the obtained data to be used for the analysis of experimental data of those works in which, for certain reasons, the extrema of the specified thermoelectric parameters are not given.

Keywords: maximum of power factor, thermoelectric module.

Introduction

An important characteristic of thermoelectric material, power factor ($PF \equiv \sigma S^2$, σ – specific electrical conductivity, S – Seebeck coefficient) often has extreme values depending on the temperature (T), composition, concentration of charge carriers (n), Fermi energy etc. [1–7]. In this paper, $PF - T$ dependence is considered. In some cases, it has a minimum, in others – a maximum, and in some cases – both. This is demonstrated in Figs (1, 2) based on literary and our data. For practical purposes, it is of interest to determine the maxima of this thermoelectric characteristic, which is included in the expression of the figure of merit $ZT \equiv \sigma S^2 T/k$ (k – thermal conductivity).

Below, a mathematical approach to the issue will be made. In particular, it turned out that despite the presence of several variable quantities in the formulas used, no need to use the Lagrange multiplier method – the usual calculation can be applied.

And then, the obtained calculated data will be compared with the experimental data.

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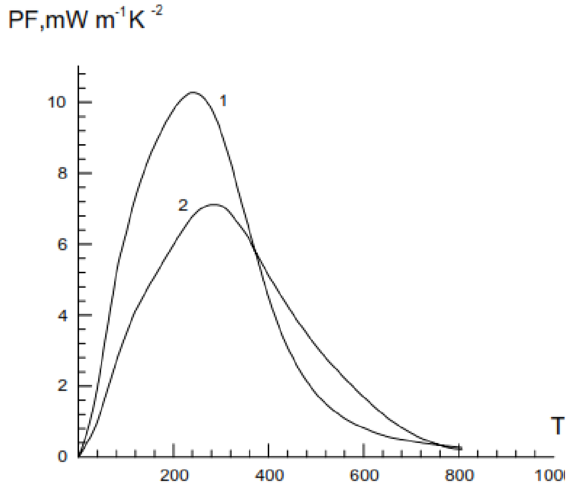

Fig. 1. Temperature dependences of PF for: (1) $Fe_2V_{0.95}Ta_{0.05}Al_{0.9}Si_{0.1}$ and (2) $Fe_2V_{0.95}Ta_{0.05}Al_{0.8}Si_{0.2}$ [1]

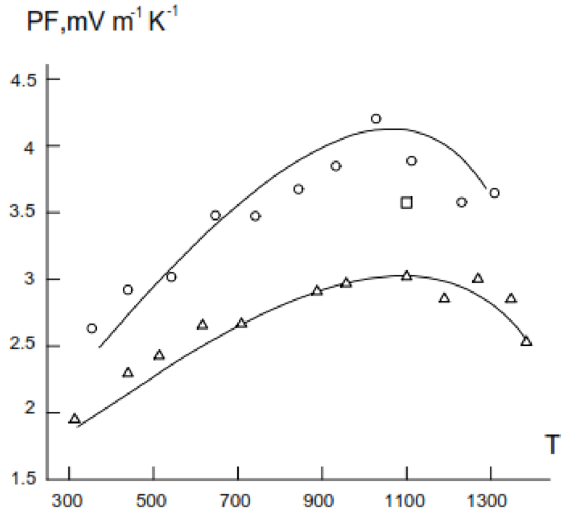

Fig. 2. Temperature dependences of PF for (o) $Si_{0.72}Ge_{0.28}$ and (Δ) $Si_{0.83}Ge_{0.17}$ of N-type conductivity, □ – point by Eq. 3 (see below)

Discission

To compile an expression for Seebeck coefficient (S), formulas known from the literature [8] relating the absolute temperature (T), effective mass (m^*), and concentration of charge carriers[(*)] the following expression can be obtained:

$$f(S)\sim\left\{\frac{\left[e^{(S_r-2)}-0.17\right]^{2/3}}{S_r\left[1+e^{-5(S_r-S_r^{-1})}\right]}+\frac{1}{1+e^{5(S_r-S_r^{-1})}}\right\}. \quad (1)$$

After of all this, we will consider the issue of maximization of the power factor $\sigma S^2 = nq_e\mu S^2$. Using the equations from [8,9] we get: $\mu\cong\left(\frac{m^*}{m_0}\right)^{-3/2}\mu_W$, $\frac{m^*}{m_0}\sim\left(\frac{n^{2/3}}{T}\right)\left\{\frac{3\left[e^{(S_r-2)}-0.17\right]^{2/3}}{1+e^{-5(S_r-S_r^{-1})}}+\frac{S_r}{1+e^{5(S_r-S_r^{-1})}}\right\}$, $\mu_W\sim\left\{\frac{e^{(S_r-2)}}{1+e^{-5(S_r-1)}}+\frac{\frac{3}{\pi^2}S_r}{1+e^{5(S_r-1)}}\right\}$ (μ, μ_W – drift and weighted mobilities, m_0 – electron rest mass, $S_r=\frac{q_e}{k_B}|S|\cong 11604|S|$ – reduced Seebeck coefficient, q_e – elementary charge, k_B – Boltzmann's constant). Using these expressions and Eq. (1) we will get:

$$PF \sim AT^{3/2}, \quad (2)$$

where

$$A=\left\{\frac{\left[e^{(S_r-2)}-0.17\right]^{2/3}}{1+e^{-5(S_r-S_r^{-1})}}+\frac{S_r}{1+e^{5(S_r-S_r^{-1})}}\right\}\left\{\frac{e^{(S_r-2)}}{1+e^{-5(S_r-1)}}+\frac{\frac{3}{\pi^2}S_r}{1+e^{5(S_r-1)}}\right\}\left\{\frac{\left[e^{(S_r-2)}-0.17\right]^{2/3}}{1+e^{-5(S_r-S_r^{-1})}}+\frac{S_r}{1+e^{5(S_r-S_r^{-1})}}\right\}^2$$

(here and below all quantites are in SI system). At $S \geq 2\cdot10^{-4}$ V/K, $A \cong [e^{(S_r-2)}-0.17]^2 e^{(S_r-2)}$ with high accuracy.

To determine $(PF)_{max}$, the Lagrange multiplier method should have been used and the function f(T, m^*, μ_W) = f(T, S_r) = f(T, S) should have been considered. But when making the additional condition$^{(**)}$, the T's are truncated and $(PF)_{max}$ is calculated more easily.

The empirical result (for our samples) is:

$$(PF)_{max} \cong 1.42\cdot10^{-8}A_{max}T^{3/2}, \qquad (3)$$

(T corresponds to S_{max}) which can be considered acceptable (see Fig. 2). In this case, $S_r \cong 3.25$ (i.e. $S \cong 2.8\cdot10^{-4}$ V/K), which is also in satisfactory agreement with experiment.

Note that $(PF)_{max}$ can be determined with other ways: from σ_{min} [11]: $(\sigma S^2)_{max} = (a/\sigma_{min}) - b$, $(\sigma S^2)_{max} = c/(\sigma_{min})^d$ (a, b, c and d are constants) or $\lg(\sigma S^2)_{max} \cong 0.583(\lg\sigma_{min})2 - 3.332\lg\sigma_{min}$; as well as from $(B_S)_{min}$ [12] ($B_S = \left[\frac{e^{S_r-2}}{1+e^{-5(S_r-1)}} + \frac{\frac{\pi^2}{3}S_r}{1+e^{5(S_r-1)}}\right]$ is the scaled power factor). You can also use the formulas [13, 14] $S = (3k_B/2q_e)\ln T + C$, where $C = (k_B/q_e)\{C_0 + \ln[2(2\pi m^* k_B)^{3/2}/(2\pi h^3)^3 n]\}$ (the constant C_0 depends on the scattering mechanism and takes values from 2 to 4, i.e. C is also constant) and [13] $S = k_1/2\sigma + [(k_1/2\sigma)^2 + k_2/\sigma]^{1/2}$ (k_1, k_2 – constants) – see Figs (3, 4).

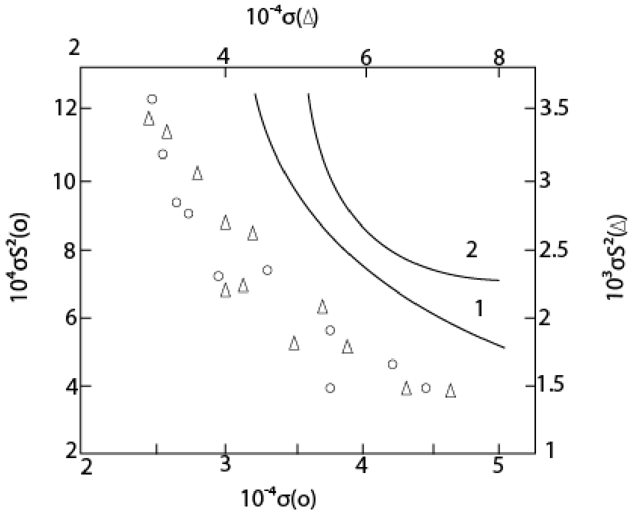

Fig. 3. Dependences $\sigma S^2 - \sigma$: (Δ) – $Si_{0.7}Ge_{0.3}$, (o) – $Tl_8Sn_2Te_6$ [15]; lines without points – shematic graphs of functions $y = x^{-1/3}$ (1) and $y = ax^{-b}$, $b\neq-1/3$ (2). $[\sigma]$ = Sim/m, $[\sigma S^2]$ = W/K²m

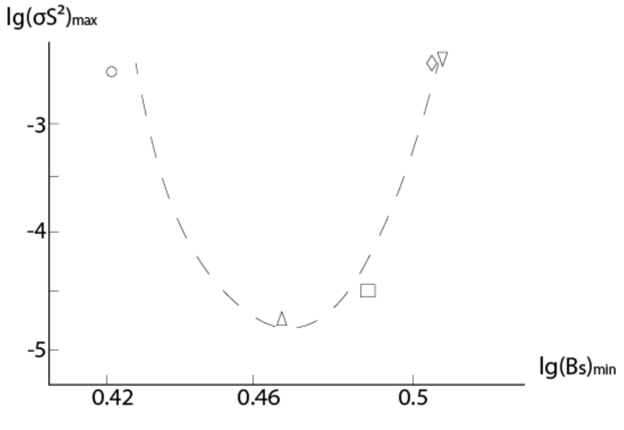

Fig. 4. Dependence $\lg(\sigma S^2)_{max} - \lg(B_S)_{min}$ in Si_xGe_{1-x}: x = 0.7 (o), 0.72 (Δ), 0.76 (□), 0.8 (◊) and 0.83 (∇)

In conclusion, it should be pointed out that a thermogenerator module has been designed based on SiGe alloy (Figs 5, 6). Its power is 4.5 W. This material has been used in spacecraft generators and in many other areas of science and technology [16–18].

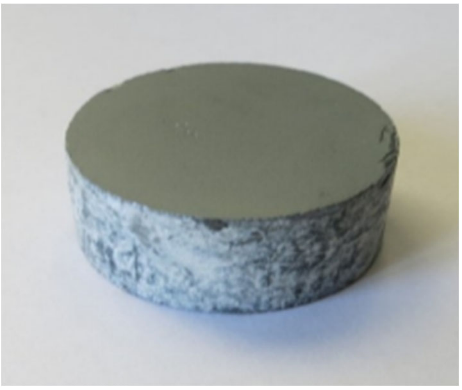

Fig. 5. Photo (×1) of briquette compacted from ultradispersed $Si_{0.7}Ge_{0.3}$+$P_{0.5}$ (wt.%) alloy powder at 1300 °C

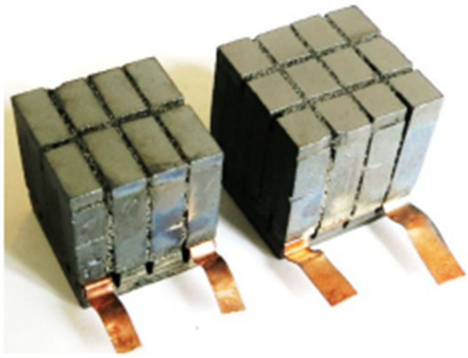

Fig. 6. Photos of modules from 16 (2.0 × 2.0 × 2.3 cm) and 24 (2.2 × 2.2 × 2.3 cm) branches

The SiGe used in spacecraft is based on alloys with x = 0.32 and 0.2. The author, together with researchers from the Sukhumi Institute of Physics and Technology, further reduced the Ge content. An alloy with the composition $Si_{0.9}Ge_{0.1}$ was prepared, which will be reported in a future publication.

Conclusions

The maximum values of thermoelectric parameter of materials - power factor is estimated. Based on the formulas known from the literature, which interconnect the thermoelectric parameters, the function of the mentioned factor is obtained and its maximum was estimated. The obtained data can be used to analyze the experimental data of those works in which, for some reason, the maxima of the specified thermoelectric parameter is not given. A thermogenerator module based on SiGe alloy has been developed for use in spacecraft. Its power is 4.5 W.

Footnotes:

$$^{(*)}\, S = (8\pi^2 k_B^2/3q_e h^2)Tm^*(\pi/3n)^{2/3} \cong 7.355\cdot 10^{40} Tm^* n^{-2/3},$$

$$m^* \cong 9.647\cdot 10^{-46} n^{2/3} T^{-1}\left\{\frac{\left[e^{(S_r-2)}-0.17\right]^{2/3}}{1+e^{-5(S_r-S_r^{-1})}}+\frac{S_r}{1+e^{5(S_r-S_r^{-1})}}\right\}.$$

$^{(**)}$ Considering $n \cong 1.331\cdot 10^{13} e^{S_r-2}/\{(e^{S_r-2}-0.17)[(1.17-0.216/[1+e^{\frac{8.617\cdot 10^{-5} S_r-1.01}{0.671}}]\}$ [10], additional condition is:

$$\varphi = S-\lambda(8\pi^2 k_B^2/3q_e h^2)Tm^*(\pi/3n)^{2/3} \cong S - 7.355\cdot 10^{40}\lambda Tm^* n^{-2/3} \cong$$

$$\cong 8.617\cdot 10^{-5} S_r - 1.987\cdot 10^{-65}\lambda\left\{\frac{\left[e^{(S_r-2)}-0.17\right]^{\frac{2}{3}}}{1+e^{-5(S_r-S_r^{-1})}}+\frac{S_r}{1+e^{5(S_r-S_r^{-1})}}\right\}$$

$$\langle e^{S_r-2}/\{(e^{S_r-2}-0.17)^{2/3}[(1.17-0.216/[1+e^{\frac{8.617\cdot 10^{-5} S_r-1.01}{0.671}}]\}\rangle^{-2/3} = 0.$$

Appendix

Technologies for manufacturing of SiGe samples and thermoelectric modules based on them

To create a thermoelectric module, $Si_{0.7}Ge_{0.3}$ alloys of n- and p-type conductivity with a charge carrier concentration of 3.2·1026 m-3 were produced by vacuum hot pressing. Bulk Si and Ge wastes were crushed with a steel rod and sifted through a sieve with a cell size of 0.2 mm. Then they were loaded into the chamber of the PM-100-SM mill and crushed for 20–25 hours. The grain size of the powder was estimated using an optical microscope (Nicon) and an X-ray diffractometer (DRON-3M). The dispersed powder obtained according to the specified mode consisted mainly of Si and Ge grains with a size of (60–80) nm. The resulting powder was pressed in a high-temperature vacuum induction chamber at a temperature of (1200–1320) °C and a pressure of 480 kg·cm^2 for 20–30 minutes. The matrix and punches were made of high-strength graphite. Profiled samples were cut out of the resulting briquettes on a diamond-disc machine. Graphite commutation plates were attached to the ends of the alloy branches. The commutated sample was placed in the vacuum chamber of the induction furnace, and sensors for measuring the temperature and electrical force were placed in its commutation plates. One side of the module was heated by a flame generated by gas combustion, which fell directly on the surface of the module. On the other side, the module was cooled with running water. Chromel-alumel thermocouples were placed on the hot and cold ends of the module. The electrical insulation unit of the cold side of the monolithic thermoelectric module was made using AlN and graphite plates (вoth of them are thermomechanically compatible with SiGe alloys in a wide temperature range). To manufacture a mini-monolithic thermoelectric module containing 16 branches, 4 plates of n- and p-type alloy (2 n-type and 2 p-type) were taken. They were arranged in the order n-p-n-p. A mini-monolithic thermoelectric module containing 24 branches was manufactured using a similar technology.

Authors' information

I. Nakhutsrishvili – Ph. D., Senior Scientist.

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Нахуцрішвілі І. (https://orcid.org/0000-0002-7961-3437)

Інститут кібернетики Грузинського технічного університету,
вул. З. Анджапарідзе 6, 0186 Тбілісі

Максимуми коефіцієнта потужності термоелектриків: математичний підхід та практика

Метою цієї статті є оцінка максимальних значень важливого термоелектричного параметра матеріалів – фактора потужності. На основі відомих з літератури формул, що зв'язують між собою термоелектричні параметри (ефективну масу та рухливість носіїв заряду, коефіцієнт Зеєбека, температуру), отримано функцію зазначеного фактора. Її обробка дозволяє використовувати отримані дані для аналізу експериментальних даних тих робіт, у яких з певних причин не наводяться екстремуми зазначеного термоелектричного параметра.

Ключові слова максимальний коефіцієнт потужності, термоелектричний модуль.

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