DOI: 10.63527/1607-8829-2025-3-37-44

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

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

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

Generalized Parameter and Compatibility Factor of Thermoelectric *n*-Si_xGe_{1-x}

The dependence of the maximum of the figure of merit $(ZT)_{max}$ of the Si_xGe_{1-x} alloy on the generalized parameter of material B is investigated. A formula is used to calculate the values of B*, which contains the quantities of band gap, specific electrical conductivity, scaled parameter B'_S and lattice thermal conductivity: $B^* \cong 7.755 \cdot 10^{-4} E_g \sigma B'_S k_L^{-1}$. This formula is derived from the combination of the formulas known from the literature that relate the thermoelectric parameters – mobility, effective mass and weighted mobility of charge carriers. This formula no longer includes effective mass, mobility and temperature – these parameters are replaced by specific electrical conductivity and the Seebeck coefficient. Dependence $(ZT)_{max}$ – B* is constructed. By calculating the generalized parameter, you can approximately estimate the maximum value of the figure of merit for almost any thermoelectric. The compatibility factor of Si_xGe_{1-x} has been determined. The possibility of creating segmented thermogenerators based on this material in combination with $YbMg_{1.8}Zn_{0.05}Bi_{1.98}$, $CuAl_{0.8}Fe_{0.2}O_2$ and $Cu_{1.98}S$ is indicated.*

Keywords: thermoelectric SiGe, generalized parameter, compatibility factor.

Unique properties of thermoelectric energy sources have determined the undeniable advantages of using thermoelectric generators as autonomous energy sources [1–4]. Among the well-known materials, alloy SiGe also occupies a prominent place. This thermoelectric has been used in spacecraft generators since the second half of the last century until recently [5–8]. This alloy is also used in many other areas of science and technology: coolers, sensors, thin-film transistors, batteries, solar cells, photodetectors [9–16]. It has good mechanical properties, thermal stability and its potential efficiency reaches 15 %.

The quality of a thermoelectric material is determined by the figure of merit $ZT = \sigma S^2 T/k$, where σ is specific electrical conductivity, S – Seebeck coefficient, T – absolute temperature and k – total thermal conductivity. For SiGe with *P*- and *N*-type conductivity, quite high values of ZT were obtained: 0.86 and 1.29, respectively [17].

Citation: I. Nakhutsrishvili (2025). Generalized Parameter and Compatibility Factor of Thermoelectric *n*-Si_xGe_{1-x}. *Journal of Thermoelectricity*, (3), 37–44. https://doi.org/10.63527/1607-8829-2025-3-37-44

The effective parameter for predicting the maximum value of ZT is generalized parameter of the thermoelectric material. It is given by the following expression [18, 19]: $B^* \cong 6.668 \cdot 10^{-2} E_g U^* k_L^{-1}$, where E_g is band gap in eV, $U^* = \mu(m^* T/m_0)^{3/2}$ (μ and m^* – mobility and effective mass of charge carriers, m_0 – electron rest mass) and k_L – lattice component of the total thermal conductivity k.

Next, we will consider generalized parameter of alloy Si_xGe_{1-x} with n-type conductivity at $x = 0.7$, 0.76 and 0.8. (N-Si_xGe_{1-x} has a number of advantages over the P-type. In particular, in addition to a larger figure of merit for the same temperatures, it is more resistant to radiation [20].)

The compatibility factor of material is also considered. This important parameter of the material characterizes its suitability for segmentation with other materials to create a thermoelectric device [21–28].

The studied samples were obtained according to the method described in the monograph [20]. Si_xGe_{1-x} samples with different compositions were used for research: $x = 0.7$, 0.76 and 0.8 (concentration of charge carriers $n = 3.2 \cdot 10^{26}$ m^3). Their conductivity is N-type, for which they were doped with phosphorus.

$$B^* \cong 7.755 \cdot 10^{-4} E_g \sigma B'_S k_L^{-1}. \quad (1)$$

($B'_S \cong \frac{3\left[e^{(S_r-2)}-0.17\right]^{2/3}}{1+e^{-5(S_r-S_r^{-1})}} + \frac{S_r}{1+e^{5(S_r-S_r^{-1})}}$. At $|S| \cong 2 \cdot 10^{-4}$V/K and above $B'_S \cong 3(e^{S_r-2} - 0.17)^{2/3}$ with high accuracy.)

As we see, formula (1) no longer includes effective mass, mobility and temperature – these parameters are replaced by specific electrical conductivity and B'_S (i.e. the Seebeck coefficient).

To determine the values of E_g at different x, we used the formula [31] $E_g = 2|S|_{max} T_{S_{max}}$ as a result of which from Eq. (1) we finally have:

$$B^* \cong 1.551 \cdot 10^{-3} |S|_{max} T_{S_{max}} \sigma B'_S k_L^{-1}. \quad (1')$$

Bulk SiGe alloys typically have total and lattice thermal conductivities close to each other (unlike nanomaterials). Therefore, in formulas (1, 1') k_L can be replaced by k.

Figure 1 shows the $(ZT)_{max} - B^*$ dependence, built on the basis of literature data for various thermoelectric materials (CoSbTe, CoSbTeSn, BiTeSe, BiSbTe, FeNbSb, $MgSn_{0.73}Ge_{0.25}$, BiSbTe [18]; P,N-Mg_2Sn, P,N-Ag_2Te, P-$YbMg_2Bi_2$, N-$Mg_3(Sb,Bi)_2$, P,N-Bi_2Te_3, P,N-PbTe, P,N-$CoSb_3$, P-MgAgSb, N-BiAgSeS, P-FeVSb, N-ZrNiSn, P,N-SiGe [19]) and data for N-Si_xGe_{1-x}. From this figure it can be seen that our data satisfactorily adds to the literature data.

The parameter B^* provides a good characterization of thermoelectrics, particularly at high temperatures, and therefore can facilitate the search for better thermoelectric materials. Thus, by calculating the generalized parameter, you can approximately estimate the maximum value of the figure of merit for almost any thermoelectric.

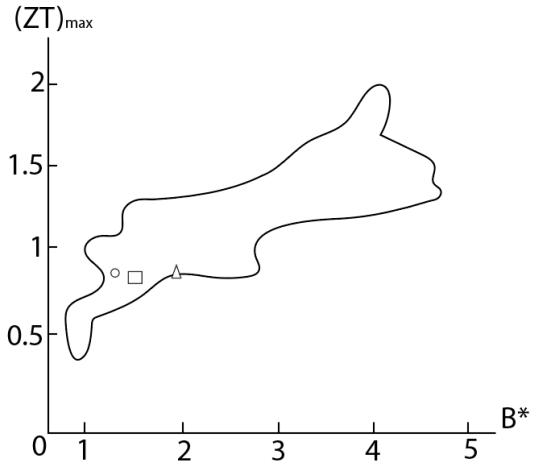


Fig. 1. Dependence $(ZT)_{max} – B^*$: data for 25 thermoelectric materials from [18, 19] (bounded area); o – $Si_{0.7}Ge_{0.3}$, Δ – $Si_{0.76}Ge_{0.24}$, □ – $Si_{0.8}Ge_{0.2}$

The effective parameter for materials is the thermoelectric quality factor $B = B_E T/k_L$ (B_E – electronic quality factor [32]) that also determines maximum of ZT. It is a good predictor for $(ZT)_{max}$ of an optimally doped sample, provides a better characterization of thermoelectrics, particularly at high temperatures, and therefore can facilitate the search for good thermoelectric materials, in the criteria of high weighted mobility, low lattice thermal conductivity, and large band gap value. We have constructed the $(ZT)_{max} – B$ dependence for a large number of thermoelectric materials (bounded area in Fig. 2). The points for our samples as well as for some SiGe-based materials are also given there. It is evident that these points fit into the overall picture well.

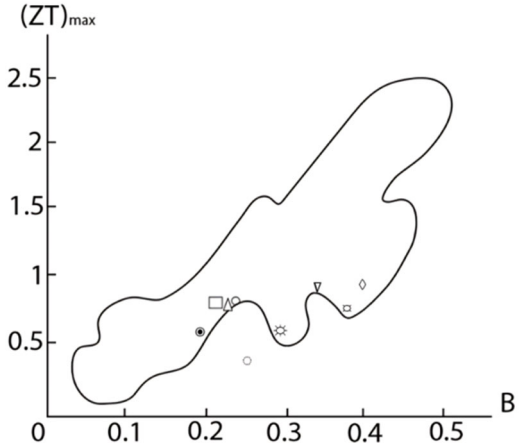
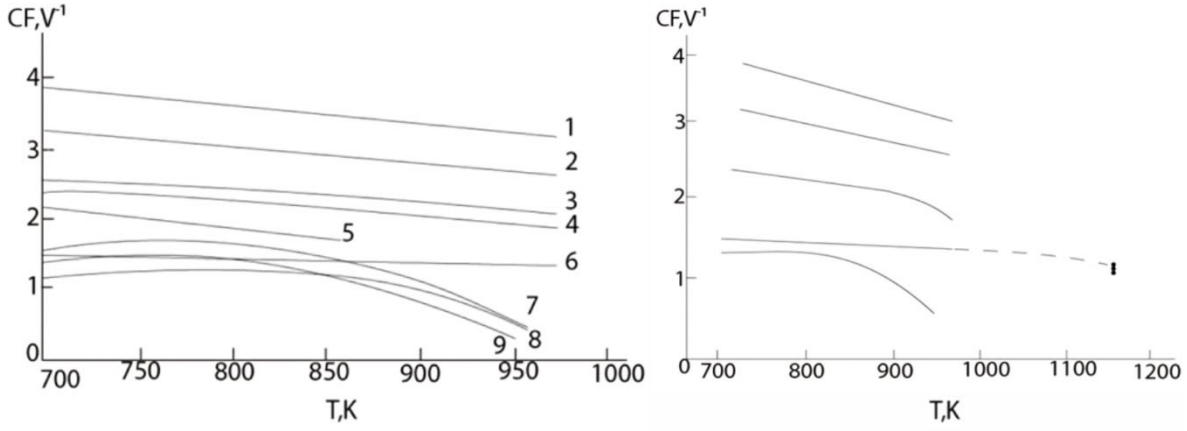


Fig. 2. Dependence $(ZT)_{max} – B$: data for a large number thermoelectric materials (bounded area); o – $Si_{0.7}Ge_{0.3}$, Δ – $Si_{0.76}Ge_{0.24}$, □ – $Si_{0.8}Ge_{0.2}$, ◊ – $(Si_{0.8}Ge_{0.2})_{0.98}P_{0.02}$ [33], ∇ – $Si_{0.8}Ge_{0.2}B_{0.8}$ [34], ¤ – $Si_{0.8}Ge_{0.2}B_{0.8}(TaC)_{0.75}$ [34], ☼ – $Si_{0.8}Ge_{0.2}B_{0.8}(NaBH_4)_{0.7}$ [35], ◌ – $Si_{0.7}Ge_{0.3}$ ($n=2.3\cdot10^{25}$ m^3) [36], ◉ – P-type nano SiGe [37]

Values of the figure of merit allows us to determine the compatibility factor: $CF=[(1+ZT)^{1/2}-1]/ST$. Figure 3(*a*) shows the temperature dependences of the compatibility factor for $Cu_{1.98}S_xSe_{1-x}$ and SiGe from [27]. The graph of SiGe can be considered the best, since the compatibility factor should not change significantly depending on temperature. Our data are presented as points at 1173 K in Figure 3(*b*). Extrapolation of the A – T dependence to these points gives a more complete picture.



a) *b)*

Fig. 3. (a) Temperature dependences of compatibility factor for: 1 – $Cu_{1.98}Se$, 2 – $Cu_{1.98}S_{0.02}Se_{0.98}$, 3 – La_2Te_3, 4 – $CoSb_3$, 5 – PbTe, 6 – SiGe, 7 – $Cu_{1.98}S$, 8 – $Cu_{1.98}S_{0.8}Se_{0.2}$, 9 – $Cu_{1.98}S_{0.9}Se_{0.1}$ from[27]; (b) Some graphs from Fig. 3(a); points are our data (these points, corresponding to different x in Si_xGe_{1-x} overlap each other)

Temperature dependences of CF for some well-known thermoelectrics are shown in Fig. 4. Our data for $Si_{0.8}Ge_{0.2}$ are also given there. It is evident from the figure that the A – T dependence for $YbMg_{1.8}Zn_{0.05}Bi_{1.98}$ [38] intersects with our dependence at approximately 350 K, for $CuAl_{0.8}Fe_{0.2}O_2$ [39] – at 750 K, and for $Cu_{1.98}S$ – at 850 K. All this indicates the possibility of creating segmented thermogenerators based on SiGe in combination with the indicated materials.

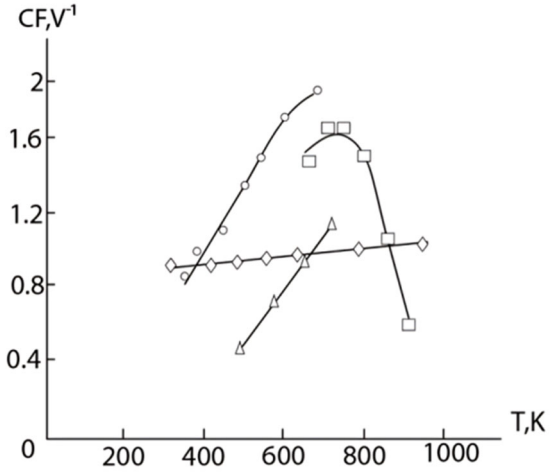


Fig. 4. Temperature dependences of compatibility factor: o – $YbMg_{1.8}Zn_{0.05}Bi_{1.98}$, Δ – $CuAl_{0.8}Fe_{0.2}O_2$, □ – $Cu_{1.98}S$ and ◊ – $Si_{0.8}Ge_{0.2}$

Authors' information

Irakli Nakhutsrishvili – Ph.D., Senior Scientist.

References

1. Anatichuk L.I., Vikhor L.N., Strutynska L.T., Termena (2011). Segmented generator modules using Bi_2Te_3-based materials. *Electron. Mat*., 40, 957. (DOI: https://doi.org/10.1007/s11664-010-1468-x)
2. Dashevsky Z., Horichok I., Maksymuk M., Muchtar A.R., Srinivasan B., Mori T. (2022). Feasibility of high performance in *p*-type $Ge_{1-x}Bi_xTe$ materials for thermoelectric modules. *American Ceram. Soc*., 105(6), 4500–4511. (DOI: https://doi.org/10.1111/jace.18371)
3. Dashevsky Z., Jarashneli A., Unigovski Y., Dzunzda B., Gao F., Shneck R.Z. (2022). Development of a high perfomance gas thermoelectric generator (TEG) with possibible use of waste heat. *Energies*, 15(11), 3960. (DOI: https://doi.org/10.3390/en15113960)
4. Parashchuk T., Wiendlocha B., Cherniushok O., Knura R., Wojciechowski K.T. (2021). High thermoelectric performance of p-type PbTe enabled by the synergy of resonance scattering and lattice softening. *ACS Appl. Mater Interf*., 13(41), 49027–49042. (DOI: https://doi.org/10.1021/acsami.1c14236)
5. Rosi F.D. (1968). Thermoelectricity and thermoelectric power generation. *SolidState Electronics*, 11(9), 849–868. (DOI: https://doi.org/10.1016/0038-1101(68)90104-4)
6. de Winter F. (1972). Xenon-filled silicon germanium thermoelectric generators. *JPL Technical Review*, 2(3), 22–31.
7. Cook B. (2022). Silicon-germanoim: The legacy lives on. Energies, 15(8), 2957. (DOI: https://doi.org/10.3390/en15082957)
8. Barbakadze K., Bokuchava G., Isakadze Z., Tabatadze, I., Rekhviashvili, M. (2022). High temperature thermoelewctricgenrator based on SiGe alloy. *Sci J LEPL – Agmashenebeli National Defence Academy of Georgia*, 47–50.
9. Schwinge C., Kühnel K., Emara J., Roy, L., Biedermann, K., Weinreich, W., Kolodinski, S., Wiatr, M.,Gerlach, G., Wagner-Reetz, M. (2022). Optimization of LPCVD phosphorous-doped Si Ge thin films for CMOS-compatible thermoelectric applications. *Applied Physics Letters*, 120(3), 031903. (DOI: https://doi.org/10.1063/5.0076945)
10. Big-Alabo A. (2021). Finite element modeling and optimization of Ge/SiGe super lattice based thermoelectric generators. *Applied Science,* 3(2), 189. (DOI: https://doi.org/10.1007/s42452-020-04122-x)
11. Jang K., Kim Y., Park J., Yi J. (2019). Electrical and structural characteristics of excimer laser-crystallized polycrystalline $Si_{1-x}Ge_x$ thin-film transistors. *Materials,* 12(11), 1739. (DOI: https://doi.org/10.3390/ma12111739)
12. Murata H., Nozawa K., Suzuki T., Kado Y., Suemasu T., Toko K. (2022). $Si_{1-x}Ge_x$ anode synthesis on plastic films for flexible rechargeable batteries. *Scientific Reports,* 12, 13779. (DOI: https://doi.org/10.1038/s41598-022-18072-4)
13. Idda A., Ayat L., Dahbi N. (2019). Improving the performance of hydrogenated amorphous

silicon solar cell using a-SiGe:H alloy. *Ovonic Research,* 15(5), 271–278. (DOI: https://doi.org/10.1016/j.solmat.2014.06.012)

14. Singh A.K., Kumar M., Kumar D. (2020). Heterostructure silicon and germanium alloy based thin film solar cell efficiency analysis. *Engineering and Manufacturing, 10(2),* 29–40. (DOI: https://doi.org/10.5815/ijem.2020.02.03)
15. Aberl J., Brehm M., Fromherz T., Schuster J., Frigerio J., Rauter P. (2019). SiGe quantum well infrared photo detectors on strained-silicon-on-insulator. *Optics Express,* 27(22), 32009. (DOI: https://doi.org/10.1364/OE.27.032009)
16. Chiang P.T., Hu Sh.M.,Yen W.T., Wu H.-J., Hsu H.-P., Lan Ch.-W. (2023). A study of iron-doped SiGe growth for thermoelectric applications. *Alloys and Compounds*, 967, 171700. (DOI: https://doi.org/10.1016/j.jallcom.2023.171700)
17. Ahmad S., Singh A. (2024). Dopant dependent microstructure of hot-pressed SiGe alloys and its implications on thermoelectric properties. *Physica B: Condensed Matter*, 674, 415534. (DOI: https://doi.org/10.1016/j.physb.2023.415534)
18. Liu W., Zhou J., Jie Q., Li Y., Kim H.S., Bao J., Chen G., Ren Z. (2016). New insight into the material parameter B to understand the enhanced thermoelectric performance of $Mg_2Sn_{1-x-y}Ge_xSb_y$. *Energy Environmental Science*, 9(2), 530–539. (DOI: https://doi.org/10.1039/C5EE02600H)
19. Liu W., Han Z., Ji J., Feng T., Yang J., Zhang W. (2023). Uplimit $(ZT)_{max}$ and effective merit parameter *B** of thermoelectric semiconductors. *Materials Today Physics*, 31, 100989. (DOI: https://doi.org/10.1016/j.mtphys.2023.100989)
20. Bokuchava G., Nakhutsrishvili I., Barbakadze K. (2023). Si_xGe_{1-x} thermoelectric: determination of electronic quality factor, universal electrical conductivity, effective mass, mobility of charge carriers andpreparation of monolithic module based on $Si_{0.7}Ge_{0.3}$ alloy. *Fundamental Research and Application of Physical Science*, 3, 113–126.
21. Snyder G.J., Caillat T. (2003). Using the compatibility factor to design high efficiency segmented thermoelectric generators. *Materials Research Society Proceedings*, 793, 37. (DOI: https://doi.org/10.1557/PROC-793-S2.1)
22. Snyder G.J. (2004). Application of the compatibility factor to the design of segmented and cascaded thermoelectric generators. *Applied Physics Letters,* 84(13), 2436. (DOI: https://doi.org/10.1063/1.1689396)
23. Lobato C.N., Esposito V., Pryds N., Christensen D.V. (2024). How efficient are thermoelectric materials? – An assessment of state-of-the-art individual and segmented thermoelectric materials. *Materialstoday-Energy*, 43, 101564. (DOI: https://doi.org/10.1016/j.mtener.2024.101564)
24. Koike S., Yanagisawa R., Jalabert L., Anufriev R., Kurosawa M., Mori T., Nomura M. (2024). Planar-type SiGe thermoelectric generator with double cavity structure. *Applied Physics Letters,* 124(12), 123902. (DOI: https://doi.org/10.1063/5.0191450)
25. Nurachman A., Permata S., Idogho Ch., Harsito C., Ilogho T., Abel Ejila J. (2025). Compatibility in thermoelectric material synthesis and thermal transport. *Unconventional Resources*, 7, 100198. (DOI: https://doi.org/10.1016/j.uncres.2025.100198)

26. Christian I., Abah E.O., Abel J.E., Harsito, C., Omoniyi M., Boriwaye T. (2025). Compatibility study of synthesized materials for thermal transport in thermoelectric power generation. *Innovation Science and Engineering*, 4(1), 2158–7205. (DOI: https://orcid.org/0000-0003-4097-9041)
27. Zhao L., Fei F.Y., Wang G., Wang F., Wang Ch., Li J., Wang J., Cheng Z., Dou Sh., Wang X. (2017). Improvement of thermoelectric properties and their correlations with electron effective mass in $Cu_{1.98}S_xSe_{1-x}$. *Scientific Reports*, 7(1), 40436. (DOI: https://doi.org/10.1038/srep40436)
28. Yang K.-I., Li X., Jiang Y. (2025). General screening rules and segmented optimization strategy for efficient thermoelectric devices validated by $Mg_3(Sb, Bi)_2/Bi_{0.5}Sb_{1.5}Te_3$-GeTe module. *Advanced Science*, 5, e2502832. (DOI: https://doi.org/10.1002/advs.202502832)
29. Snyder G.J., Pereyra A., Gurunathan R. (2022). Effective mass from Seebeck coefficient. *Advanced Functional Materials*, 32(20), 2112772. (DOI: https://doi.org/10.1002/adfm.202112772)
30. Namiki H., Nagata K., Kobayashi M., Saito Y., Tachibana N., Ota Y. (2022). Relationship between the density of states effective mass and carrier concentration of thermoelectric phosphide $Ag_6Ge_{10}P_{12}$ with strong mechanical robustness. *Materials Today Sustainability*, 18, 100116. (DOI: https://doi.org/10.1016/j.mtsust.2022.100116)
31. Gibbs Z.M., Kim H.S., Wang H., Snyder G.J. (2015). Band gap estimation from temperature dependent Seebeck measurement – Deviations from the $2e|S|_{max}T_{max}$ relation. *Applied Physics Letters*,106(2), 022112. (DOI: https://doi.org/10.1063/1.4905922)
32. Zhang X., Bu Z., Shi X., Lin S., Shan B., Wood M., Snyder A.H., Chen L., Pei Y. (2020). Electronic quality factor for thermoelectric. *Science Advances*, 6(46), eabc0726. (DOI: https://doi.org/10.1126/sciadv.abc0726)
33. Zhao T., Li X., Wu W., Gu J., Han Y., Tang X. (2025). Enhancing the thermoelectric properties and delaying their attenuation in *n*-type SiGe alloy through SiC nanoparticle doping. *ACS Omega*, 10(28), 30023–30030. (DOI: https://doi.org/10.1021/acsomega.4c10843)
34. Fan Z., Liang J.Sh., Chen J.-L., Peng Y., Lai H., Nong J., Liu Ch., Ding W., Miao L. (2023). Realizing high thermoelectric performance for p-type SiGe in medium temperature region via TaC compositing. *Materiomics*, 9(5), 984-991. (DOI: https://doi.org/10.1016/j.jmat.2023.03.004)
35. Lahwal A., Zeng X., Bhattacharya S., Zhou M., Hitchcock D., Karakaya M., He J., Rao A.M., Tritt T.M. (2015). Enhancing thermoelectric properties of $Si_{80}Ge_{20}$ alloys utilizing the decomposition of $NaBH_4$ in the spark plasma sintering process. *Energies*, *8*(10), 10958–10970. (DOI: https://doi.org/10.3390/en81010958)
36. Xu Q., Zhou J., Liu T-H., Chen G. (2021). First-principles study of all thermoelectric properties of SiGe alloys showing large phonon drag from 150 to 1100 K. *Physical Review Applied*, 16(6), 064052. (DOI: https://hdl.handle.net/1721.1/138801)
37. Vishwakarma A., Chauhan N.S., Bhardwaj R., Johari K.K., Dhakate S.R., Gahtori B., Bathula S. (2021). Melt-spun SiGe nano-alloys: Microstructural engineering towards high

thermoelectric efficiency. *Electronic Materials*, 50(1), 364–374. (DOI: https://doi.org/10.1007/s11664-020-08560-6)

38. Wei S., Qin N., Wu G. (2024). Thermoelectric properties of Zn-doped $YbMg_{1.85-x}Zn_xBi_{1.98}$. *Materials*, 17(5), 973. (DOI: https://doi.org/10.3390/ma17050973)
39. Feng Y., Joo J.H., Han G., Lu N. (2023). The effects of Fe addition for enhanced thermoelectric performance in p-type $CuAlO_2$. *Engineered Science*, 22, 822. (DOI: https://doi.org/10.30919/es8d822)

Submitted: 26.06.2025

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

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

Узагальнений параметр і фактор сумісності термоелектричного *n*-Si_xGe_{1-x}

Досліджено залежність максимуму коефіцієнта добротності $(ZT)_{max}$ сплаву Si_xGe_{1-x} від узагальненого параметра матеріалу B. Для розрахунку значень B* використовується формула, яка містить величини ширини забороненої зони, питомої електропровідності, масштабованого параметра B'_S та теплопровідності решітки: $B^* \cong 7.755 \cdot 10^{-4} E_g \sigma B'_S k_L^{-1}$. Ця формула виведена з комбінації відомих з літератури формул, що пов'язують термоелектричні параметри – рухливість, ефективну масу та зважену рухливість носіїв заряду. Дана формула більше не включає ефективну масу, рухливість та температуру – ці параметри замінюються питомою електропровідністю та коефіцієнтом Зеєбека. Побудовано залежність $(ZT)_{max}$ – B*. Обчислюючи узагальнений параметр, можна приблизно оцінити максимальне значення добротності практично для будь-якого термоелектрика. Визначено фактор сумісності Si_xGe_{1-x} Вказано на можливість створення сегментованих термогенераторів на основі цього матеріалу в поєднанні з $YbMg_{1.8}Zn_{0.05}Bi_{1.98}$, $CuAl_{0.8}Fe_{0.2}O_2$ та $Cu_{1.98}S$.*

Ключові слова: термоелектричний SiGe, узагальнений параметр, фактор сумісності.

Надійшла до редакції 26.06.2025