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Some Thermoelectric Characteristics of $\text{Si}_{0.95}\text{Ge}_{0.05}$ Alloy and Monolithic Module Performance

Si-Ge alloys serve as benchmark materials for high-temperature thermoelectric generators, particularly in aerospace power systems. To lower fabrication costs and expand terrestrial applications, reducing the Germanium content while maintaining competitive conversion efficiency remains a critical engineering objective. In this work, we investigate the high-temperature thermoelectric characteristics of a low-Ge content alloy, $\text{Si}_{0.95}\text{Ge}_{0.05}$. The transport metrics, the temperature-dependent trajectories of the electronic quality factor (B_E) and the thermoelectric compatibility factor (CF) are analyzed to elucidate underlying charge carrier scattering and system segmentation viability. Furthermore, the material parameter (B) and generalized material parameter (B^) are calculated to predict the upper bounds of the dimensionless the gap between material properties and practical device-level implementation, monolithic thermoelectric generator modules with 16 and 24 legs were fabricated using vacuum induction hot pressing. The 24-leg module achieved a peak power output of 2.25 W and a practical thermal-to-electrical energy conversion efficiency of 9.2% under a hot-junction temperature of 480 °C, establishing a highly competitive benchmark for low-Ge thermoelectric systems.*

Keywords: silicon-germanium alloy, low Germanium content, thermoelectric characteristics, monolithic module, conversion efficiency.

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Introduction

Thermoelectric energy conversion offers a robust pathway for the direct transformation of thermal gradients into electrical energy via the Seebeck effect. Characterized by the total absence of moving parts, zero mechanical emissions, high operational reliability, and an exceptionally long service life, thermoelectric generators (TEGs) have long been deployed as autonomous power sources in deep-space exploration, remote marine navigation, and strategic pipeline monitoring. Recent decades have witnessed a significant resurgence of interest in these solid-state devices, driven both by the urgent need to harvest industrial waste heat and by advancements in nanostructuring that mitigate lattice thermal conductivity without penalizing electronic transport.

In the realm of high-temperature operations (above 900 K), silicon-germanium (Si-Ge) alloys represent the industry standard [1, 2]. State-of-the-art space power configurations traditionally rely on compositions with substantial Germanium fractions, such as Si_{0.68}Ge_{0.32} [3, 4] and Si_{0.8}Ge_{0.2} [5–8]. However, the high economic cost ⁽¹⁾ and supply volatility of raw Germanium create severe barriers to widespread terrestrial commercialization. Consequently, synthesizing and optimizing Si-Ge formulations with heavily minimized Germanium concentrations has emerged as a high-priority research vector.

While the basic transport trends of the Si_{0.95}Ge_{0.05} have been studied fundamentally [9–12], assessment using advanced thermodynamic descriptors – such as the electronic quality factor, compatibility factor, and predictive scaling parameters – coupled with practical, multi-couple module validation remains sparse. This paper addresses this gap by presenting a analysis of the high-temperature characteristics of Si_{0.95}Ge_{0.05}, tracking its compatibility with other material classes for segmented structures, and demonstrating the manufacturing and performance of functional, high-efficiency monolithic modules.

Material synthesis and processing

The Si_{0.95}Ge_{0.05} alloy coupons investigated in this work were synthesized via vacuum hot pressing of nanostructured powders derived from zone-melting ingots. High-purity bulk Silicon and Germanium precursor materials were mechanically crushed using a steel rod and sieved through a 0.2 mm mesh. The sieved mixtures were loaded into a high-energy planetary ball mill (REK PM-100 SM) and subjected to continuous mechanical machining for 20–25 hours. The structural characteristics and grain size distribution of the processed powders were characterized using a Nikon optical microscope and an HZG-4A X-ray diffractometer. The milling configuration consistently yielded a highly dispersed Si-Ge powder with an average grain size ranging between 60 and 80 nm.

The nanostructured powder was consolidated using a high-temperature vacuum induction hot-pressing system. The densification process was executed within high-strength graphite dies at temperatures between 1200 °C and 1320 °C under an axial mechanical pressure of ~ 47 MPa for a dwell time of 20–30 minutes. Profiled rectangular parallelepiped specimens measuring 10×10×20 mm were precision-cut from the dense consolidated briquettes using a diamond-disc cutter for subsequent transport property characterization.

To induce p-type electrical conductivity, Boron was incorporated into the alloy matrix as an acceptor dopant. The room-temperature majority charge carrier concentration was determined to be $3.2 \cdot 10^{26} \text{ m}^{-3}$, derived from Hall coefficient measurements.

Thermoelectrical characteristics were evaluated over operational range of 30 °C to 1150 °C, where the upper temperature limit was limited by the stability region of the alloy. The measurement errors were: the Seebeck coefficient (S) $\pm 3\%$, electrical resistivity ($\rho = \sigma^{-1}$, σ – electrical conductivity) via the standard four-probe technique within $\pm 5\%$, and total thermal conductivity (k) with an uncertainty not exceeding $\pm 7\%$.

Theoretical estimations

Below are the thermoelectric characteristics of Si_{0.95}Ge_{0.05} that have not been studied in other works. Specifically, these characteristics are the electronic quality and the compatibility factors as well as the material and generalized parameters of the thermoelectrics. They are given by expressions $B_E = \sigma S^2 / B_S$, [13], $CF = [(1+ZT)^{1/2} - 1] / ST$ [14–20], $B = B_E T / k_L$ [13] and $B^* \cong 6.668 \cdot 10^{-2} E_g U^* k_L^{-1}$ [21, 22], respectively. Here, $B_S = \left[\frac{S_r^2 e^{2-S_r}}{1+e^{-5(S_r-1)}} + \frac{\frac{\pi^2}{3} S_r}{1+e^{5(S_r-1)}} \right] \cong \left[\frac{S_r^2 e^{2-S_r}}{1+e^{-5(S_r-1)}} + \frac{3.29 S_r}{1+e^{5(S_r-1)}} \right]$ is the scaled power factor, $S_r = (q_e / k_B) |S| \cong 1.1604 \cdot 10^4 |S|$ is reduced Seebeck coefficient (q_e – elementary charge, k_B – Boltzmann's constant), 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 is lattice thermal conductivity.

By combining of known from the literature formulas [23–25]: $\mu = (m^* / m_0)^{-3/2} \mu_W$, $\mu_W \cong 3.31 \cdot 10^{-7} (T/300)^{-3/2} \sigma B'_S \cong 1.72 \cdot 10^{-3} T^{-3/2} \sigma B'_S$ (weighted mobility) we will have: $B^* \cong 7.755 \cdot 10^{-4} E_g \sigma B'_S k_L^{-1}$ ($B'_S \cong \frac{3[e^{(S_r-2)} - 0.17]^{2/3}}{1+e^{-5(S_r-S_r^{-1})}} + \frac{S_r}{1+e^{5(S_r-S_r^{-1})}}$). At $|S| \geq 2 \cdot 10^{-4} \text{ V/K}$, $B_S \cong S_r^2 e^{(2-S_r)}$ and $B'_S \cong 3[e^{(S_r-2)} - 0.17]^{2/3}$ with high accuracy. If there is no direct data on band gap (this is the case in the overwhelming majority of cited works), then the formula $E_g = 2|S|_{\max} T_{S_{\max}}$ [26] is used (the temperature dependence of the Seebeck coefficient must have an extreme point – a maximum). As a result, we will have: $B^* \cong 1.551 \cdot 10^{-3} |S|_{\max} T_{S_{\max}} \sigma B'_S k_L^{-1}$. In instances where specific cited literature data lacked direct experimental parameters for the lattice thermal conductivity, a semi-empirical approximation was implemented to isolate the lattice component from the total thermal conductivity: $k_L \cong k - L' \cdot 10^{-8} \sigma T$, where $L' \cong 1.5 + e^{-|S|/116}$ (S is in $\mu\text{V/K}$) represents the modified Lorenz number parameterized as a function of the Seebeck coefficient. For calculation of B , B^* and CF all parameters were extracted at the specific temperatures where thermoelectric figure of merit reaches its peak value $(ZT)_{\max}$.

Data on the temperature dependences of the above parameters are presented in Fig. 1.

The electronic quality factor serves as a fundamental metric to evaluate the electronic transport capability of a material independently of its lattice thermal conductivity.

Figure 2 shows the B_E – T dependence schematically from work [13]. As illustrated in Fig. 2, the temperature-dependent profile of B_E can be divided into three distinct regimes:

region I points toward the presence of additional scattering mechanisms, region II reveals the onset of band convergence that drives the factor to its peak, and region III shows the degradation caused by the bipolar effect at elevated temperatures.

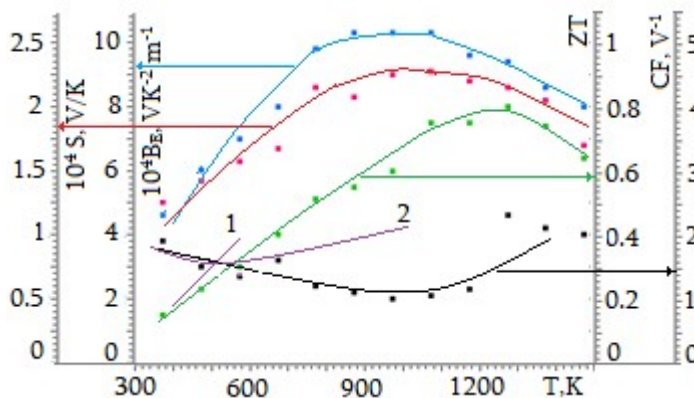


Fig. 1. Temperature dependences of Seebeck coefficient, electronic quality factor, figure of merit and compatibility factor of alloy $\text{Si}_{0.95}\text{Ge}_{0.05}$; 1 and 2 – $\text{CF}-T$ dependences for $\text{Cu}_{1.98}\text{Se}$ [27] and $\text{Si}_{0.62}\text{Ge}_{0.32}\text{Ni}_{0.03}\text{B}_{0.07}$ [28]

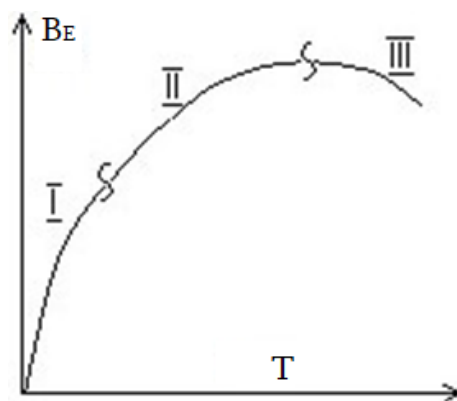


Fig. 2. Schematic representation of temperature dependence of electronic quality factor: I – additional scattering, II – band convergence, III – bipolar

While ZT dictates the absolute efficiency potential of an isolated material, the engineering execution of multiple materials within a segmented leg requires matching their compatibility factors. If two materials with vastly different CF values are joined in a segmented leg, the forced continuity of electric current forces one of the materials to operate far from its thermodynamic optimum, leading to severe efficiency penalties or parasitic heat accumulation.

In addition to our data for $\text{Si}_{0.95}\text{Ge}_{0.05}$, Fig.1 shows the $\text{CF}-T$ dependences for $\text{Cu}_{1.98}\text{Se}$ and $\text{Si}_{0.62}\text{Ge}_{0.32}\text{Ni}_{0.03}\text{B}_{0.07}$, calculated from the experimental results of [27] and [28], respectively. As can be seen from this figure, they intersect the corresponding dependence for $\text{Si}_{0.95}\text{Ge}_{0.05}$ at ~ 500 K. This will allow segmented thermogenerators to be manufactured using these materials.

Parameters B and B^* are predictors for forecasting the maximum values of the figure of merit of thermoelectric materials. The $(ZT)_{\text{max}} - B$ and $(ZT)_{\text{max}} - B^*$ dependences for $\text{Si}_{0.95}\text{Ge}_{0.05}$ are shown in Figs. 2 and 3. The same figures also presents data on some thermoelectric materials

containing Si and/or Ge, calculated on the basis of works [29-53]. It is evident from the figures that the data for $\text{Si}_{0.95}\text{Ge}_{0.05}$ fit satisfactorily into the general dependences. The latter can be described by empirical formulas $(ZT)_{\max} \cong 1.165B + 0.474$ and $(ZT)_{\max} \cong 0.011 B^* + 0.472$.

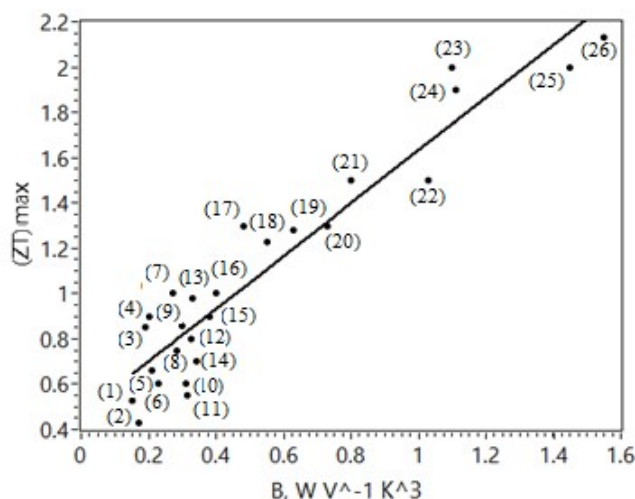


Fig. 3. $(ZT)_{\max} - B$ dependences for: 1 – $\text{Si}_{0.8}\text{Ge}_{0.2}\text{B}_{0.005}$, 2 – $\text{Si}_{0.94}\text{P}_{0.06}$, 3 – $\text{Si}_{0.58}\text{Ge}_{0.42}$, 4 – $\text{Si}_{0.8}\text{Ge}_{0.2}\text{Pt}^*$, 5 – $\text{SiGe} + 0.01\text{SiMo}$, 6 – melt-spun SiGe^{**} , 7 – nano-Si, 8 – $\text{Si}_{0.8}\text{Ge}_{0.9}(\text{NaBH}_4)_{0.7}$, 9 – $\text{Si}_{0.8}\text{Ge}_{0.2}\text{P}_{0.01}$, 10 – $\text{Si}_{0.8}\text{Ge}_{0.2}\text{P}_{0.02}$, 11 – nano-Si, 12 – $\text{Si}_{0.95}\text{Ge}_{0.05}$ [this work], 13 – melt-spun SiGe^{**} , 14 – $\text{Si}_{0.8}\text{Ge}_{0.2}\text{B}_{0.008}$, 15 – $\text{Si}_{0.8}\text{Ge}_{0.2}\text{B}_{0.008}(\text{TaC})_{0.0075}$, 16 – $\text{SiGe} + 0.03\text{SrTiO}_3$, 17 – $\text{Si}_{0.8}\text{Ge}_{0.2}\text{P}_{0.02}\text{Sn}_{0.02}$, 18 – $\text{Si}_{0.9}\text{Ge}_{0.1}\text{P}_{0.02}\text{Zn}_{0.003}$, 19 – $\text{SiGe} + 0.05\text{Mg}_2\text{Si}$, 20 – nano-SiGe^{**}, 21 – nano-SiGe^{**}, 22 – $\text{Ge}_{0.91}\text{Sb}_{0.09}\text{Te}$, 23 – $\text{Ge}_{0.93}\text{Ti}_{0.01}\text{Bi}_{0.06}\text{Te} + 0.05\text{Cu}$, 24 – $\text{Ge}_{0.893}\text{Sb}_{0.1}\text{In}_{0.007}\text{Te}$, 25 – $\text{Ge}_{0.96}\text{Bi}_{0.04}\text{Te}$, 26 – $\text{Ge}_{0.93}\text{In}_{0.01}\text{Bi}_{0.06}\text{Te}$. (*Data from our as yet unpublished work; **The samples were obtained under different technological conditions).

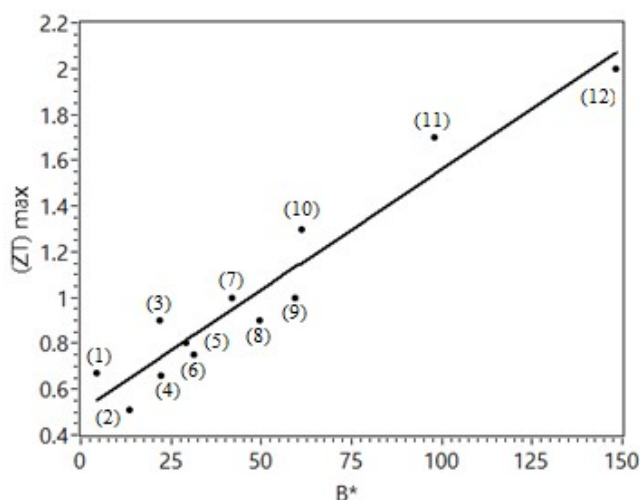


Fig. 4. 1 – PtTiGe^* , 2 – PtTiPb^* , 3 – GeTe , 4 – $\text{SiGe} + 0.01\text{SiMo}$, 5 – $\text{Si}_{0.95}\text{Ge}_{0.05}$ [this work], 6 – $n\text{-Si}_{0.83}\text{Ge}_{0.17}$, 7 – GeTe , 8 – $\text{Si}_{0.8}\text{Ge}_{0.2}\text{P}_{0.0006}$, 9 – GeTe , 10 – nano-SiGe, 11 – $\text{Ge}_{0.95}\text{Bi}_{0.04}\text{In}_{0.01}\text{Te}$, 12 – $\text{Ge}_{0.96}\text{Bi}_{0.04}\text{Te}$. (*Data from our as yet unpublished work)

All this indicates that the nanostructured $\text{Si}_{0.95}\text{Ge}_{0.05}$ alloy effectively optimizes transport properties, ensuring the high device performance metrics that will be demonstrated below.

Manufacturing and performance of monolithic modules

To evaluate the practical device-level viability of the synthesized nanostructured $\text{Si}_{0.95}\text{Ge}_{0.05}$ alloy, monolithic thermoelectric modules were designed and fabricated. The core architecture relies on an alternating segmented arrangement of p-type (boron-doped) and n-type (phosphorus-doped) legs arrayed in an n-p-n-p matrix. Electrical insulation between adjacent structural branches was achieved by applying a high-temperature glass-ceramic suspension layer across the active plates.

The structural integrity and dense consolidation of the multi-leg package were achieved by diffusion bonding within a high-temperature vacuum induction chamber. The assembly process was executed at a localized bonding temperature of 1050 °C under a pressure of 10 Pa, resulting in a robust, monolithic module block with nominal dimensions of $2.4 \times 1.6 \times 2.0$ cm (Fig. 4).

The power generation capacity ($P = E^2/4R$, E and R are the EMF and internal resistance of the module, respectively) and thermal-to-electrical energy conversion efficiencies (η) of the fabricated prototypes were systematically evaluated under distinct thermal gradients. A module with 16 legs was studied. The hot-side temperature (T_h) was varied up to 520 °C while the cold-side junction (T_c) was actively maintained (23 °C) via a water-cooled copper block exchanger⁽²⁾.



Fig. 4. Photo of a thermoelectric module attached to a water cooler (1×0.4)

The measured energy conversion parameters are tabulated in Table 1. Under a maximal thermal gradient $\Delta T = 497$ °C, the module generated a peak output power of 1.83 W, demonstrating a maximum device efficiency of 7.5 %.

To increase power output, a more compact module with 24 legs was tested. Preliminary data indicate a conversion efficiency of $\eta = 9.2$ % at $\Delta T = 432$ °C. While the theoretical efficiency threshold for optimized bulk silicon-germanium systems can scale between 14 % and 15 % under ideal operational regimes, practical laboratory prototypes typically report values ranging from ~ 9 % to ~ 12 % due to localized thermal contact resistances and parasitic electrical contact losses at the commutation boundaries. Within this context, the realization of a 9.2 % represents a highly competitive benchmark compared to traditional alloys with higher germanium content.

Table 1

*Thermoelectric performance characteristics
of the fabricated 16-leg $\text{Si}_{0.95}\text{Ge}_{0.05}$ monolithic module*

T_c , °C	T_h , °C	P , W	$Z \cdot 10^{-3}$, K ⁻¹	η , %
23	450	1.54	3.48	6.9
23	480	1.73	7.11	7.2
23	520	1.83	6.84	7.5

Conclusions

The high-temperature thermoelectric performance of nanostructured Si_{0.95}Ge_{0.05} alloy and its integrated monolithic modules were systematically evaluated, yielding the following core conclusions:

1. The temperature dependence of the electronic quality factor serves as an effective diagnostic tool, revealing additional alloy/impurity scattering at intermediate ranges and the emergence of band convergence/bipolar transport at elevated temperatures.
2. Thermoelectric compatibility factor confirmed a definitive intersection with Cu_{1.98}Se and Si_{0.62}Ge_{0.32}Ni_{0.03}B_{0.07}, at ~ 500 K, establishing a thermodynamic justification for high-efficiency segmented generator architectures.
3. The calculated coordinates for Si_{0.95}Ge_{0.05} fit tightly within global empirical linear scaling laws mapped against multiple Si/Ge-based materials, confirming the predictive validity of material parameters B and B* for evaluating peak performance boundaries.
4. The 16-branch module exhibited conversion efficiency of 7.5 % and a peak power output of 1.83W, validating the commercial potential of low-germanium thermoelectrics for cost-effective, high-temperature power generation.

Footnotes:

(1) Today's price is \$4.670.20 per kg.

(2) $\eta = \frac{T_h - T_c}{T_h} \frac{\sqrt{1 + Z \frac{T_h + T_c}{2}} - 1}{\sqrt{1 + Z \frac{T_h + T_c}{2} + \frac{T_c}{T_h}}}$. The first term of this formula represents the thermodynamic part

of η , which increases with increasing operating temperature, and the second term represents the material part, which increases with increasing efficiency of the thermoelectric material. Therefore, the creation of a high-temperature TEG based on high-efficiency thermoelectric materials is promising from an energetic point of view.

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Деякі термоелектричні характеристики сплаву Si_{0.95}Ge_{0.05} та робочі характеристики монолітного модуля

Сплави Si-Ge є еталонними матеріалами для високотемпературних термоелектричних генераторів, зокрема в аерокосмічних енергетичних системах. Зменшення вмісту германію за умови збереження конкурентоспроможної ефективності перетворення залишається важливим інженерним завданням, спрямованим на зниження витрат на виробництво та розширення сфери наземного застосування. У цій роботі досліджено високотемпературні термоелектричні характеристики сплаву Si_{0.95}Ge_{0.05} із низьким вмістом германію. Проаналізовано транспортні параметри, а також температурні залежності електронного фактора якості (B_E) та фактора термоелектричної сумісності (CF) з метою з'ясування механізмів розсіяння носіїв заряду та доцільності сегментації системи. Крім того, для прогнозування верхніх меж безрозмірного розриву між властивостями матеріалу та їхньою практичною реалізацією на рівні пристрою було розраховано матеріальний параметр (B) і узагальнений матеріальний параметр (B^*); методом вакуумного індукційного гарячого пресування було виготовлено монолітні модулі термоелектричних генераторів із 16 та 24 гілками. Модуль із 24 гілками продемонстрував пікову вихідну потужність 2.25 Вт і практичний коефіцієнт перетворення теплової енергії в електричну на рівні 9.2 % за температури гарячого спаю 480 °C, встановивши висококонкурентний орієнтир для термоелектричних систем із низьким вмістом германію.

Ключові слова: кремній-германієвий сплав, низький вміст германію, термоелектричні характеристики, монолітний модуль, ефективність перетворення.