### **DOI:** 10.63527/1607-8829-2025-2-17-24

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# Universal Relation for Thermoelectric Figure of Merit of Two-Phase Composites

In the paper, a universal expression for the effective thermoelectric figure of merit of a composite two-phase material is found based on the isomorphism method. It is shown that to determine the effective thermoelectric figure of merit, a set of values of local kinetic coefficients of the phases, namely electrical conductivity, thermal conductivity, and thermoEMF, and the effective value of the thermoEMF coefficient is quite sufficient to use. To determine the thermoelectric figure of merit, it is not necessary to know the effective coefficients of electrical conductivity and thermal conductivity. Therefore, the effective figure of merit does not depend on the choice of approximation (effective medium approximation (EMA), flow theory, Maxwell approximation, etc.) for calculating the effective values of electrical conductivity and thermal conductivity.

**Keywords:** composites, isomorphism theory, effective thermoelectric properties, effective thermoelectric figure of merit.

### Introduction

Thermoelectric figure of merit is a key parameter that determines the efficiency of converting thermal energy into electrical energy and vice versa. In modern technologies, where the main directions are sustainable development and energy saving, the control of thermoelectric properties of materials, in particular composite materials, is of primary importance. Composite materials, due to the possibility of targeted selection of components and structure, open up broad prospects for optimizing thermoelectric figure of merit and creating efficient thermoelectric converters.

A high thermoelectric figure of merit indicates the ability of a material to efficiently

**Citation:** A.O. Snarskii, L.M. Vikhor, S.O. Podlasov (2025). Universal Relation for Thermoelectric Figure of Merit of Two-Phase Composites. *Journal of Thermoelectricity*, (2), 17–24. https://doi.org/10.63527/1607-8829-2025-2-17-24

convert energy. This property is significant in such areas as the conversion of heat generated by industrial installations, cooling of electronic devices, and many others. Composites enable combining materials with high thermoEMF, low thermal conductivity, and high electrical conductivity, which ensures optimization of a thermoelectric material.

It should be emphasized that there is a direct relationship between the thermoelectric figure of merit and the efficiency of a thermoelectric device. The higher the figure of merit, the closer the efficiency to the theoretical limit is. Thus, an optimization of the figure of merit directly leads to an increase in the energy efficiency of thermoelectric systems.

The aim of the paper was to establish a universal relation for the effective figure of merit of a randomly inhomogeneous medium, i.e., a composite, thus connecting it to the effective coefficient of thermoEMF.

### 2. Effective kinetic coefficients of thermoelectric composite materials

Let us consider a sample of volume V with macroscopically random heterogeneity of the properties of the medium, by which we will understand such a medium in which locally, in the vicinity of each point of the medium, phenomenological expressions can be written, namely local relations between the vectors of electric current density **j**, heat flux density **q**, temperature gradient  $\nabla T$  and electric field strength **E**, in the form [1–3]

$$\begin{aligned} \mathbf{j} &= \mathbf{\sigma} \mathbf{E} + \gamma \mathbf{g} \\ \mathbf{s} &= \gamma \mathbf{E} + \chi \mathbf{g} \end{aligned}$$
 (1)

where  $\mathbf{s} = \mathbf{q} / T$ ,  $\mathbf{g} = -\nabla T$ ,  $\gamma = \alpha \sigma$ ,  $\chi = \sigma \alpha^2 + \frac{\kappa}{T}$ ,  $\alpha$ ,  $\sigma$ ,  $\kappa$  are coefficients of thermoEMF,

electrical conductivity and thermal conductivity. Local kinetic coefficients  $\alpha(\mathbf{r})$ ,  $\sigma(\mathbf{r})$ ,  $\kappa(\mathbf{r})$  depend on the coordinate  $\mathbf{r}$  and in the case of a two-phase composite take the values  $\alpha_1$ ,  $\sigma_1$ ,  $\kappa_1$  in the first phase and  $\alpha_2$ ,  $\sigma_2$ ,  $\kappa_2$  in the second one.

For the stationary case under consideration, the following conditions are fulfilled

$$\operatorname{div} \mathbf{j} = 0, \ \operatorname{div} \mathbf{s} = 0, \ \operatorname{rot} \mathbf{E} = 0, \ \operatorname{rot} \mathbf{g} = 0.$$
 (2)

The properties of a heterogeneous medium as a whole are described by the effective kinetic coefficients  $\alpha_e$ ,  $\sigma_e$ ,  $\kappa_e$ , which by definition connect the local thermodynamic fields **E** and **g** averaged over the volume *V* with the flows **j** and **s** by the following relations

where  $\gamma_e = \alpha_e \sigma_e$ ,  $\chi_e = \sigma_e \alpha_e^2 + \frac{\kappa_e}{T}$  and <...> denotes averaging over volume, namely

$$\langle ... \rangle = 1 / V \int_{V} ... dV \,. \tag{4}$$

Calculation of effective kinetic coefficients is a complex problem, and its exact solution

for inhomogeneous thermoelectric media in the entire region of phase concentrations with different values of local kinetic coefficients has no solution. There exist various approximations that, in some cases, allow obtaining approximate concentration expressions for effective coefficients. In the case of a two-phase composite, the concentration p denotes the relative volume of the first phase in the sample of the material.

One of the most important parameters of an inhomogeneous medium is the local dimensionless thermoelectric figure of merit [3, 4], determined by the formula

$$ZT = \frac{\sigma \alpha^2}{\kappa} T \,. \tag{5}$$

To describe composite materials, the effective figure of merit should be determined as

$$Z_e T = \frac{\sigma_e \alpha_e^2}{\kappa_e} T, \qquad (6)$$

that in addition to knowing the local kinetic coefficients, demands calculation of the effective coefficients  $\alpha_e$ ,  $\sigma_e$ ,  $\kappa_e$ . We will demonstrate that for a two-phase randomly inhomogeneous medium, being generally isotropic, the effective thermoelectric figure of merit can be determined by establishing the value of only one of the effective kinetic coefficients, namely the effective coefficient of thermoEMF.

### 3. Isomorphism method

Calculation of effective kinetic coefficients in thermoelectric media is possible in various approximations, however, there is a so-called isomorphism method, whose details are described in [3], where all references to primary sources for this method are provided. The idea of the method is to move from a double-flow problem, in this case with flows **j** and **s**, which are determined by relations (1), to some single-flow problem. This allows obtaining, in some cases, expressions for the effective coefficients of a thermoelectric composite, having determined the properties of the single-flow problem.

Let us present the isomorphism theory necessary for further relations. By introducing some constant K, (1) can be written in the form

$$\mathbf{j} + K\mathbf{s} = (\mathbf{\sigma} + K\gamma)\mathbf{E} + (\gamma + K\chi)\mathbf{g}.$$
(7)

The definition  $\omega = \frac{\gamma + K\chi}{\sigma + K\gamma}$  should be used to obtain

$$\mathbf{j} + K\mathbf{s} = (\mathbf{\sigma} + K\gamma) (\mathbf{E} + \boldsymbol{\omega} \cdot \mathbf{g}).$$
(8)

Based on (8), one can enter a single-flow system with flow i and field  $\varepsilon$ , specified by the relations

$$\mathbf{i} = \mathbf{j} + K\mathbf{s}, \qquad \mathbf{\varepsilon} = \mathbf{E} + \boldsymbol{\omega} \cdot \mathbf{g}.$$
 (9)

In the new single-flow system (9), as in the double-flow system, equations for the flow and field similar to (2) must be satisfied, namely

$$\operatorname{div}\mathbf{i} = 0, \quad \operatorname{rot}\mathbf{\varepsilon} = 0. \tag{10}$$

These equations will follow from (2) if we require that the introduced constants *K* and  $\omega$  do not depend on the coordinates, that is, they are the same for each of the two phases:  $K = K_I = K_{II}$ . This requirement leads to the following condition

$$\frac{\gamma_1 + K\chi_1}{\sigma_1 + K\gamma_1} = \frac{\gamma_2 + K\chi_2}{\sigma_2 + K\gamma_2}.$$
(11)

Thus, having determined from (11) two possible values of the constants  $K_I$  i  $K_{II}$ 

$$K_{I,II} = \frac{\chi_2 \sigma_1 - \chi_1 \sigma_2 \pm \sqrt{(\chi_2 \sigma_1 - \chi_1 \sigma_2)^2 - 4(\chi_1 \gamma_2 - \chi_2 \gamma_1)(\gamma_1 \sigma_2 - \gamma_2 \sigma_1)}}{2(\chi_1 \gamma_2 - \chi_2 \gamma_1)},$$
 (12)

and two constants  $\omega_I$  and  $\omega_{II}$ , according to (8) we pass from the double-flow problem (1) – (2) to the single-flow problem with the local coefficient  $f(\mathbf{r})$ , which is written in the form

$$\mathbf{i}(\mathbf{r}) = f(\mathbf{r}) \cdot \boldsymbol{\varepsilon}(\mathbf{r}), \text{ where } f(\mathbf{r}) = \sigma(\mathbf{r}) + K\gamma(\mathbf{r}).$$
 (13)

A reverse transition also exists, which means the presence of isomorphism.

The effective coefficient of a single-flow system is determined similarly to (3), i.e.

$$\langle \mathbf{i}(\mathbf{r}) \rangle = f^e \langle \varepsilon(\mathbf{r}) \rangle.$$
 (14)

Now, averaging (9), taking into account the presence of two constants  $K_I$  and  $K_{II}$ , we will have

whence obtain

$$\langle \mathbf{j} \rangle = \frac{K_{II} f_{I}^{e} - K_{I} f_{II}^{e}}{K_{II} - K_{I}} \langle \mathbf{E} \rangle + \frac{K_{II} f_{I}^{e} \omega_{I} - K_{I} f_{II}^{e} \omega_{II}}{K_{II} - K_{I}} \langle \mathbf{g} \rangle,$$

$$\langle \mathbf{s} \rangle = \frac{f_{I}^{e} - f_{II}^{e}}{K_{II} - K_{I}} \langle \mathbf{E} \rangle + \frac{f_{I}^{e} \omega_{I} - f_{II}^{e} \omega_{II}}{K_{II} - K_{I}} \langle \mathbf{g} \rangle.$$

$$(16)$$

By comparing (16) and (3), we obtain the relationship between the effective coefficients of the single-flow and double-flow systems in the following form:

$$\sigma_{e} = \frac{K_{II}f_{I}^{e} - K_{I}f_{II}^{e}}{K_{II} - K_{I}}, \quad \gamma_{e} = \frac{K_{II}f_{I}^{e}\omega_{I} - K_{I}f_{II}^{e}\omega_{II}}{K_{II} - K_{I}}, \quad \chi_{e} = \frac{f_{I}^{e}\omega_{I} - f_{II}^{e}\omega_{II}}{K_{II} - K_{I}}.$$
 (17)

In this case, the equalities  $\omega_I K_{II} = -1$  and  $\omega_{II} K_I = -1$  were used, which must be satisfied so that the matrix of effective coefficients in (16) is symmetric, i.e. the condition is satisfied

$$\frac{K_{II}f_{I}^{e}\omega_{I} - K_{I}f_{II}^{e}\omega_{II}}{K_{II} - K_{I}} = \frac{f_{I}^{e} - f_{II}^{e}}{K_{II} - K_{I}}.$$
(18)

#### 4. Universal relation for effective figure of merit

The effective kinetic coefficients  $f_I^e$ ,  $f_{II}^e$  of a single-flow system can be determined using various approximations, for example, Maxwell's approximation [1–3], effective medium approximation (EMA) [5–7], flow theory methods [1, 3]. However, the relations (17) between the single-flow and double-flow systems enable obtaining the relationship for the effective thermoelectric figure of merit of the two-phase composite without using these approximations. For this purpose, based on (13) and (14), let us write

$$f_1 = \sigma_1 + K\gamma_1, \quad f_2 = \sigma_2 + K\gamma_2, \qquad f_I^e = \sigma_e + K_I\gamma_e, \quad f_{II}^e = \sigma_e + K_{II}\gamma_e.$$
(19)

By substituting (19) in  $\chi_e$ , one can find from (17) the following:

$$\chi_e = \frac{\omega_I - \omega_{II}}{K_{II} - K_I} \sigma_e + \frac{K_I \omega_I - \omega_{II} K_{II}}{K_{II} - K_I} \gamma_e.$$
(20)

Considering that  $\omega_I = -1/K_{II}$ ,  $\omega_{II} = -1/K_I$  and  $\chi_e = \frac{\kappa_e}{T}(1+Z_eT)$ , the following is obtained

$$1 + \frac{1}{Z_e T} = \frac{1 + (K_I + K_{II})\alpha_e}{K_I \cdot K_{II}\alpha_e^2}$$
(21)

In conformance with (12), it can be shown that

$$K_{I} \cdot K_{II} = \frac{\gamma_{1}\sigma_{2} - \gamma_{2}\sigma_{1}}{\chi_{1}\gamma_{2} - \chi_{2}\gamma_{1}}, \qquad K_{I} + K_{II} = \frac{\chi_{2}\sigma_{1} - \chi_{1}\sigma_{2}}{\chi_{1}\gamma_{2} - \chi_{2}\gamma_{1}}.$$
(22)

Thus, substituting (22) into (21) and taking into account the notations  $\gamma_1$ ,  $\gamma_2$ ,  $\chi_1$ ,  $\chi_2$ , we finally find the following expression for the effective figure of merit of the two-phase composite:

$$Z_{e}T = \frac{(\alpha_{2} - \alpha_{1})\alpha_{e}^{2}}{\alpha_{1}^{2}\left(1 + \frac{1}{Z_{1}T}\right)(\alpha_{2} - \alpha_{e}) + \alpha_{2}^{2}\left(1 + \frac{1}{Z_{2}T}\right)(\alpha_{e} - \alpha_{1}) - (\alpha_{2} - \alpha_{1})\alpha_{e}^{2}}$$
(23)

where  $Z_1T$  and  $Z_2T$  are dimensionless figures of merit of the first and second phases.

This relation can be called universal, for it provides an opportunity to determine the effective figure of merit of a two-phase composite without any of the above approximations. To do this, it is enough to know the figure of merit and thermoEMF coefficients of individual phases and, e.g., to experimentally estimate only the effective value of the thermoEMF coefficient of the composite, the methods of measuring which are simpler and more accurate than those for other thermoelectric parameters of the composite.

To confirm the above theory and the validity of the universal relation (23), we calculated

the dependence of  $Z_e T(\alpha_e)$  of the effective figure of merit on the effective thermoEMF in two ways, namely by formula (23) and by calculating in the effective medium approximation (EMA). For example, we used a composite whose first phase is a metal with thermoelectric parameters  $\alpha_1 = 10^{-8}$  V/K,  $\sigma_1 = 5 \cdot 10^6$  Ohm<sup>-1</sup>m<sup>-1</sup>,  $\kappa_1 = 40$  W/m·K, the second phase is a thermoelectric material with parameters  $\alpha_2 = 2 \cdot 10^{-4}$  V/K,  $\sigma_2 = 10^5$  Ohm<sup>-1</sup>m<sup>-1</sup>,  $\kappa_2 = 2$  W/m·K,  $Z_2T = 0.6$ , being close to the parameters of Bi<sub>2</sub>Te<sub>3</sub>-based alloys at a temperature of T = 300 K.

To calculate  $Z_e T(\alpha_e)$  in the EMA, the concentration dependences of the effective thermoEMF coefficients  $\alpha_e(p)$ , electrical conductivity  $\sigma_e(p)$ , thermal conductivity  $\kappa_e(p)$  and the figure of merit  $Z_e T(p)$ , where p is the concentration of the first phase in the composite, were calculated in the first place. The results are illustrated in Fig. 1. It should be noted that similar concentration dependences can be obtained by applying other approximations and, obviously, they will differ [3].



Fig. 1. Concentration dependences of the effective coefficients of the two-phase composite, calculated in EMA. a) thermoEMF  $\alpha_e(p)$ , b) electrical conductivity  $\sigma_e(p)$ , c) thermal conductivity  $\kappa_e(p)$ , d) figure of merit  $Z_eT(p)$ 

Using the concentration p as a parameter, the dependence  $Z_e T^{(1)}(\alpha_e)$  is built according to

the data in Fig. 1*a* and 1*d*, which is shown in Fig. 2. The same figure presents a similar dependence  $Z_e T^{(2)}(\alpha_e)$ , calculated with the universal relation (23), which does not depend on the approximation chosen for calculating the concentration dependences of the effective kinetic coefficients of the composite. As expected, both dependences  $Z_e T(\alpha_e)$  coincide.



Fig. 2. Dependences of the effective figure of merit of the composite on the effective thermoEMF.  $1 - Z_e T^{(1)}(\alpha_e)$  dependence, calculated in the EMA,  $2 - Z_e T^{(2)}(\alpha_e)$ , dependence, calculated using the universal relation

# Conclusions

For a two-phase randomly inhomogeneous composite with isotropic kinetic coefficients, the isomorphism method is applied and an analytical universal relation between the effective thermoelectric figure of merit and the effective thermoEMF coefficient is obtained. It is shown that the relationship between these effective parameters does not depend on the approximation used to calculate the concentration dependences of the effective kinetic coefficients of the composite and can be easily established using the obtained universal expression.

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# References

- 1. Torquato S. (2002). Random heterogeneous materials: Microstructure and macroscopic properties. Springer. https://doi.org/10.1115/1.1483342
- 2. Choy T.C. (2016). Effective medium theory: Principles and applications. *Oxford University Press*. https://doi.org/10.1093/acprof:oso/9780198705093.001.0001
- 3. Snarskii A., Bezsudnov I.V., Sevryukov V.A., Morozovskiy A., & Malinsky J. (2016).

Transport processes in macroscopically disordered media: From mean field theory to percolation. Springer. https://doi.org/10.1007/978-1-4419-8291-9

- 4. Rowe D.M. (Ed.). (2006). Thermoelectrics handbook: Macro to nano. Taylor & Francis.
- Bruggeman V.D. (1935). Berechnung verschiedener physikalischer Konstanten von heterogenen Substanzen. I. Dielektrizitätskonstanten und Leitfähigkeiten der Mischkörper aus isotropen Substanzen. Annalen der Physik, 416(7), 636–664. https://doi.org/10.1002/andp.19354160705
- Bergman D.J. (1978). The dielectric constant of a composite material a problem in classical physics. *Physics Reports*, 43(9), 407–411. https://doi.org/10.1016/0370-1573(78)90024-1
- Snarskii A., Zorinets D., Shamonin M., & Kalita V. (2019). Theoretical method for calculation of effective properties of composite materials with reconfigurable microstructure: Electric and magnetic phenomena. *Physica A: Statistical Mechanics and its Applications*, 535, 122467. https://doi.org/10.1016/j.physa.2019.122467

Submitted: 24.05.2025

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# Універсальне співвідношення для термоелектричної добротності двофазних композитів

У роботі на основі метода ізоморфізму знайдено універсальний вираз для ефективної термоелектричної добротності композитного двофазного матеріалу. Показано, що для визначення ефективної термоелектричної добротності достатньо набору значень локальних кінетичних коефіцієнтів фаз, а саме електропровідності, теплопровідності, і термоЕРС, та ефективного значення коефіцієнта термоЕРС. Для визначення термоелектричної добротності не потрібно знати ефективні коефіцієнти електропровідності та теплопровідності. Відтак ефективна добротність не залежить від вибору наближення (теорії середнього поля, теорії протікання, наближення Максвелла та інші) для обчислення ефективних значень електропровідності та теплопровідності в

**Ключові слова**: композити, теорія ізоморфізму, ефективні термоелектричні властивості, ефективна термоелектрична добротність.

Надійшла до редакції 24.05.2025