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Study of Thermal Rectification in a Bi-Material with Interfacial Inhomogeneities

Abstract: Thermal rectification is a phenomenon of heat exchange that allows heat to be transferred in one direction to a lesser extent than in the other. The study of this process enables the control of temperature, energy conversion, and the creation of potentially new materials. Studies of the thermal rectification effect using nanofiber compounds are known in the literature, in which the heat flow causes different heat transfer in both directions by changing the operating temperature, and thus, in one direction, the connected structure plays the role of a dielectric, in the other – a conductor. In this article, the phenomenon of thermal rectification is studied based on a model of thermos-elastic behaviour of a bi-material with interfacial inhomogeneities. It is assumed that the interfacial inhomogeneities are filled with some substance and are characterised by a given thermal conductivity coefficient. It is demonstrated that inhomogeneities along the interfacial line of the bi-material result in varying heat transfer depending on the direction of the heat flow and the properties of the bi-material components. The phenomenon of thermal rectification for such a model consists in increasing the difference between the values of effective thermal resistance for two opposite directions of heat flow. It has been established that the lower the thermal conductivity of the inhomogeneities and the greater the density of their location, the more pronounced the phenomenon of thermal rectification becomes.

Keywords: bi-material, interfacial inhomogeneities, thermal conductivity, thermal rectification.

Introduction

Developing novel materials with predictable properties such as thermal conductivity, electrical conductivity, and mechanical compliance is crucial for modern technologies. These properties can be imparted through various methods, including combining different materials, creating geometric and physical surface inhomogeneities, doping, and applying influencing factors like electric and magnetic fields. A key application of such material engineering is in thermal management. For instance, experimental studies on a thin film of vanadium dioxide deposited on a silicon wafer have demonstrated a radiative thermal rectifier (*Ito, K. et al., 2014*). In this system, the operating temperatures are precisely adjusted by doping the film with tungsten.

Thermal rectification is a phenomenon that is often used to regulate the electrical conductivity of a material by changing the temperature. For example, mass-loaded carbon and boron nitride nanotubes exhibit asymmetric axial thermal conductance, with greater heat flow occurring in the direction of decreasing mass density (*Wang et al., 2014*). Similarly, the thermal rectification coefficient is enhanced by increasing the geometric asymmetry in nanostructures such as graphene (*Wang et al., 2017*). To investigate these principles, experimental studies on defect-engineered graphene have utilized focused ion beam methods to create defects with precisely controlled sizes and locations (*Nobakht et al., 2018*). In some materials, this temperature-dependent phenomenon is also coupled with changes in electrical conductivity, offering a potential route for its regulation.

Thermal rectification occurs in bi-material structures in the presence of surface roughness at the material contact points, a thermal potential barrier between the material contacts, and a difference in the temperature dependence of thermal conductivity between different materials at the contact point (*Roberts et al., 2011; Chumak et al., 2012*). Nanoscale bi-material thermal rectification induced by a bi-material interface has been experimentally verified and its underlying mechanism investigated using molecular dynamics simulations (*Ye et al., 2017*). The thermal diode consists of polyamide (PA) and silicon (Si) nanowires in contact with each other. It has been found that temperature has a negligible effect on the rectification coefficient, while decreasing the contact length or increasing the temperature difference can enhance the rectification coefficient. These results are related to the development of solid-state thermal diodes based on the interface. The thermal rectification effect of a solid is demonstrated in the article (*Shrestha et al., 2020*), using the heterogeneous transition of "irradiated-pure" polyethylene from nanofibers using electron irradiation. For irradiated nanofiber samples, it is shown that the heat flux can be rectified by changing the operating temperature, and the average thermal rectification coefficient is significantly higher than the experimental values obtained in previous studies.

However, achieving a large and controllable rectification effect remains a significant challenge, as it requires either a macroscale or a substantial temperature shift, and experimental methods are typically quite expensive. This article proposes a theoretical approach to study the phenomenon of thermal rectification based on a bi-material endowed with interfacial inhomogeneities, which cause the appearance of thermal resistance under the action of a heat flow.

Materials and Methods

Consider the bi-material, which consists of two isotropic materials D_1 and D_2 with different thermomechanical properties. A periodical system crack is located at the bi-material interface (*Figure 1*). The height of the crack is given by $h_0(x)$, the length is $2a$, period of the location of the cracks is d. At infinity, the bi-material is subjected to uniformly distributed tensile and shear forces p, S_1, S_2, respectively, and a stationary homogeneous heat flow q. Under the action of the load the cracks aare opening The resulting height of the gaps will be $h(x)$,. The cracks are filled with a substance that penetrates the crack from the external environment or material by diffusion or filtration. We assume that the crack filler does not resist deformation of the body and is ccharacterisedby a thermal conductivity coefficient λ_c. When heat and force are transferred across a bi-material interface, imperfect thermal contact occurs between faces of the cracks. Outside the cracks, mechanical and thermal contact is ideal.

The heat transfer between the faces of the cracks is modelled by the thermal resistance and the longitudinal thermal conductivity of the filler (*Martynyak & Serednytska, 2017*). The thermal resistance is directly proportional to the thermal conductivity coefficient of the filler and inversely proportional to the height of the gap formed during the loading process. The longitudinal thermal conductivity is equal to the product of the thermal conductivity coefficient of the filler and the height of the crack. We assume that the heat flow between the faces of the cracks in the transverse direction is continuous.

The thermal and mechanical boundary conditions on the crack are as follows:

$x \in (-a+kd, a+kd)$:

$\tau_{xy}^{+}(x) = \tau_{xy}^{-}(x) = 0,\ \sigma_y^{+}(x) = \sigma_y^{-}(x) = 0$

$$\lambda_c h(x) \frac{\sigma^2}{\sigma x^2}\left(T^{-}(x) - T^{+}(x)\right) + 12 {q_y}^{+}(x) - 12 \frac{\lambda_c}{h(x)}\left(T^{-}(x) - T^{+}(x)\right) = 0,\ q_y^{-}(x) = q_y^{+}(x) \quad (1)$$

where the superscript "+" and "–" denote the boundary values of temperature T, normal components of heat flow q_y, normal and tangential stress components τ_{xy} and σ_y on the x-axis in the upper and lower half-plane, respectively.

Using the method of complex potentials (*Chumak et al., 2012*) and contact boundary conditions (1), the formulated problem is reduced to a nonlinear system of singular integrao-differential equations with a Hilbert kernel with respect to functions that have the physical meaning of the temperature jump $\gamma(x)$ between the crack surfaces and the height $h(x)$ of the formed gaps:

$$\frac{1}{d}\int_{-a}^{a} h(t)\, ctg\left(\frac{\pi(t-x)}{d}\right) dt + \frac{\lambda\eta}{2}\left(\gamma(x) - \gamma_{ef}\right) = -\frac{G^*}{2} p + \frac{1}{d}\int_{-a}^{a} h_0'(t)\, ctg\left(\frac{\pi(t-x)}{d}\right) dt,\ h(a) = 0,$$

$|x| < a,$

$$\lambda_c h \gamma''(x) + \frac{6\lambda}{\pi}\int_{-a}^{a} \gamma'(t)\, ctg\left(\frac{\pi(t-x)}{d}\right) dt - \frac{12\lambda_c}{h(x)}\gamma(x) = -12q,\ \gamma(a) = 0,\ |x| < a, \quad (2)$$

where

$\gamma_{ef} = \frac{1}{d}\int_{-a}^{a} \gamma(x)\, dx,\ G^* = \frac{(1-k_1 k)}{G_1(1-k_2)},\ G_1(1-k_2) = G_2(1-k_1),\ k = 3 - 4\upsilon_n,$

$\lambda = \frac{2\lambda_1\lambda_2}{(\lambda_1+\lambda_2)},\ \lambda_2 = \lambda_1,\ \eta = \eta_2 - \eta_1,\ \eta_n = \frac{\alpha_n(1+\upsilon_n)}{\lambda},\ n = 1, 2;\ \upsilon_1, \upsilon_2$ are Poisson's ratios,

G_1, G_2 are shear moduli,

α_1, α_2 are coefficients of linear thermal expansion,

λ_1, λ_2 are thermal conductivities of materials D_1 and D_2.

The resulting system (2) was solved using a modified analytical-numerical procedure (*Serednytska et al. 2019*) based on the methods of collocations and successive approximations.

Effective temperature jump γ_{ef} is determined by the solution of the system (2). The value of the temperature jump γ_{ef} characterises the additional temperature distribution caused by the periodic system of cracks. The effective temperature jump is a function of the heat flow $\gamma_{ef}(q)$.

Effective thermal resistance is a parameter that characterises the interfacial contact thermal resistance of a bi-material and is defined as differentiation of effective temperature jump function with respect heat flow $R_{ef}(q) = \frac{\delta\lambda(q)}{\delta q}$.

The effective temperature jump γ_{ef} and the effective thermal resistance R_{ef} depend on the density and direction of the heat flow.

The phenomenon of thermal rectification consists of increasing the difference between the values of effective thermal resistance for two opposite directions of heat flow.

The direction of the heat flow is determined by the parameter η, which is the difference in thermal distortivity of materials. The coefficient of thermal distortivity of a material $\eta_n (n = 1, 2)$ characterises the curvature of a rectilinear element due to a heat flow q of unit intensity perpendicular to this element. The coefficient of thermal distortivity is determined by the thermomechanical properties of the material. It is believed that if the difference in thermal distortions is positive $\eta > 0$, then the heat flow is directed to the material with a greater thermal distortivity. If the difference in thermal distortivity is negative $\eta < 0$, then the heat flow is directed to the material with a lower thermal distortivity.

The thermal rectification parameter δ determines the relative error between two values of effective thermal resistance R_{ef}^{+} and R_{ef}^{-} for two cases of heat flow direction towards the material with greater thermal distortivity and towards the material with less thermal distortivity, respectively $\delta = \left|\frac{R_{ef}^{+} - R_{ef}^{-}}{R_{ef}^{+}}\right| \times 100\%$.

Thus, to assess the phenomenon of thermal rectification, it is sufficient to analyse the change in the parameter δ. The larger the parameter δ, the greater the thermal rectification of the bi-material.

Results

The main results of the thermal rectification study are illustrated in the appendix (*Figure 2*; *Figure 3*; *Figure 4*; *Figure 5*; *Figure 6*). Based on the solution of system (2), the value of the effective thermal resistance for the considered bi-material was determined. The difference between the values of the thermal resistance for the two directions of the heat flow was analysed.

Numerical calculations were performed for a bi-material characterized by the following dimensionless quantities:

$$\bar{x} = \frac{x}{d},\ \bar{a} = \frac{a}{d},\ \overline{h_0} = \frac{h_0}{d},\ \bar{q} = qd\eta,\ \bar{p} = pG^*,\ \bar{\lambda}_c = \frac{\lambda_c}{\lambda},\ \bar{\gamma}_{ef} = \gamma_{ef}\lambda\eta,\ \bar{R}_{ef} = \frac{R_{ef}d}{\lambda},\ \bar{k}_t = 2\bar{a},$$

$$\bar{\delta} = \left|\frac{R_{ef}^{+} - R_{ef}^{-}}{R_{ef}^{+}}\right| \times 100\%,\ \bar{h}_0(\bar{x}) = 0.001(1 - \bar{x}^2)^{3/2}.$$

The change in the effective thermal resistance of the bi-material $\bar{R}_{ef}$ depending on the direction and density of the heat flow $\bar{q}$ for different fixed values of the forces $\bar{p}$, the coefficient of thermal conductivity $\bar{\lambda}_c$ and the coefficient of interface heterogeneity $\bar{k}_t$. Note that the coefficient of interface heterogeneity $\bar{k}_t$ determines the density of the cracks' location. The larger the value of the coefficient $\bar{k}_t$, the more densely the cracks are located, the smaller the value $\bar{k}_t$, the further the cracks are from each other. The direction of the heat flow depends on the value $\bar{q}$: if $\bar{q} > 0$, then the heat flow is directed to the material with greater thermal distortivity, if $\bar{q} < 0$, then the heat flux is directed to the material with less thermal distortivity. The dependence of the thermal rectification parameter on the heat flow is determined by the relative error between the values of the dimensionless effective thermal resistance for the two directions of the heat flow. Figure 2 shows the dependence of the effective thermal resistance $\bar{R}_{ef}$ on the heat flow $\bar{q}$ for different values of the thermal conductivity $\bar{\lambda}_c$ (*Figure 2*). It can be seen that with increasing heat flow density, thermal resistance increases in the case of a flow directed to a material with greater thermal distortivity and decreases in the case of a flow directed to a material with less thermal distortivity. An increase in the thermal conductivity $\bar{\lambda}_c$ leads to a decrease in thermal resistance $\bar{R}_{ef}$. The effect of tensile forces on the change in effective thermal resistance $\bar{R}_{ef}$ is proportional to the intensity of the forces $\bar{p}$ (*Figure 3*). Thermal resistance $\bar{R}_{ef}$ increases with increasing the forces $\bar{p}$ for both directions of the heat flow. With increasing $\bar{k}_t$, the effective thermal resistance $\bar{R}_{ef}$ increases and the difference between the values of the thermal resistance for two opposite directions of the heat flow increases (*Figure 4*). The effective thermal resistance acquires greater values in the case of a flow directed to a material with greater thermal distortivity.

A nonlinear dependence of the thermal rectification parameter $\bar{\delta}$ on the heat flow density $|\bar{q}|$ was found (*Figure 5*) for different values of the thermal conductivity of the crack filler $\bar{\lambda}_c$. An increase in the heat flux density leads to an increase in the thermal rectification parameter. With an increase in thermal conductivity $\bar{\lambda}_c$, the value of the parameter $\bar{\delta}$ decreases, which means a decrease in thermal rectification. The thermal rectification parameter simultaneously increases with an increase in the density of the gaps and a decrease in the intensity of tensile forces (*Figure 6*). The dependence of thermal rectification on the density of the cracks' location, which indicates a different thermal distortivity of the bi-material depending on the number of cracks located along a unit length of the interface.

Therefore, an increase in the values of the effective thermal resistance and the thermal rectification parameter of the bi-material manifests itself with an increase in the heat flow density and a decrease in the resistance to heat transfer through the interface. Accordingly, the ability of the interface to transmit heat is characterised by the presence of inhomogeneities such as cracks, their density of location, and the thermal conductivity of the substance that fills them.

Discussion

The phenomenon of thermal rectification demonstrates how, by altering the temperature, it is possible to control the electrical conductivity of materials. Alternatively, by adjusting the dimensions and geometry of the material structure, it is also possible to achieve the desired heat transfer. This effect can be used in engineering developments to create new devices or materials that can convert thermal energy into valuable electrical energy. Experimental studies on various types of nanostructured materials enable us to gradually increase the thermal distortion parameter, confirming the effect itself and refining existing methods for converting thermal motion into directed current. Theoretical approaches to studying the phenomenon of thermal rectification can facilitate the development of a mathematical model for a device based on a material with controllable properties, such as thermal conductivity and electrical conductivity. Therefore, theoretical studies of thermal rectification for bi-materials can logically be continued for electrically conductive interface inhomogeneities and piezoelectric bi-materials.

Conclusion

The phenomenon of thermal rectification is studied based on a model of a bi-material consisting of components characterised by different thermomechanical properties, and at the interface of which there is a periodic system of heat-conducting inhomogeneities, such as cracks.

Interface inhomogeneities introduce an additional temperature difference, resulting in a change in thermal resistance during heat transfer through the interface, which depends on the direction of the heat flow. The problem of thermoelasticity for a bi-material with interfacial cracks is reduced to a system of nonlinear singular integro-differential equations concerning the functions of crack opening and the temperature jump between their surfaces. Using analytical-numerical methods for solving such systems, the additional temperature distribution as a function of the heat flow, as well as the effective interfacial thermal resistance, are determined. The thermal rectification parameter is analysed based on the values of the effective thermal resistance determined for two opposite directions of the heat flow. It is shown that changing the direction of the heat flow leads to qualitatively different values of thermal resistance, and the difference between these values increases with increasing heat flow and significantly depends on the thermal conductivity of the crack filler and the parameter characterising the density of the crack location, as well as on the influence of the force load. The thermal rectification parameter determines the relative error in percentage between the values of the effective thermal resistance for two opposite directions of the heat flow and increases with increasing flow. Thus, the phenomenon of thermal rectification in a bi-material with different coefficients of thermal distortivity of its components is manifested to a greater extent at high values of the heat flow density, low thermal conductivity of the interface and low intensity of tensile forces. The results obtained show a qualitative change in the thermal rectification parameter and can be used as a model for engineering calculations.

Conflict of interest

The author declares that there is no conflict of interest.

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Appendix

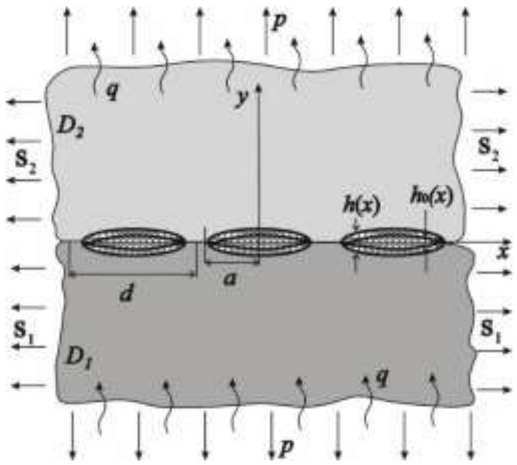

Figure 1. Shema of bi-material

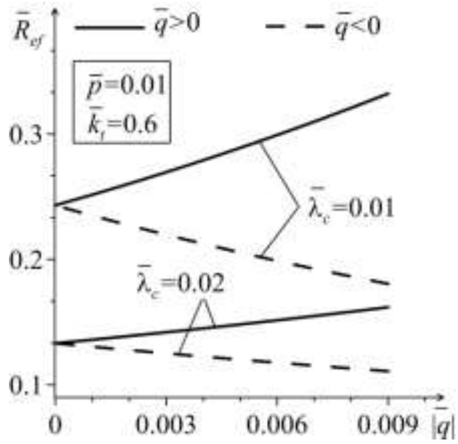

Figure 2. Dependencies of the thermal resistance $\bar{R}_{ef}$ on the heat flow $\bar{q}$ for different values of the thermal conductivity $\bar{\lambda}_c$.

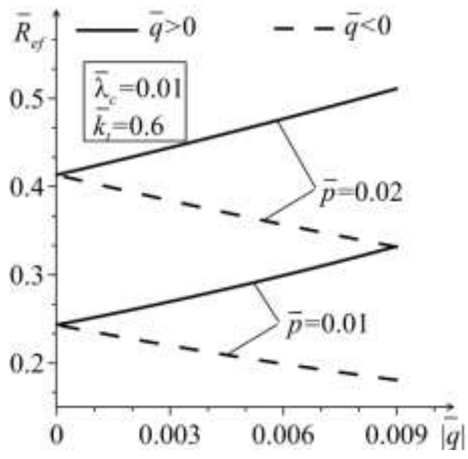

Figure 3. Dependencies of the thermal resistance $\bar{R}_{ef}$ on the heat flow $\bar{q}$ for different values of the intensity of forces $\bar{p}$.

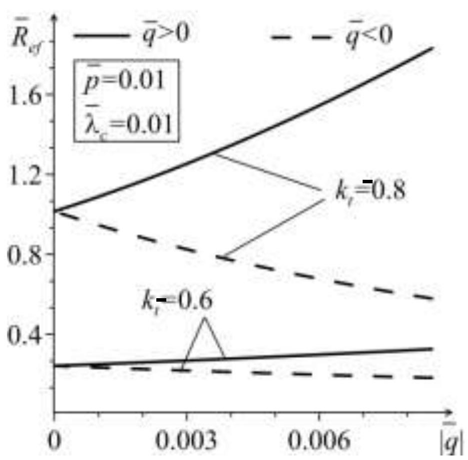

Figure 4. Dependencies of the thermal resistance $\bar{R}_{ef}$ on the heat flow $\bar{q}$ for different values of parameter $\bar{k}_t$.

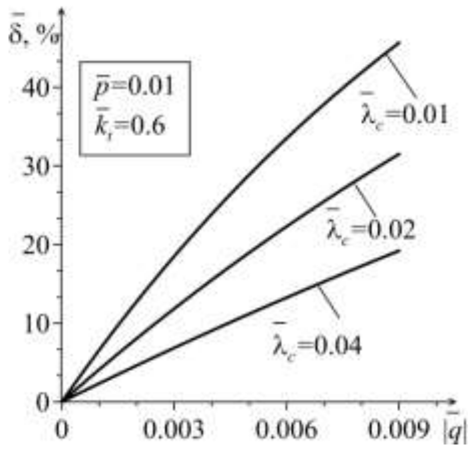

Figure 5. Dependencies of parameter of thermal rectification $\bar{\delta}$ on the heat flow density $|\bar{q}|$ for different values of the thermal conductivity $\bar{\lambda}_c$.

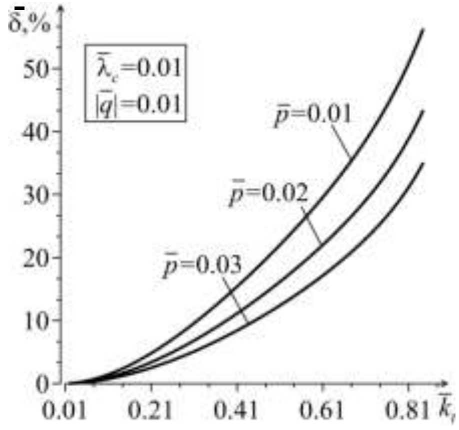

Figure 6. Dependencies of parameter of thermal rectification $\bar{\delta}$ on the coefficient of interface heterogeneity $\bar{k}_t$ for different values of the intensity of forces $\bar{p}$.