

Article

Finite Element Analysis of Hybrid Piezo- and Pyroelectric Energy Harvesting

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Abstract

Pyropiezoelectric energy harvesting has the potential to utilize both environmental vibrations and time-dependent temperature changes to increase the amount of energy harvested compared to harvesting from only one of the two sources. So far, the investigation of such hybrid energy harvesting approaches has mainly been experimental. This makes it difficult to distinguish between their individual physical effects and complicates the optimization of such harvesters. This work presents a numerical framework for solving transient coupled pyropiezoelectric equations using the finite element method. The numerical method can be applied to simulate hybrid energy harvesters by taking into account external electrical circuits. The numerical simulations enable a targeted analysis of the contributions of mechanical, electrical and thermal effects to the harvested energy. This is illustrated by various numerical examples, such as a simple piezoelectric cuboid, a unimorph, a bimorph and a bimetallic beam with a piezoelectric patch. These are subjected to oscillating deformations and/or temperature changes. The simulations calculate the harvested energy resulting from the individual physical effects, depending on the excitation frequency, the external resistance, and the geometric configuration of the harvester. For a bimetallic beam with a piezoelectric patch, which is used as a low frequency hybrid energy harvester, a geometric optimization based on the simulation results showed a possible increase in the harvested energy of up to 386% under idealized circuit conditions compared to the initial design from the literature.

Keywords: hybrid energy harvesting; finite element method; coupled simulation; pyropiezoelectricity



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1. Introduction

The increasing importance of microelectromechanical systems (MEMS) in the context of digitalization and the Internet of Things (IoT) has created a need for reliable, maintenance-free and sustainable energy sources [1,2]. Batteries are often used for power, but have a significant environmental impact when disposed of and limits in their possible applications. Replacement, maintenance, malfunction, etc., can lead, for example, to production downtime and thus, additional production costs [3].

Piezoelectric MEMS, with their high energy density, ref. [4] are a promising candidate to reduce the number of batteries needed by harvesting ambient vibrations and converting them into electrical energy via the piezoelectric effect [5]. Typically, a basic piezoelectric structure is excited near one of its eigenfrequencies and the electrical energy is extracted using a circuit connected via electrodes. The circuit has the task of rectifying, conditioning and storing the electrical energy generated by the piezoelectric structure. A comprehensive

review on the state of the art of piezoelectric energy harvesting can be found, for example, in the cited review articles [6–11]. Possible application examples can be found, e.g., in [12–14].

In order to increase the amount of energy harvested, it is possible to use other effects in addition to the piezoelectric effect. Shaukat et al. [15] and Liu et al. [16] provide an overview of different types of such hybrid energy harvesting approaches. One possibility is to also use ambient temperature fluctuations and thus exploit the pyroelectric effect [17]. From a materials science perspective, 32 crystal classes or crystallographic point groups can be distinguished [18,19], 10 of which exhibit both piezoelectric and pyroelectric behavior [20] (p. 63) and are therefore suitable for hybrid pyropiezoelectric energy harvesting. Bai et al. [21] explain that it is crucial for such harvesting devices that the two energy conversion effects do not conflict. Nevertheless, there is only a very limited number of publications to date that have investigated the combination of both effects in the context of energy harvesting.

Experimentally, Chen et al. [22] describe a fabricated nanogenerator (NG) based on a (PVDF-TrFE) nanowire array. It showed an increased output voltage under combined periodic bending and thermal radiation. Ko et al. [23] investigated the harvesting behavior of a PZT-based NG mounted on the exhaust pipe of a car. A high current output was observed under normal working conditions. Lee et al. [24] describe a highly stretchable pyropiezoelectric NG. By applying a line-based micropattern, the stretchability and robustness of the device could be further increased. In Yamamoto et al. [25], the current and voltage curves of a stainless steel beam to which a BCZT50 sample is attached are investigated. They show an increased integrated voltage output for pyropiezoelectric harvesting compared to the pure piezoelectric case for certain resistances. Kang and Yeatman [26,27] describe an experimental setup for pyropiezoelectric energy harvesting with a heat source attached to a slider oscillating at low frequencies (0.02 Hz to 0.1 Hz) under a bimetallic beam. A decisive influence of the phase shift between the pyroelectric and piezoelectric effect on the output power of the energy harvester is reported.

Physical models are often based on simplified analytical solutions or use equivalent circuit models or finite element simulations to predict the behavior of energy harvesting structures. Usually, beam-like structures, such as unimorphs, bimorphs or multimorphs, are investigated for the pure piezoelectric case [11]. The piezoelectric analytical solutions of Erturk and Inman [28–30] for serial and parallel unimorphs and bimorphs, for example, are based on the Euler–Bernoulli beam theory and predict the steady-state response for harmonic excitation at arbitrary frequencies quite well. Their approach is still used in more recent literature, see, for example, [31,32]. Recently, Hegendörfer et al. investigated in a series of publications [33–35] the piezoelectric energy harvesting behavior for various base excitations and electrical circuits by means of the finite element method (FEM). Electrical circuits are incorporated via appropriate boundary conditions or by coupling to an electronic circuit simulation method [36]. Martins et al. [37,38] used the FEM as part of the uncertainty optimization of an energy harvesting device with imperfect clamping. An overview of the various approaches to simulating piezoelectric energy harvesting devices is provided by Gedeon et al. [39]. Simulations including thermal or pyroelectric effects by adding a thermal field usually focus only on the pyropiezoelectric structure, without an external electric circuit attached, and are thus typically outside the scope of energy harvesting. For example, Toledo et al. [40,41] studied the effect of temperature-dependent material properties. In addition to the pyroelectric effect, they took into account the temperature dependency of the piezoelectric strain coefficients for a multimorph, with the example of a stratospheric balloon. Their custom simulation framework was validated using an analytical solution for a two-dimensional laminate configuration from Tauchert [42], which is also explained in detail in the work from Görnant and Gabbert [43]. Häusler et al. [44]

and Milde et al. [45] examine pyroelectric sensor arrays in their works by using a staggered simulation scheme. In a preliminary thermal analysis, the temperature distribution in space and time is calculated and used as input for subsequent electromechanical analysis. Herth et al. [46] investigate numerically and experimentally the design and performance of hybrid thermopiezoelectric U-shaped cantilevers in connection with microactuators. They also predict potential for applications in the field of vibration energy harvesting.

Since piezoelectric and pyroelectric effects not only add up but can also interfere with each other, it is necessary to be able to distinguish between advantageous and disadvantageous combinations in order to increase the energy harvested. Understanding the complex coupling of physical effects and their impacts on the energy harvested is important for designing and optimizing hybrid harvesters. Numerical analysis offers the possibility of separating individual effects that influence each other, which is often impossible or very difficult to achieve in experimental setups. However, there is a lack of these kinds of fully coupled transient system simulations of energy harvesting structures that take into account piezoelectric and pyroelectric effects and compute the resulting energy output. This work aims to close this gap. The novelties of this work are therefore as follows:

- Consideration of thermal influences in a finite element energy-harvesting simulation together with a connected external circuit.
- Calculation of the pyropiezoelectric energy output with an analysis of the different contributions to it.

First, in Section 2, the theoretical background for solving the equations of linear pyropiezoelectricity together with an attached external electric circuit is discussed. Second, the influence of piezo- and pyroelectric effects on the resulting voltage and current is explained schematically by means of a cuboid under pressure and temperature oscillations attached to a resistor. The main chapters of the work follow with an investigation of the impact of present temperature gradients on two typical energy harvesting structures, a unimorph and bimorph, in series connection with a single resistor. Finally, the harvesting structure of Kang and Yeatman [27] is investigated in more detail to study an application under a low-frequency condition. All the presented results are obtained using a custom FEM C++ code using the open source library *deal.ii* [47,48]. *DeepL* [49] was used to assist with the translation into English and to improve sentence structure during the writing and editing process.

2. Theoretical Background

In order to model the small-signal behavior of a pyropiezoelectric body $\mathcal{B}$ together with its temperature distribution, the mechanical, electrical and thermal fields and their coupling must be specified. The complete set of differential equations was first derived by Mindlin [50] and can also be found in more recent literature, see, e.g., [51] (p. 210) or [52] (p. 3888). Nowacki [53,54] derived a uniqueness and reciprocity theorem for this set of equations. A comprehensive overview and further information on variational principles in the field of thermopiezoelectricity and beyond is given by Altay et al. [55].

2.1. Equations of Linear Pyropiezoelectricity

The complete set of pyropiezoelectric differential equations can be divided into gradient, balance and constitutive equations, which must be solved for the unknown displacement u_i , the electric potential φ and the temperature change $\theta = T - T_0$ as the difference between the current temperature T and an arbitrary reference temperature T_0 under the assumption $|\theta| \ll T_0$. Here, index notation is used together with the summation convention for repeated indices, following the *IEEE Standard on Piezoelectricity* [56]. The partial

derivative $\frac{\partial \{\bullet\}_i}{\partial x_j}$ of the i -th component of a vector-valued quantity $\{\bullet\}$ with respect to the spatial coordinate x_j is written as $\{\bullet\}_{i,j}$.

The linear mechanical strain tensor ε_{ij} , the electric field E_i and the heat flux q_i are defined by means of the gradients of the unknown displacements u_i , electric potential φ and temperature change θ as

$$\varepsilon_{ij} = \frac{1}{2} [u_{i,j} + u_{j,i}] \quad (1)$$

$$E_i = -\varphi_{,i} \quad (2)$$

$$q_i = -k_{ij}\theta_{,j} \quad (3)$$

where Equation (3) is *Fourier's law of heat conduction* with the symmetric heat conduction tensor k_{ij} . The balance equations

$$\rho \ddot{u}_i - \sigma_{ij,j} = 0 \quad (4)$$

$$D_{i,i} = 0 \quad (5)$$

$$T_0 \dot{S} + q_{i,i} = 0 \quad (6)$$

with density ρ , mechanical stress tensor σ_{ij} , electric displacement D_i and entropy density S are independent of the material behavior. The first and second derivatives with respect to time t are denoted by overdots. Equations (4)–(6) are the *balance of linear momentum* in absence of body forces, *Gauss's law* without free electric charges and the *balance of energy*. In order to model the material behavior and the coupling between the different fields, a set of constitutive equations is required, which can be derived from the electric Gibbs potential $\mathcal{G}$ [52] (p. 3900), in the form

$$\mathcal{G} = \frac{1}{2} C_{ijkl}^{\varepsilon, \theta} \varepsilon_{ij} \varepsilon_{kl} - \frac{1}{2} \epsilon_{ij}^{\varepsilon, \theta} E_i E_j - \frac{1}{2} \frac{\rho c_v^{\varepsilon, \theta}}{T_0} \theta^2 - e_{ijk}^{\theta} E_i \varepsilon_{jk} - p_i^{\varepsilon} \theta E_i - \lambda_{ij}^{\varepsilon} \varepsilon_{ij} \theta \quad (7)$$

with the elasticity tensor at constant electric field and temperature $C_{ijkl}^{\varepsilon, \theta}$, the electric permittivity tensor at constant strain and temperature $\epsilon_{ij}^{\varepsilon, \theta}$, the specific heat at constant strain and electric field $c_v^{\varepsilon, \theta}$, the piezoelectric coupling tensor at constant temperature e_{ijk}^{θ} , the pyroelectric coupling tensor at constant strain p_i^{ε} and the thermal stress tensor at constant electric field $\lambda_{ij}^{\varepsilon}$. To improve readability, the superscripts of the constant physical quantities (ε , E , θ) are omitted in the following. The assumption of linear material behavior made here is justified as long as the excitation amplitudes do not cause geometric or material nonlinearities [39]. The constitutive equations for the mechanical stress σ_{ij} , the electric displacement D_i and the entropy density S are calculated from Gibbs potential (7) as

$$\sigma_{ij} = \frac{\partial \mathcal{G}}{\partial \varepsilon_{ij}} = C_{ijkl} \varepsilon_{kl} - e_{kij} E_k - \lambda_{ij} \theta \quad (8)$$

$$D_i = -\frac{\partial \mathcal{G}}{\partial E_i} = e_{ijk} \varepsilon_{jk} + \epsilon_{ij} E_j + p_i \theta \quad (9)$$

$$S = -\frac{\partial \mathcal{G}}{\partial \theta} = \lambda_{ij} \varepsilon_{ij} + p_i E_i + \frac{\rho c_v}{T_0} \theta \quad (10)$$

with the independent variables strain ε_{ij} , electric field E_i and temperature change θ . Equations (8)–(10) are the so-called *e-form* of the constitutive equations. Different thermodynamic potentials with other independent variables are possible; an overview is given by Hetnarski [52] (p. 3896), for example. A graphical representation of their relationship in the form of the *Heckmann diagram* [57] can be found in the book from Rupitsch [20] (p. 48).

From an experimental point of view, it is generally more practical to measure the piezoelectric coupling coefficients d_{ijk} instead of e_{ijk} and the thermal expansion coefficients α_{ij} instead of λ_{ij} . The material parameters of the *e-form* can be derived using the conversions

$$e_{kij} = d_{klm} C_{lmij} \quad (11)$$

$$\lambda_{ij} = C_{ijkl} \alpha_{kl} . \quad (12)$$

Equations (1)–(3), (4)–(6) and (8)–(10) can be solved on a body $\mathcal{B}$ if appropriate boundary and initial conditions are prescribed. The surface of the body $\partial\mathcal{B}$ is divided into subsurfaces where either Dirichlet or Neumann boundary conditions (subscripts D and N) are prescribed as

$$u_i = \bar{u}_i \quad \text{on } \partial\mathcal{B}_D^u \quad \text{and} \quad \sigma_{ij} n_j = \bar{t}_i \quad \text{on } \partial\mathcal{B}_N^u , \quad (13)$$

$$\varphi = \bar{\varphi} \quad \text{on } \partial\mathcal{B}_D^\varphi \quad \text{and} \quad D_i n_i = -\bar{\sigma}_f \quad \text{on } \partial\mathcal{B}_N^\varphi , \quad (14)$$

$$\theta = \bar{\theta} \quad \text{on } \partial\mathcal{B}_D^\theta \quad \text{and} \quad q_i n_i = -\bar{q} \quad \text{on } \partial\mathcal{B}_N^\theta , \quad (15)$$

with introduction of the outward unit normal vector n_i , the prescribed surface tractions $\bar{t}_i$, the prescribed free surface charge density $\bar{\sigma}_f$ and the prescribed scalar heat flux $\bar{q}$, such that $\partial\mathcal{B} = \partial\mathcal{B}_D^u \cup \partial\mathcal{B}_N^u = \partial\mathcal{B}_D^\varphi \cup \partial\mathcal{B}_N^\varphi = \partial\mathcal{B}_D^\theta \cup \partial\mathcal{B}_N^\theta$ and $\partial\mathcal{B}_D^u \cap \partial\mathcal{B}_N^u = \partial\mathcal{B}_D^\varphi \cap \partial\mathcal{B}_N^\varphi = \partial\mathcal{B}_D^\theta \cap \partial\mathcal{B}_N^\theta = \emptyset$. The initial conditions

$$u_i(x_i, t_0) = u_i^0 , \quad \dot{u}_i(x_i, t_0) = \dot{u}_i^0 \quad \text{and} \quad \theta(x_i, t_0) = \theta^0 \quad (16)$$

are necessary to complete the initial boundary value problem, which we want to solve for the unknown solution variables u_i , φ and θ .

For the numerical solution of the coupled problem with the finite element method, we derive the weak forms by multiplying Equations (4)–(6) with scalar or vector-valued test functions, integrating them over the entire body $\mathcal{B}$ and applying partial integration and the divergence theorem [58] (p. 80). Using a vector-valued test function η_i for the mechanical field and scalar-valued test functions ζ and ψ for the electrical and thermal field, the weak forms result as

$$\int_{\mathcal{B}} \rho \eta_i \ddot{u}_i dV + \int_{\mathcal{B}} \eta_{i,j} \sigma_{ij} dV = \int_{\partial\mathcal{B}_N^u} \eta_i \bar{t}_i dA \quad (17)$$

$$\int_{\mathcal{B}} \zeta_{,i} D_i dV = - \int_{\partial\mathcal{B}_N^\varphi} \zeta \bar{\sigma}_f dA \quad (18)$$

$$\int_{\mathcal{B}} \psi T_0 \dot{S} dV - \int_{\mathcal{B}} \psi_{,i} q_i dV = \int_{\partial\mathcal{B}_N^\theta} \psi \bar{q} dA . \quad (19)$$

To solve the continuous Equations (17)–(19), their discretization in time and space is necessary. In the following, the derivations to obtain the discretized equations are given in condensed form. For a more detailed description please refer to Appendix A.

2.2. Discretization in Time and Space

The discretization of the weak forms (17) to (19) results in the semi-discrete equations in matrix format

$$\begin{bmatrix} \mathbf{M}_{uu} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} \cdot \begin{bmatrix} \ddot{\mathbf{u}} \\ \ddot{\varphi} \\ \ddot{\theta} \end{bmatrix} + \begin{bmatrix} \mathbf{D}_{uu} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{D}_{\theta u} & \mathbf{D}_{\theta \varphi} & \mathbf{D}_{\theta \theta} \end{bmatrix} \cdot \begin{bmatrix} \dot{\mathbf{u}} \\ \dot{\varphi} \\ \dot{\theta} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\varphi} & \mathbf{K}_{u\theta} \\ \mathbf{K}_{\varphi u} & \mathbf{K}_{\varphi\varphi} & \mathbf{K}_{\varphi\theta} \\ \mathbf{0} & \mathbf{0} & \mathbf{K}_{\theta\theta} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{u} \\ \varphi \\ \theta \end{bmatrix} = \begin{bmatrix} \mathbf{F}_u \\ \mathbf{F}_\varphi \\ \mathbf{F}_\theta \end{bmatrix} . \quad (20)$$

The submatrix D_{uu} was introduced to account for Rayleigh-type damping with

$$D_{uu} = \alpha_R M_{uu} + \beta_R K_{uu} \quad (21)$$

where the Rayleigh parameters α_R and β_R describe the frequency-dependent Lehr's damping ratio $D_i = \frac{1}{2} \left(\frac{\alpha_R}{\omega_i} + \beta_R \omega_i \right)$.

Harvesting energy from a pyroelectric structure requires the integration of an electrical circuit, which has the function of rectifying, conditioning, and storing the electrical energy generated. Usually, the circuit is connected to two electrodes, one of which is grounded. The grounded electrode is modeled by setting the electric potential φ^G on ∂B_0 to zero; see Figure 1. The electrical potential φ^N of all electrical degrees of freedom N on the nongrounded electrode ∂B_{el} is set to the same value φ_{el} . This value is not known a priori, but is determined by the simulation in each time step. The coupling between the finite element structure and the electric circuit is then realized by means of the electric potential φ_{el} and the electric current $\dot{Q}_{el}$, as indicated in Figure 1.

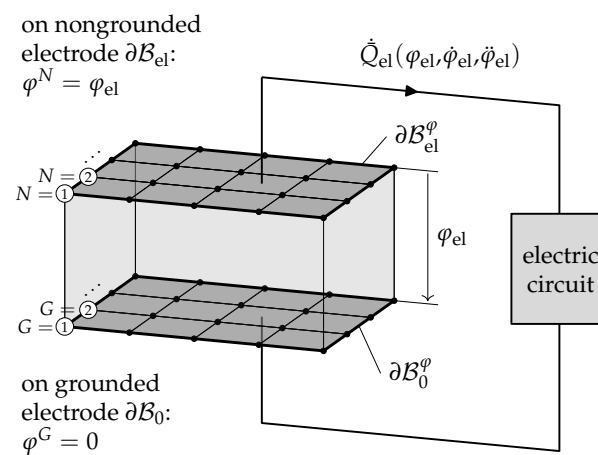


Figure 1. Exemplary attachment of an electric circuit to a cubic example geometry with a grounded and nongrounded electrode ∂B_0^{φ} and $\partial B_{el}^{\varphi}$.

The relationship between the two variables is on the one hand determined by the piezoelectric structure but on the other hand simultaneously by the electric circuit in the form of a differential equation

$$\dot{Q}_{el} = \dot{Q}_{el}(\varphi_{el}, \dot{\varphi}_{el}, \ddot{\varphi}_{el}) . \quad (22)$$

This relation is included in the FE simulation as a mixed boundary condition that defines the relationship between $\dot{F}_{\varphi}$ and the electric potential φ_{el} at the electrode. If the electric circuit consists, e.g., of a simple resistor with resistance R , relation (22) becomes

$$\dot{Q}_{el} = \frac{1}{R} \varphi_{el} . \quad (23)$$

Since this relation is defined for $\dot{F}_{\varphi}$, it can more easily be incorporated into the FE simulation by taking the time derivative of the electrical part in Equation (20) [34,59]. The matrix formulation with an incorporated electric circuit can then be written in a condensed form as

$$M\ddot{x} + D\dot{x} + Kx = F . \quad (24)$$

Since the numerical solution of the transient Equation (24) requires its discretization in time, in the following, the Bossak–Newmark integration scheme [60] is used. It solves Equation (24) at time t_{n+1} coming from a previous known time step t_n by

$$\mathbf{M}[(1 + \alpha_B)\ddot{\mathbf{x}}_{n+1} - \alpha_B\ddot{\mathbf{x}}_n] + \mathbf{D}\dot{\mathbf{x}}_{n+1} + \mathbf{K}\mathbf{x}_{n+1} = \mathbf{F}_{n+1}. \quad (25)$$

The introduced Bossak parameter α_B can be chosen as $\alpha_B \in [0, 1]$. In the following we will set $\alpha_B = 0.5$ to introduce slight numerical damping, which stabilizes the numerical method while keeping the error through artificial damping low; see also [61]. After the solution of one time step, the harvested energy in this time step can be calculated as

$$\mathcal{E}_{n+1} = \mathcal{E}_n + \int_{t_n}^{t_{n+1}} \mathcal{P} dt = \mathcal{E}_n + \int_{t_n}^{t_{n+1}} \varphi_{el} \dot{Q}_{el} dt \quad (26)$$

which is numerically evaluated by means of the backward Euler method.

To verify the custom C++ code that implements the equations mentioned, the benchmark problem from Tauchert [42] and Görnandt and Gabbert [43] was analyzed, and the results were compared. All results are explained in detail in Appendix B and demonstrate excellent agreement between the custom code and the results from the literature, thereby confirming the correctness of the developed numerical method.

3. Voltage and Current for a Simple Cuboid

To better understand the combination of the piezoelectric and pyroelectric effects together with a connected external resistor, a pyropiezoelectric cuboid under oscillating pressure and temperature is considered. The attachment of an external resistor is particularly important for measurements in which the open-circuit voltage is to be determined, as has already been highlighted by Su et al. [62] and Li et al. [63]. There the resistance represents the internal resistance of the voltmeter used.

The geometry and the boundary conditions are specified in Figure 2a. Electrodes $\partial\mathcal{B}_{el}$ and $\partial\mathcal{B}_0$ are placed on the top and bottom of the cuboid and are connected to a resistance R . Prescribed displacement $\bar{u}_z(t)$ and temperature $\bar{\theta}(t)$, whose time curves are shown in Figure 2b,c, are applied on the top surface. The bottom face of the cube is fixed and grounded ($u_z = 0$, $\varphi = 0$, $\theta = 0$), such that a quasi-one-dimensional problem with constant strains, stresses, electric field and electric displacement results. The maxima and minima of the prescribed loading are chosen so that the resulting electrical potential φ_{el} for piezoelectricity and pyroelectricity alone is of the same order of magnitude as for PZT-5H; see Table A3 in Appendix C. Depending on whether only $\bar{u}_z(t)$, only $\bar{\theta}(t)$, or both are applied, pure piezoelectric, pure pyroelectric, or pyropiezoelectric simulations are performed. In the following, the height h is set equal to the width/length a or to $\frac{1}{10}a$ in order to show geometric influences due to heat conduction. The resistance R takes values between $R = 10^{13} \Omega$ (close to open circuit), $R = 10^{10} \Omega$ and $R = 1 \Omega$ (close to closed circuit). For simplicity, damping effects are neglected ($\alpha_R = 0$, $\beta_R = 0$).

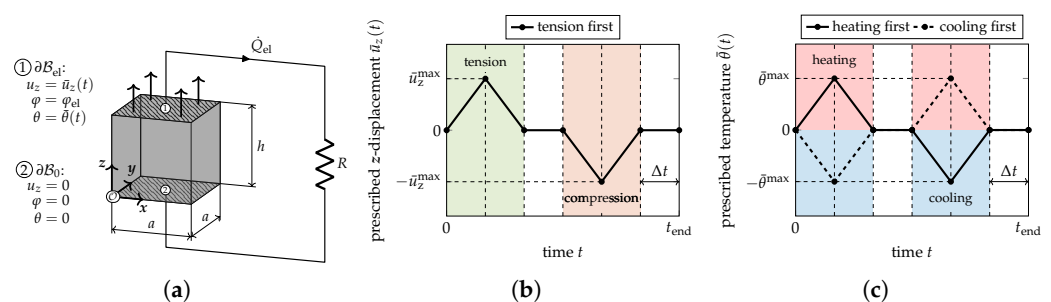
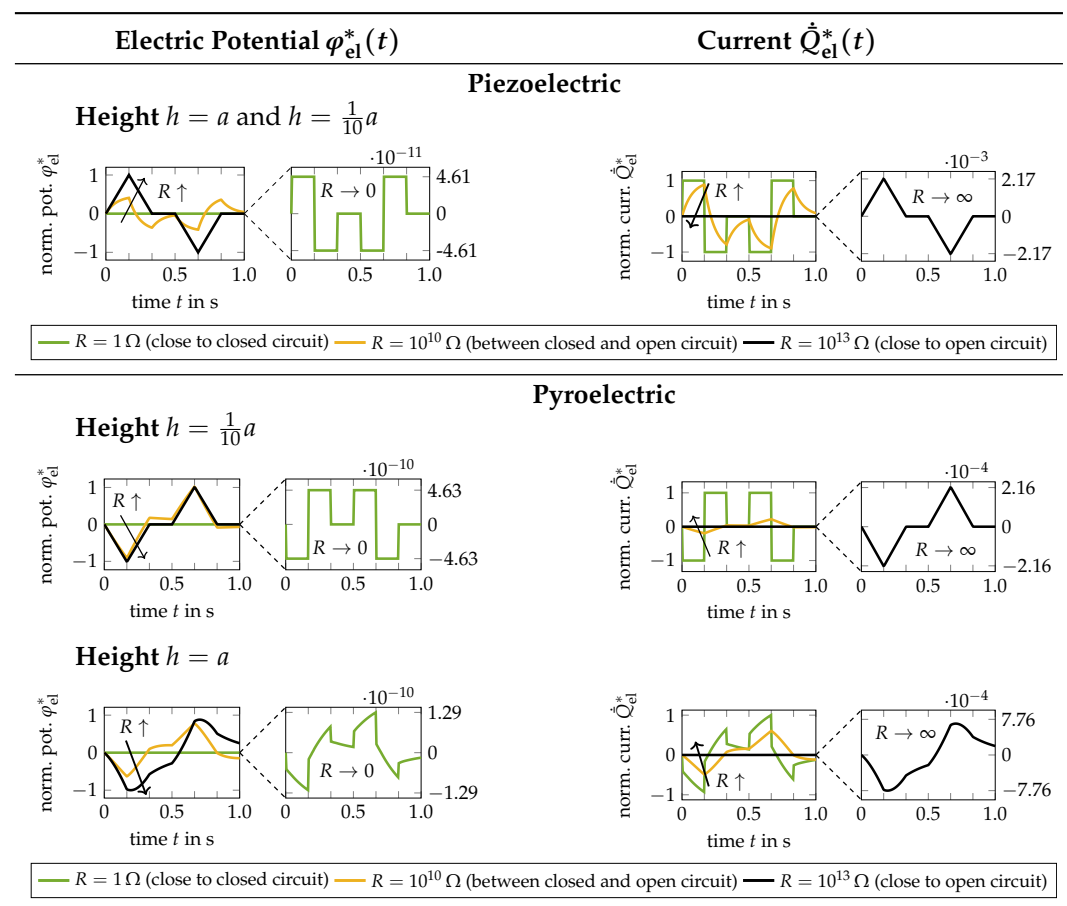


Figure 2. Geometry and boundary conditions of the cuboid: (a) Geometry of the cuboid. (b) Displacement input $\bar{u}_z(t)$ over time t on the top electrode $\partial\mathcal{B}_{el}$. (c) Temperature input $\bar{\theta}(t)$ over time t on the top electrode $\partial\mathcal{B}_{el}$.

3.1. Piezoelectric Results

The normalized results for the piezoelectric simulations are shown in the upper part of Table 1. For all results in this chapter, normalization was performed based on the maximum value of each variable for the three resistance values investigated. Close to open circuit ($R = 10^{13} \Omega$, black lines), the normalized electric potential φ_{el}^* has the same triangular shape as the displacement input, so that $\varphi_{el}^*(t) \propto \bar{u}_z(t)$. Tensile stress results in a positive voltage φ_{el}^* due to the positive value of the piezoelectric parameter d_{33} . The normalized current $\dot{Q}_{el}^*$ exhibits the same proportionality $\dot{Q}_{el}^*(t) \propto \dot{\bar{u}}_z(t)$, but the absolute values of $\dot{Q}_{el}^* \approx 0$ since the resistance is large and $\dot{Q}_{el} = \varphi_{el}/R$. Close to closed circuit ($R = 1 \Omega$, green lines), the electric potential and current now have a rectangular shape and are therefore proportional to the time derivative of the prescribed displacement $\varphi_{el}^*(t) \propto \dot{\bar{u}}_z(t)$ and $\dot{Q}_{el}^*(t) \propto \ddot{\bar{u}}_z(t)$, respectively. The electrical potential $\varphi_{el}^* \approx 0$ since the resistance is small and $\varphi_{el} = \dot{Q}_{el}R$. If a resistance value between open and closed circuit (here $R = 10^{10} \Omega$, yellow lines) is prescribed, a mixture of the two limiting cases results. Regardless of the resistance used, the values of φ_{el}^* and $\dot{Q}_{el}^*$ remain the same when two different heights $h = a$ and $h = \frac{1}{10}a$ are used.

Table 1. Normalized electric potential $\varphi_{el}^*(t)$ and normalized electric current $\dot{Q}_{el}^*(t)$ of the cuboid for the piezoelectric and pyroelectric cases for different resistances R and heights h .



3.2. Pyroelectric Results

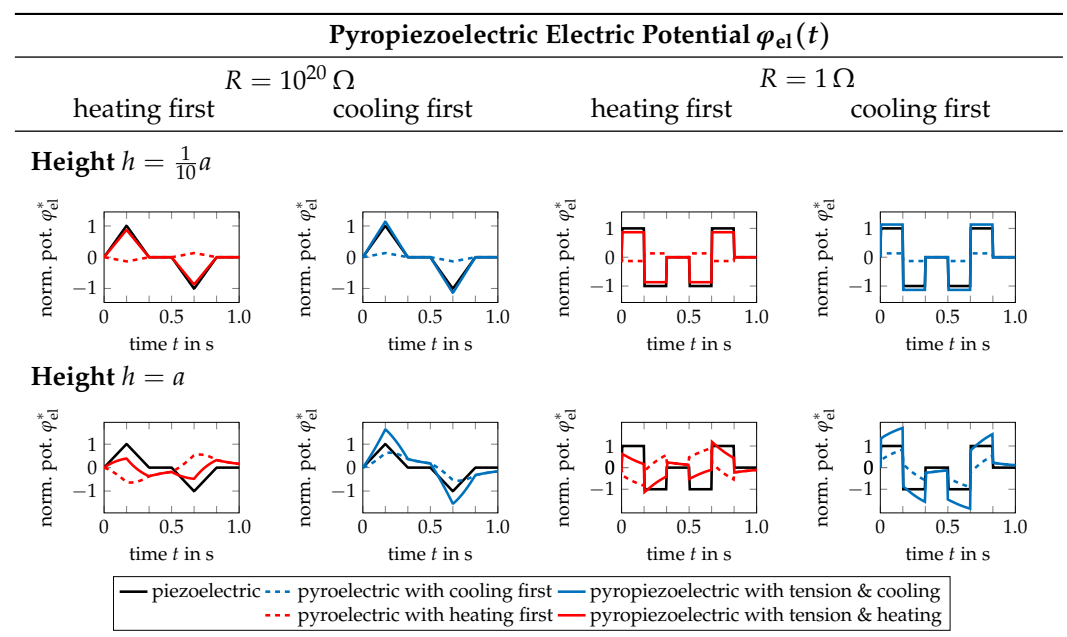
In order to investigate the pyroelectric effect, the temperature boundary condition $\theta = \bar{\theta}(t)$ is applied. The middle part of Table 1 shows the resulting electric potential φ_{el}^* and the current $\dot{Q}_{el}^*$ for $h = \frac{1}{10}a$, the lower part for $h = a$. The evolution of the electric potential φ_{el}^* is inverted compared to the piezoelectric case, since the pyroelectric coefficient p_3 is negative, but is otherwise similar in shape. The yellow line again shows the result

for an intermediate resistance between the open and closed circuits ($R = 10^{10} \Omega$). The pyroelectric results for $h = a$ look different, since heat conduction takes more time. This can be explained using the Fourier number $Fo \equiv \frac{t}{t_0} = \frac{\alpha t}{L_c^2}$ which can be interpreted as the ratio between the current time t and the characteristic time $t_0 = \frac{L_c^2}{\alpha}$ that is needed to diffuse a characteristic length L_c with thermal diffusivity $\alpha = \frac{k}{\rho c_p}$. If $Fo > 1$, steady-state is reached at time t , if $Fo \ll 1$, the temperature profile at time t deviates from the steady-state case. For the two cases here, the Fourier numbers can be estimated using the material parameters of PZT-5H given in Table A3, the dimension of the cuboid $a = 1 \text{ mm}$, $L_c = h$, and the total time $t_{\text{end}} = 1 \text{ s}$. For $h = \frac{1}{10}a$, $Fo \approx 6.06 > 1$, and for $h = a$, $Fo = 0.06 \ll 1$. In the latter case, steady-state is not reached during the temperature oscillations, which results in “rounded” or “delayed” signals for the electric potential and the current. The influence of resistance is independent of the height h and similar to the purely piezoelectric case.

3.3. Pyropiezoelectric Results

In the following, the pyropiezoelectric results are studied by applying $u_z = \bar{u}_z(t)$ and $\theta = \bar{\theta}(t)$ simultaneously. In the first step, a combination of tension and heating is investigated. The resulting electric potential φ_{el}^* is shown in Table 2 (solid red lines) in comparison to the piezoelectric case (solid black lines) and the pyroelectric case (dashed red lines) for the four combinations of $R = 10^{20} \Omega$ and $R = 1 \Omega$ with $h = \frac{1}{10}a$ and $h = a$. Close to open circuit ($R = 10^{20} \Omega$) for $h = \frac{1}{10}a$ with heating first, it can be seen that the pyropiezoelectric voltage is lower than in the piezoelectric case. The two effects have opposite signs and therefore weaken each other. When the temperature input $\bar{\theta}(t)$ is inverted (cooling first), a combination of tension and cooling results. This inverts the sign of the pyroelectric contributions (dashed blue lines) and the combination of tension and cooling as well as compression and heating increases the electrical potential φ_{el}^* compared to the purely piezoelectric or purely pyroelectric case. The two effects add up.

Table 2. Normalized electric potential $\varphi_{\text{el}}^*(t)$ of the cuboid for the pyropiezoelectric case for different resistances R and heights h if tension and heating (heating first) or tension and cooling (cooling first) are combined.



The influence of the resistance R and the height h on φ_{el}^* remains unchanged. Close to open circuit, $\varphi_{\text{el}}^*(t) \propto \bar{u}_z(t)$ and $\dot{\varphi}_{\text{el}}^*(t) \propto \bar{u}_z(t)$, while close to closed circuit $\varphi_{\text{el}}^*(t) \propto \dot{\bar{u}}_z(t)$

and $\dot{Q}_{el}^*(t) \propto \dot{u}_z(t)$. For $h = \frac{1}{10}a$, the heating rate is low enough to reach steady-state almost immediately with $Fo > 1$. For $h = a$, heat conduction takes more time to reach the steady-state ($Fo \ll 1$) and the electric potential deviates from the steady-state response.

4. Energy Harvesting Behavior of a Unimorph and Bimorph

In practice, structures such as unimorph or bimorph cantilevers are typically used for piezoelectric energy harvesting. Here, the transverse d_{31} -mode is mainly used, in which the change in electrical polarization occurs perpendicular to the largest stress within the material. Since $d_{33} > 0$ and $d_{31} < 0$, the preferred combination of piezoelectric and pyroelectric effects changes. Now, the simultaneous occurrence of tensile stress and heating or compressive stress and cooling leads to an increase in the resulting electrical potential and the harvested energy; see Equation (9). This section analyses the significance of the pyroelectric contribution to energy harvesting under typical operating conditions. A unimorph and a bimorph cantilever are examined under mechanical excitation close to its first natural frequency and a time-dependent temperature change.

4.1. Unimorph Cantilever Beam

A unimorph cantilever, consisting of a phosphor bronze (substrate) layer and a PZT layer, is shown in Figure 3. Electrodes are attached to the top and bottom of the PZT layer and are connected to an external resistor R . The resistor acts as a consumer of the energy harvested and dissipates it completely. On the left hand side, the beam is excited by a sinusoidal z -displacement near the first natural frequency of the beam. The beam oscillates in a temperature gradient field. This is represented by heat flux boundary conditions, which are switched on once points on the surface ∂B_{el} or ∂B_b move above the surface S_t or below S_b ; see Figure 3. The geometric parameters and the boundary conditions are given in Table 3. The excitation parameters were chosen such that a base acceleration of $|a_0| \approx 1.76 \text{ m/s}^2$ at 47.2 Hz results. According to Roundy et al. [64] and Priya et al. [5], these values are at the lower end of typical working conditions. The same applies to the applied heat flux $\bar{q} = 10 \text{ kW/m}^2$; see Mohammadnia and Rezania [65].

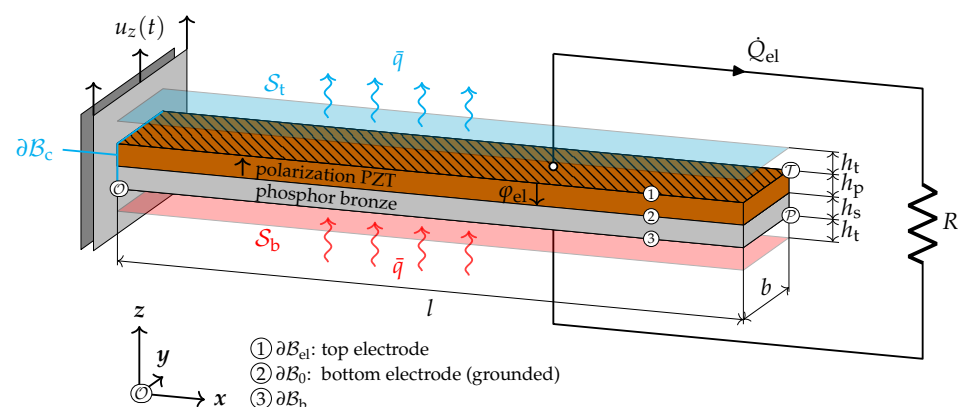


Figure 3. Unimorph cantilever beam with a resistor connected in series for the top cooling case.

Since the changes in temperature remain small, the material parameters are assumed to be constant and are provided in Table A2 in Appendix C. For the FE simulation, the unimorph is discretized with 180 elements with quadratic ansatz functions for the displacements u_i and linear ansatz functions for the potential φ and the temperature change θ . In all cases, a time period of 1 s is simulated, using a constant time step size of $\Delta t = 0.5 \text{ ms}$. The error in the z -displacement, the electric potential, and the temperature was thus less than approximately 1 % compared to a reference solution with 330 elements and a time step size of $\Delta t = 0.25 \text{ ms}$. In order to investigate the pyropiezoelectric energy harvesting behavior,

the cases *top cooling* and *top heating* are compared with the purely piezoelectric case below. In top cooling, $\partial\mathcal{B}_{\text{el}}$ and $\partial\mathcal{B}_{\text{b}}$ are cooled when the surface $\mathcal{S}_{\text{t}}$ is crossed, and heated when they cross the surface $\mathcal{S}_{\text{b}}$. In top heating, heating and cooling are reversed. Figure 4a,b, left, show the resulting z -displacement $u_z(t)$ at the tip point $\mathcal{T}$ (see Figure 3) and the electric potential $\varphi_{\text{el}}(t)$ between the electrodes for top cooling and top heating compared to the purely piezoelectric case. During the simulation, both variables reach a steady-state.

Table 3. Parameters of the serial unimorph cantilever beam.

Variable	Value	Unit
Length l	100	mm
Width b	20	mm
Substrate layer height h_{s}	0.5	mm
PZT layer height h_{p}	0.4	mm
Heating surface distance h_{t}	0.04	mm
Excitation amplitude u_0	0.02	mm
Excitation frequency f	47.2	Hz
Resistance R	26	k Ω
Heat flux $\bar{q}$	10	kW/m ²

Figure 4a,b, right, show one steady-state period in more detail. For the purely piezoelectric case (black curves), the responses for u_z and φ_{el} are symmetric as expected. Taking this as a reference, in the case of top cooling (blue curves), the total displacement and potential amplitudes increase. The signals reach their maxima at t_1^{u} and t_1^{φ} and their minima at t_2^{u} and t_2^{φ} , where the phase shift between the two signals is determined by the resistance $R = 26 \text{ k}\Omega$. The opposite behavior can be observed in the case of top heating (red curves). This behavior results from the fact that in both cases, different combinations of tension and compression with heating and cooling of the PZT layer are present. For top cooling, compression of the PZT layer and cooling or tension and heating are combined, resulting in an increase in u_z and φ_{el} . Furthermore, the pyroelectric displacement curve is not symmetric. The reason for that is the different heat expansion of the substrate layer and the PZT layer, which, in practical applications, can also lead to additional shear stresses at the interface. Since the thermal expansion coefficient α of phosphor bronze (PB) is higher than that of PZT, the thermal expansion of the PB layer dominates. This is confirmed by the temperature evolution at the lower end of the tip at point $\mathcal{P}$ as shown in Figure 5.

For top cooling, the substrate is heated from below, such that the temperature at point $\mathcal{P}$ is always oscillating around positive temperatures $\theta > 0$. The substrate therefore expands and the beam bends upwards. Bending in the opposite direction occurs for top heating, when the PB layer on average cools down. In both cases, the beam oscillates around a bent equilibrium position. Figure 5 also shows a steady decrease in temperature in both cases over the simulation time t , indicating that the temperature profile deviates from the steady-state. This is due to the high oscillation frequency f under typical working conditions for piezoelectric energy harvesting. The estimation of the Fourier number using the material parameters in Table A2 results in $\text{Fo} \ll 1$ and further confirms this.

Heat expansion seems to have a strong influence on the resulting deformation of the beam. To analyze this, the individual physical effects are examined separately by means of simulations. For the favourable load case of top cooling, simulations are repeated, either by neglecting thermal expansion ($\lambda_{ij} = 0$) or the pyroelectric effect ($p_i = 0$). Thermodynamic consistency of the model is preserved. However, the results cannot be obtained experimentally, since in reality all effects always occur simultaneously. In Figure 6, the tip displacement and electric potential for these cases are compared. Neglecting heat expansion (green curve) has, as expected, a strong influence on the displacement, which is then approximately symmetric to the time axis and almost equal to the piezoelectric case.

This also influences the electric potential: if heat expansion (and the resulting additional piezoelectric effect due to the increased deformation) is not taken into account, a larger reduction in the maximum electric potential results than by neglecting the pyroelectric effect (yellow curve). The influence of thermal expansion is therefore greater than the influence of pyroelectricity. In reality, however, the two effects cannot be separated.

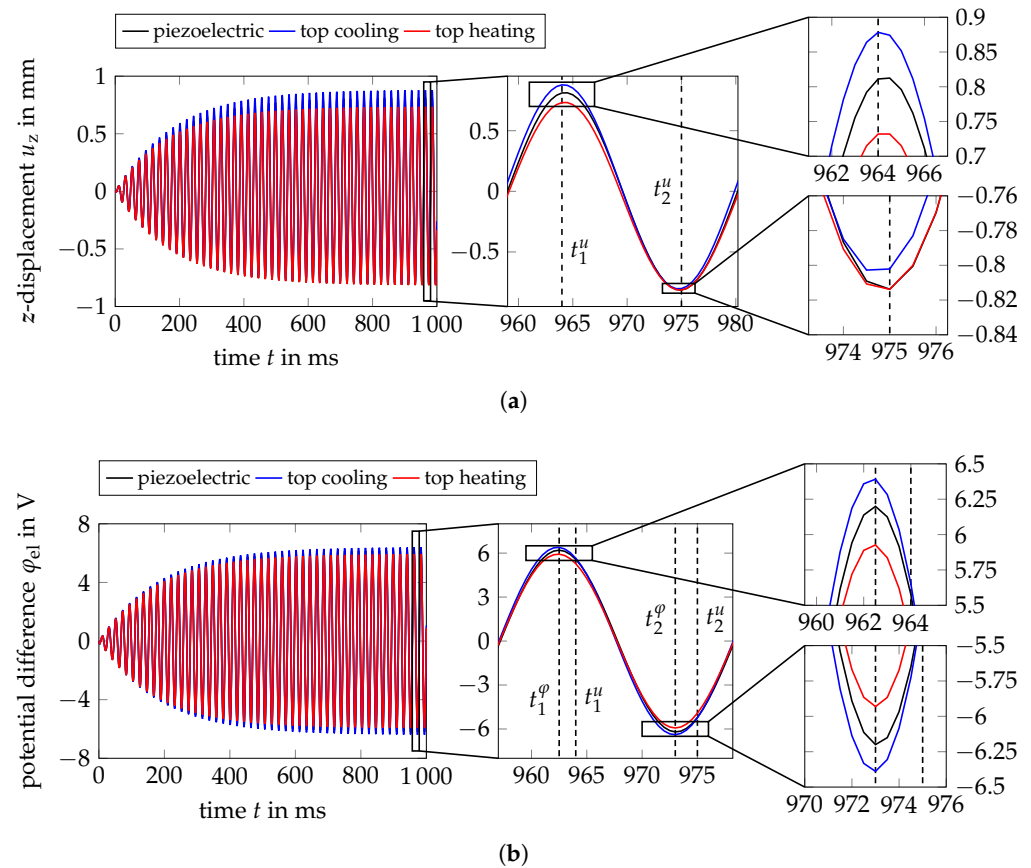


Figure 4. Resulting quantities for the unimorph cantilever: (a) z-displacement u_z at point $\mathcal{T}$ on the tip. (b) Electric potential difference $\varphi_{el}(t)$ between top and bottom electrode $\partial\mathcal{B}_{el}$ and $\partial\mathcal{B}_0$.

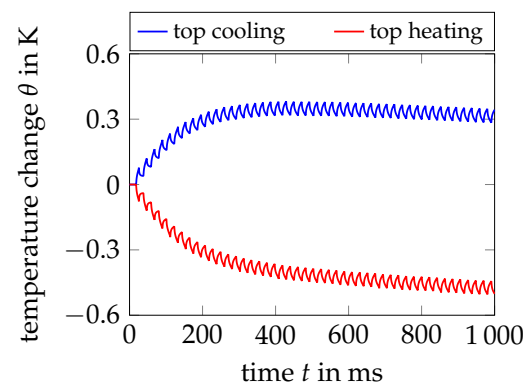


Figure 5. Temperature change $\theta(t)$ at point $\mathcal{P}$ on the lower end of the unimorph cantilever tip.

Since the harvested energy $\mathcal{E}$ is the decisive quantity for energy harvesting, it was calculated using Equation (26) for top cooling, top heating and piezoelectricity; see Figure 7. The time-dependent behavior is the same in all cases, with an exponential increase in the beginning and an approximately linear increase subsequently.

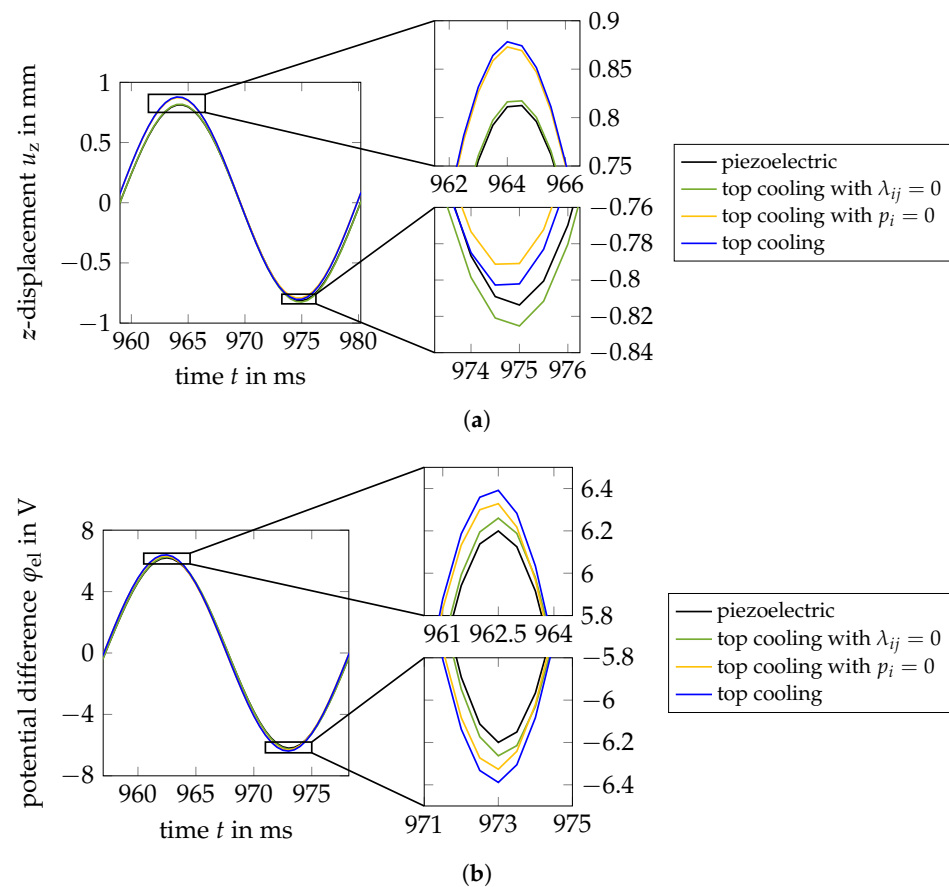


Figure 6. Resulting quantities for the unimorph cantilever for different parameter sets: (a) z-displacement $u_z(t)$ at point $\mathcal{T}$ on the tip. (b) Electric potential difference $\varphi_{el}(t)$ between top and bottom electrode $\partial\mathcal{B}_{el}$ and $\partial\mathcal{B}_0$.

With an energy harvested of $\mathcal{E} = 0.548$ mJ after 1 s for the piezoelectric case (black line) as reference, $\mathcal{E}$ increases for top cooling and decreases for top heating. The combination of pyroelectricity and thermal expansion ultimately results in an energy harvested of 0.579 mJ (+5.7%) for top cooling and 0.507 mJ (−7.5%) for top heating (see the boxed values in Figure 7).

The harvested energy $\mathcal{E}$ depends on the excitation frequency f and the resistance R . In Figure 8a, the normalized peak power $\mathcal{P}^{\max}$ frequency response function (FRF) was calculated for the piezoelectric and top cooling case in steady-state for $R = 26$ k Ω . Normalization was performed with respect to the excitation acceleration a_0 . A clear peak can be seen at approximately 47.2 Hz.

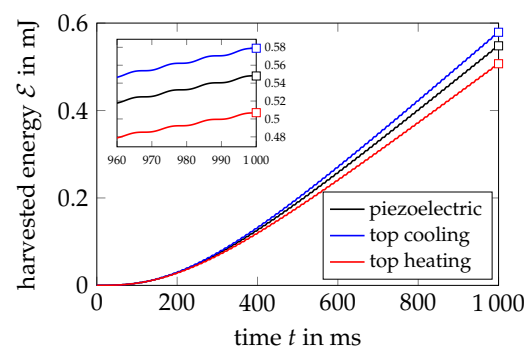


Figure 7. Harvested energy $\mathcal{E}(t)$ for the unimorph cantilever at $f = 47.2$ Hz and a resistance $R = 26$ k Ω .

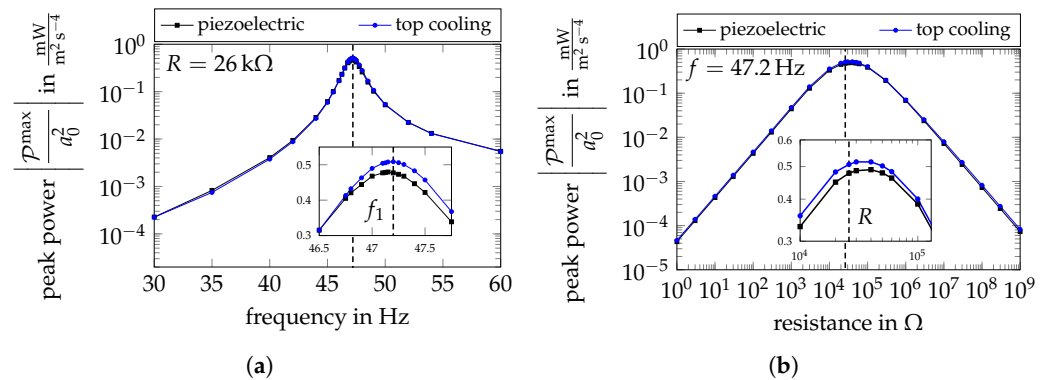


Figure 8. Normalized peak power for different external resistances R and frequencies f : (a) Peak power $\mathcal{P}^{\max}$ frequency response function (FRF) for an external resistance of $R = 26 \text{ k}\Omega$. (b) Peak power amplitude $\mathcal{P}^{\max}$ for an excitation frequency of $f = 47.2 \text{ Hz}$.

For this frequency in Figure 8b, the normalized peak power $\mathcal{P}^{\max}$ over the resistance R is shown. The maximum power is reached close to a resistance of $26 \text{ k}\Omega$. The differences in peak power between the piezoelectric and pyropiezoelectric cases are small, also at different frequencies and resistances. In summary, thermal expansion and pyroelectricity together result, in the present setting, in a difference in energy of $+5.7\% / -7.5\%$ as compared to the piezoelectric case. Of course, the values of $\mathcal{E}$ depend on the exact boundary conditions, but the oscillation around the natural frequency in a realistic temperature range applied here is representative for typical operating conditions. Even though the influences of pyroelectricity and thermal expansion are minor compared to the piezoelectric effect, unimorph energy harvesters should be aligned correctly in the presence of temperature gradients to ensure that thermal influences are beneficial rather than detrimental.

4.2. Bimorph Cantilever Beam

The bimorph cantilever has an additional active layer (here again PZT), resulting in a symmetrical geometry; see Figure 9. A series connection with an external resistor requires two additional short-circuited electrodes $\partial\mathcal{B}_{\text{el}}^{\text{um}}$ and $\partial\mathcal{B}_{\text{el}}^{\text{lm}}$ with the same electric potential and polarization of the two PZT layers in opposite directions. The geometric parameters are chosen to correspond to those of a commercially available bimorph from *Fuji Ceramics Corporation* [66], see Table 4. All material parameters are listed in Table A2 in Appendix C. The cantilever is excited on the left hand side by a sinusoidal displacement at a frequency of 65.5 Hz , which is close to the first natural frequency of the beam. Furthermore, heating and cooling takes place at the surfaces, depending on their vertical position, as in the previous example. A time period of 1 s is simulated, using a constant time step size of $\Delta t = 0.5 \text{ ms}$ with 360 elements. As for the unimorph, the deviation in the z -displacement, the electric potential, and the temperature was less than about 1% compared to the results of a reference solution with sufficient refinement.

In Figure 10a, the amplitude of the displacement u_z remains the same for all cases and is only shifted in the z -direction upwards and downwards. In Figure 10b the electric potential does not change at all. These results are based on the symmetry of the bimorph cantilever. The changes in displacement and potential amplitude for the top and bottom PZT layer compensate each other due to opposite signs. In all cases, this results in the same energy harvested of $\mathcal{E} = 1.32 \text{ mJ}$ in 1 s ; see the boxed value in Figure 11. Thus, for the symmetric geometry of the bimorph, the thermal influences on the energy harvested are negligible and it is not possible to harvest more energy through the pyroelectric effect.

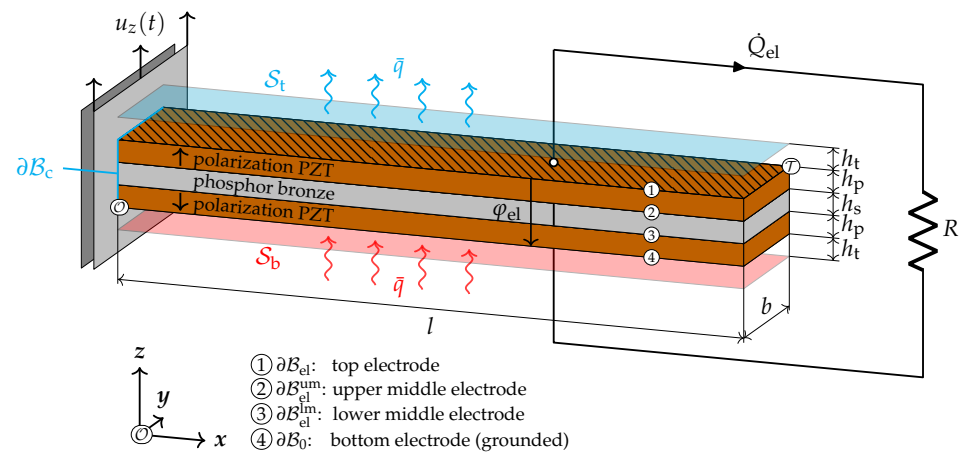


Figure 9. Bimorph cantilever beam with a resistor connected in series for the top cooling case.

Table 4. Parameters of the serial bimorph cantilever beam.

Variable	Value	Unit
Length l	85	mm
Width b	20	mm
Substrate layer height h_s	0.1	mm
PZT layer height h_p	0.45	mm
Heating surface distance h_t	0.04	mm
Excitation amplitude u_0	0.02	mm
Excitation frequency f	65.5	Hz
Resistance R	26	k Ω
Heat flux $\bar{q}$	10	kW/m ²

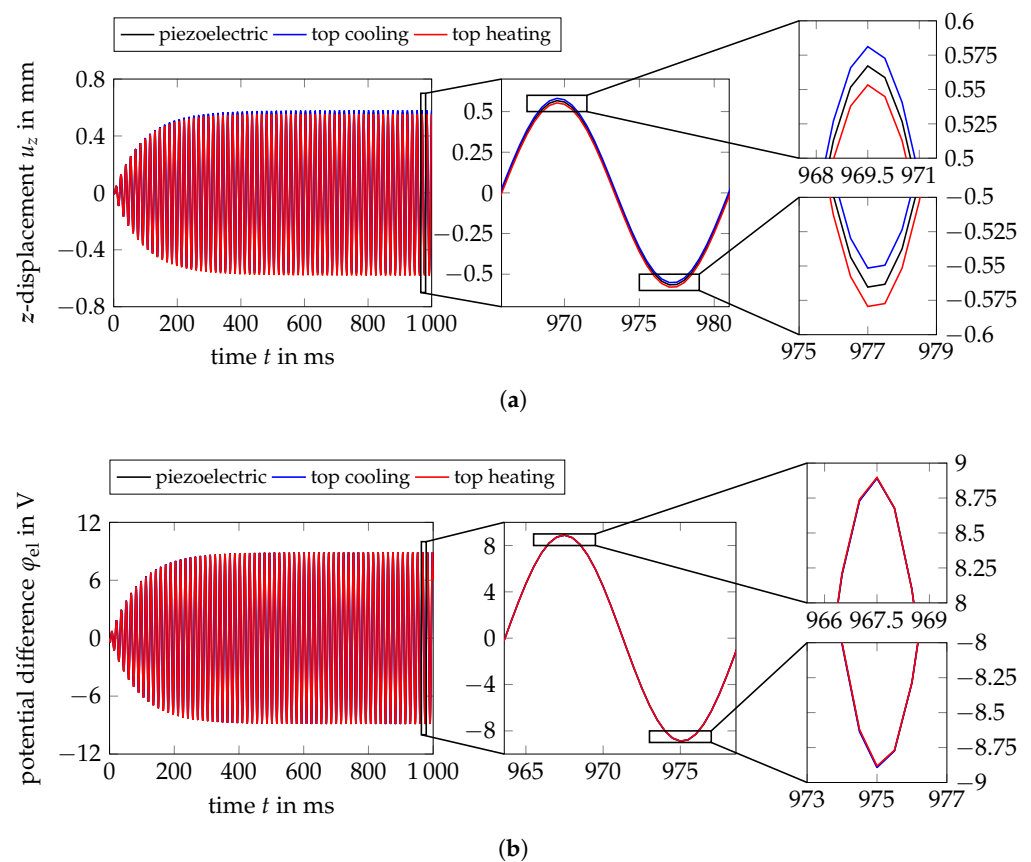


Figure 10. Resulting quantities for the bimorph cantilever: (a) z-displacement u_z at point $\mathcal{T}$. (b) Electric potential difference ϕ_{el} between top and bottom electrode $\partial \mathcal{B}_{el}$ and $\partial \mathcal{B}_0$.

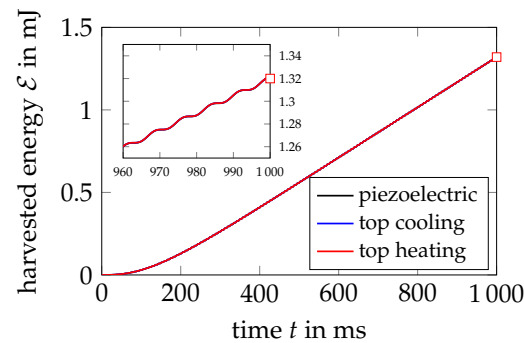


Figure 11. Harvested energy $\mathcal{E}(t)$ for the bimorph cantilever at $f = 65.5$ Hz and $R = 26$ k Ω .

5. Application Example for Low Frequency Temperature Fluctuations

The basic working principle of the pyropiezoelectric energy harvester (PPEH) from Kang and Yeatman [26,27] is to use ambient low-frequency temperature fluctuations and harvest energy by exploiting the piezoelectric and pyroelectric effects simultaneously. In contrast to the previously investigated unimorph and bimorph, no ambient vibrations are present. Heat conduction is the main driver of the harvesting cycle, which depends highly on the applied temperature fluctuation frequency. The following investigations aim to analyze the working principle of the PPEH in detail, to determine the influence of temperature fluctuation frequency and to derive the resulting energy harvested.

The PPEH consists of a bimetal beam made of two layers with low and high coefficients of thermal expansion (CTEs) from Ni-Fe and Ni-Cr-Fe and a centrally attached PZT-5H patch on top; see Figure 12. To realize simultaneous piezoelectric and pyroelectric energy harvesting, in the experiments in [27], a position-controlled slider with a heat source mounted on it oscillates below the bimetallic beam in the y -direction. When the PPEH is heated, it bends downwards due to the different thermal expansion coefficients α of the Ni-Fe and Ni-Cr-Fe layers. The bending caused by thermal expansion triggers the piezoelectric effect, while the temperature change itself initiates the pyroelectric effect. To reflect the experimental setup in the FE simulation, the two ends $\partial\mathcal{B}_c$ and $\partial\mathcal{B}_l$ are clamped and the temperature is kept constant ($\theta = 0$ K). The heating is modeled by a sinusoidal heat flux $\bar{q}(t) = q_0 \times \sin(2\pi ft - \frac{\pi}{2}) - q_0$, which is prescribed uniformly on the lower surface $\partial\mathcal{B}_h$. The in series attached external resistor takes into account the resistance of the voltage measurement setup. In the present numerical study, the dimensions of prototype P3 from [27] are used; see Table 5. Since Kang and Yeatman [27] do not specify all required material parameters, the parameters in Table A3 in Appendix C are partly estimated. Furthermore, since no further details are available, it is assumed that the material parameters remain constant across the resulting temperature range. For the FE simulation, the PPEH is discretized with 200 elements using quadratic ansatz functions for the displacement u_i and linear ansatz functions for the potential φ and the temperature change θ . A time period of 1000 s was simulated, using a constant time step size of $\Delta t = 0.5$ s. The resulting error in the z -displacement, the electric potential, and the temperature was less than about 1 % compared to the results of a sufficiently refined reference solution.

The heat flux $q_0 = 1.14$ kW/m² was chosen so that similar temperature changes θ and output voltages φ_{el} , as in [27], result in steady-state. $R = 100$ M Ω was taken from [27]. Figure 13 shows the resulting variables evaluated at point $\mathcal{D}$ in the center of the PZT-5H patch for periodic heating at a frequency of 0.02 Hz. In the first row, the displacement u_z and the temperature change θ are depicted. After approximately 800 s, both variables reach a steady-state in which the beam oscillates around a bent equilibrium state. Interestingly, however, the displacement and temperature are not in phase and therefore reach their maximum values not at the same time. Instead, there is a phase shift $\phi_u = \Delta t_u \times f \times 360^\circ \approx 47^\circ$

between them. This phase shift results heavily from the heat expansion of the PZT-5H patch on the bimetallic beam. During heating, the patch expands and thereby counteracts the downward deflection of the bimetallic beam. The maximum absolute deflection is reached when the temperature is already decreasing again. For the bimetallic beam, without the PZT-5H patch, the phase shift ϕ_u decreases significantly. A delay through thermal conductivity plays here only a minor role since the steady-state temperature profile across the thickness is present almost immediately, due to the low excitation frequency ($Fo > 1$ using the material parameters in Table A3).

The oscillation of u_z and θ leads to an oscillation of the strain and stress components ε_{11} and σ_{11} ; see the second row in Figure 13. The total strain is mainly composed of a (negative) mechanical contribution due to bending and a (positive) thermal contribution due to heat expansion. Since the mechanical contribution is in phase with u_z , this results in a phase shift of $\phi_\varepsilon = \Delta t_\varepsilon \times f \times 360^\circ \approx -32^\circ$ relative to the temperature signal.

The stress σ_{11} also varies periodically, but remains negative at all times. The compressive stresses are due to bending of the beam. Therefore, the stress signal is nearly in phase with the displacement u_z and has a phase shift of $\phi_\sigma = \Delta t_\sigma \times f \times 360^\circ \approx 36^\circ$ relative to the temperature.

In a steady-state, the electric potential φ_{el} (third row in Figure 13) oscillates around $\varphi_{el} \approx 0$ V, as expected. It is phase-shifted relative to θ , with a phase shift of $\phi_\varphi = \Delta t_\varphi \times f \times 360^\circ \approx 126^\circ$, which results from the combination of the piezoelectric and pyroelectric effects and the influence of the resistance. To isolate these effects from one another, the phase shift is considered for the open circuit case ($R \rightarrow \infty$). In the purely pyroelectric case, it is 180° , since the pyroelectric effect generates a negative voltage when heated. The pyropiezoelectric phase shift can be computed to be only slightly lower with 173° for $R \rightarrow \infty$, which shows that the pyroelectric effect dominates here. A further reduction in the phase shift to the $\phi_\varphi \approx 126^\circ$ observed here is due to the resistance, which is $100\text{ M}\Omega$ and significantly lower than in the open circuit case.

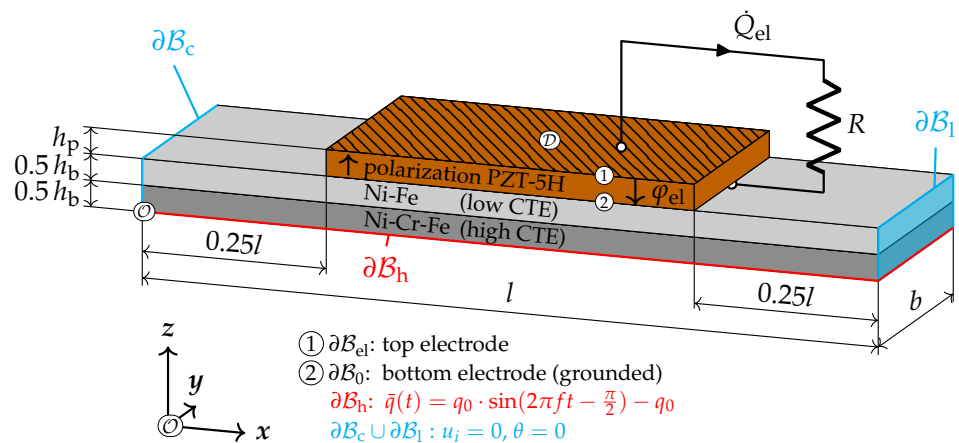


Figure 12. Pyropiezoelectric energy harvester from Kang and Yeatman [27] with a resistor connected in series where the evaluation point $\mathcal{D}$ in the center of the PZT-5H patch is marked.

Table 5. Parameters for modeling prototype P3 from Kang and Yeatman [27].

Variable	Value	Unit
Length l	50	mm
Width b	14	mm
Bimetal beam height h_b	0.3	mm
PZT-5H patch height h_p	0.127	mm
Resistance R	100	M Ω
Heat flux q_0	1.14	kW/m ²

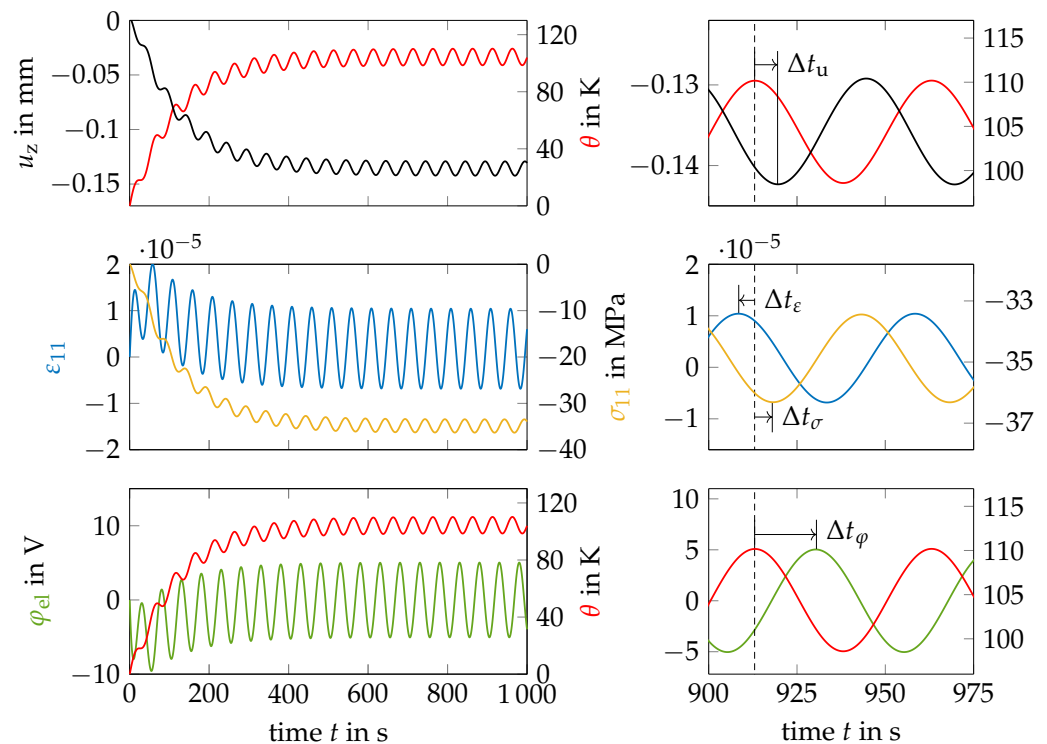


Figure 13. Resulting z-displacement u_z , strain-component ε_{11} , stress-component σ_{11} and electric potential φ_{el} in comparison with the resulting temperature change θ at point D for a frequency of $f = 0.02$ Hz.

Since the temperature increase in the PZT-5H patch depends heavily on the frequency f of the oscillating heat flux, the electric potential φ_{el} and the harvested energy $\mathcal{E}$ also depend on f . To illustrate this behavior, the peak potential $\varphi_{el}^{\max}$ is plotted over f in Figure 14a. Figure 14b shows the energy harvested after 1000 s. It can be seen that $\varphi_{el}^{\max}$ and $\mathcal{E}$ decrease exponentially with increasing frequency f . Figure 14a,b show the pyropiezoelectric response (green line), the pure pyroelectric response (red line) and the pure piezoelectric response (black line). The last two results were obtained by setting the piezoelectric coefficients d_{ijk} or the pyroelectric coefficients p_i to zero in the simulation. Comparing the three cases, the peak voltage $\varphi_{el}^{\max}$ and energy $\mathcal{E}$ increase if the piezoelectric effect disappears and only thermal expansion and pyroelectricity are present. In the pyropiezoelectric case, $\varphi_{el}^{\max}$ and thus $\mathcal{E}$ are reduced, because heating and compression of the PZT-5H patch occur simultaneously. This results in electrical potential contributions of opposite signs and thus in a reduction in the total electric potential.

This problem only becomes apparent because the various signals can be analyzed separately in the simulation. It then seems obvious to suggest an improvement to the harvester design by reversing the Ni-Fe and Ni-Cr-Fe layers of the bimetallic beam. When heated, the bimetallic beam then bends upwards and the PZT-5H patch is stretched instead of compressed. The maximum electric potential and the harvested energy for this case are shown as blue lines in Figure 14. The advantageous combination of tension and heating causes the piezoelectric and pyroelectric contributions to $\varphi_{el}^{\max}$ to add up, which also leads to an increase in $\mathcal{E}$. Taking the pyropiezoelectric case without reversing for 0.02 Hz with an harvested energy of 0.148 mJ as a reference, $\mathcal{E}$ increases by 386 % if the layers are reversed (boxed points in Figure 14b). This value should be regarded only as a theoretical upper bound under idealized circuit conditions; however, it shows the potential for improvement that can be achieved.

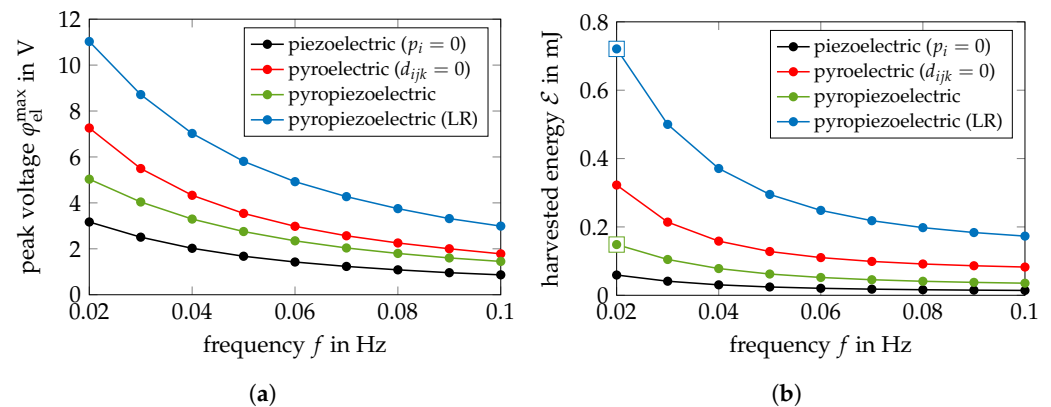


Figure 14. Resulting quantities for the piezoelectric case, pyroelectric case, pyropiezoelectric case and pyropiezoelectric case with Ni-Fe and Ni-Cr-Fe layers reversed (LR): (a) Peak voltage φ_{el}^{max} over the heat flux excitation frequency f . (b) Harvested energy $\mathcal{E}$ over the heat flux excitation frequency f .

In summary, the example from Kang and Yeatman shows that the combination of the piezoelectric and pyroelectric effects and the frequency of the heat input have a decisive influence on the harvested energy for low-frequency applications. Coupled simulations of mechanical, electrical and thermal behavior help to optimize such multi-modal harvester designs.

6. Conclusions

Simultaneous energy harvesting from the piezoelectric and pyroelectric effects was investigated using a numerical framework based on the finite element method. The fully coupled transient mechanical, electrical and thermal equations were solved, taking into account the connection to an electrical circuit by means of appropriate boundary conditions. An example problem consisting of a piezoelectric cuboid under oscillating pressure and temperature was used to analyze the shape of signals depending on the external resistance and the superposition of pyro- and piezoelectric effects. In open circuit, the electric potential and current are proportional to the prescribed input. In closed circuit they are proportional to the time derivative of the input. For resistance values in between, a combination of both limiting cases results. The voltage signal from the pyroelectric effect depends further on the Fourier number Fo . At high heating rates or with thick layers of pyroelectric materials, $Fo \ll 1$, which means that the temperature profile does not reach steady-state and the pyroelectric effect is not being utilized optimally. Furthermore, for the d_{33} -mode analyzed herein, the combination of tension and cooling as well as compression and heating is advantageous, as both effects add up. However, due to the different signs of the piezoelectric parameters, this relationship is reversed in the unimorph and bimorph beam structures (d_{31} -mode) that are typically used for piezoelectric energy harvesting. For these structures under typical operating conditions, the gain in energy harvested due to thermal effects was investigated. For an asymmetric unimorph, a change in harvested energy of $+5.7\%$ / -7.5% as compared to the piezoelectric case was computed. The influence of thermal expansion is thereby more significant than that of the pyroelectric effect. For the bimorph, no significant change in the energy harvested was observed due to symmetry. Finally, the pyropiezoelectric low-frequency energy harvesting device of Kang and Yeatman [27] was studied. Here, the pyroelectric effect is the main factor in the energy harvested, and the frequency of the oscillating heat flux therefore has a significant influence. By analyzing the various physical effects separately, a geometric optimization of the energy harvester was determined, resulting in a theoretical 386 % increase in harvested energy compared to the original design under idealized circuit conditions. In summary, it

was demonstrated that transient coupled simulations of mechanical, electrical, and thermal effects contribute to the understanding and optimization of multi-modal pyropiezoelectric energy harvesters.

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Conflicts of Interest: The authors declare no conflicts of interest.

Appendix A. Discretization Details

Starting from the weak forms (17) to (19), the constitutive Equations (8)–(10) and the gradient Equations (1)–(3) can be introduced to obtain

$$\int_B \rho \eta_i \ddot{u}_i dV + \int_B \eta_{i,j} C_{ijkl} u_{k,l} dV + \int_B \eta_{j,k} e_{ijk} \varphi_{,i} dV - \int_B \eta_{i,j} \lambda_{ij} \theta dV = \int_{\partial B_N^u} \eta_i \bar{t}_i dA \quad (A1)$$

$$\begin{array}{ccccccc} \hookrightarrow M_{uu} \cdot \ddot{u} & \hookrightarrow K_{uu} \cdot u & \hookrightarrow K_{u\varphi} \cdot \varphi & \hookrightarrow K_{u\theta} \cdot \theta & \hookrightarrow F_u \end{array}$$

$$\int_B \xi_{,i} e_{ijk} u_{j,k} dV - \int_B \xi_{,i} \epsilon_{ij} \varphi_{,j} dV + \int_B \xi_{,i} p_i \theta dV = - \int_{\partial B_N^\varphi} \xi \bar{\sigma}_f dA \quad (A2)$$

$$\begin{array}{ccccccc} \hookrightarrow K_{\varphi u} \cdot u & \hookrightarrow K_{\varphi\varphi} \cdot \varphi & \hookrightarrow K_{\varphi\theta} \cdot \theta & \hookrightarrow F_\varphi \end{array}$$

$$\int_B \psi T_0 \lambda_{ij} \dot{u}_{i,j} dV - \int_B \psi T_0 p_i \dot{\varphi}_{,i} dV + \int_B \psi \rho c_v \dot{\theta} dV + \int_B \psi_{,i} k_{ij} \theta_{,j} dV = \int_{\partial B_N^\theta} \psi \bar{q} dA \quad (A3)$$

$$\begin{array}{ccccccc} \hookrightarrow D_{\theta u} \cdot \dot{u} & \hookrightarrow D_{\theta\varphi} \cdot \dot{\varphi} & \hookrightarrow D_{\theta\theta} \cdot \dot{\theta} & \hookrightarrow K_{\theta\theta} \cdot \theta & \hookrightarrow F_\theta \end{array}$$

The matrix terms listed under the integrals refer to their counterparts after discretization of the weak forms, which are given in Equation (A13).

If the solution variables are approximated element-wise by scalar- or vector-valued polynomial ansatz functions N_i^a , $\hat{N}^a$ or $\tilde{N}^a$ and nodal values u^a , φ^a and θ^a in the form

$$u_i^e = \sum_{a=1}^{n_u} N_i^a u^a, \quad \varphi^e = \sum_{a=1}^{n_\varphi} \hat{N}^a \varphi^a \quad \text{and} \quad \theta^e = \sum_{a=1}^{n_\theta} \tilde{N}^a \theta^a, \quad (A4)$$

the submatrices M_{uu} , D_{uu} , $D_{\theta u}$, $D_{\theta\varphi}$, $D_{\theta\theta}$, K_{uu} , $K_{u\varphi}$, $K_{u\theta}$, $K_{\varphi u}$, $K_{\varphi\varphi}$, $K_{\varphi\theta}$, $K_{\theta\theta}$ and subvectors F_u , F_φ , F_θ with coefficients

$$M_{uu}^{AB} = \mathbf{A} \int_{\mathcal{B}^e} N_i^a \rho N_i^b dV, \quad (A5)$$

$$D_{uu}^{AB} = \alpha_R M_{uu}^{AB} + \beta_R K_{uu}^{AB}, \quad D_{\theta u}^{AB} = \mathbf{A} \int_{\mathcal{B}^e} \tilde{N}^a T_0 \lambda_{ij} N_{i,j}^b dV, \quad (A6)$$

$$D_{\theta\varphi}^{AB} = -\mathbf{A} \int_{\mathcal{B}^e} \tilde{N}^a T_0 p_i \hat{N}_{i,i}^b dV, \quad D_{\theta\theta}^{AB} = \mathbf{A} \int_{\mathcal{B}^e} \tilde{N}^a \rho c_v \tilde{N}^b dV, \quad (A7)$$

$$K_{uu}^{AB} = \mathbf{A} \int_{\mathcal{B}^e} N_{i,j}^a C_{ijkl} N_{j,k}^b dV, \quad K_{u\varphi}^{AB} = \mathbf{A} \int_{\mathcal{B}^e} N_{i,j}^a e_{kij} \hat{N}_{j,k}^b dV, \quad (A8)$$

$$K_{u\theta}^{AB} = -\mathbf{A} \int_{\mathcal{B}^e} N_{i,j}^a \lambda_{ij} \tilde{N}^b dV, \quad K_{\varphi u}^{AB} = \mathbf{A} \int_{\mathcal{B}^e} \hat{N}_{i,i}^a e_{ijk} N_{j,k}^b dV, \quad (A9)$$

$$K_{\varphi\varphi}^{AB} = -\mathbf{A} \int_{\mathcal{B}^e} \hat{N}_{i,i}^a \epsilon_{ij} \hat{N}_{j,j}^b dV, \quad K_{\varphi\theta}^{AB} = \mathbf{A} \int_{\mathcal{B}^e} \hat{N}_{i,i}^a p_i \tilde{N}^b dV, \quad (A10)$$

$$K_{\theta\theta}^{AB} = \mathbf{A} \int_{\mathcal{B}^e} \tilde{N}_{i,i}^a k_{ij} \tilde{N}_{j,j}^b dV, \quad F_u^A = \mathbf{A} \int_{\partial\mathcal{B}_N^{e,u}} N_i^a \bar{t}_i dA, \quad (A11)$$

$$F_\varphi^A = -\mathbf{A} \int_{\partial\mathcal{B}_N^{e,\varphi}} \tilde{N}^a \bar{\sigma}_f dA, \quad F_\theta^A = \mathbf{A} \int_{\partial\mathcal{B}_N^{e,\theta}} \tilde{N}^a \bar{q} dA, \quad (A12)$$

result, where the assembly operator $\mathbf{A}$ maps the local degrees of freedom $a, b \in \{1, \dots, n_{\text{dof}}\}$ to their corresponding global counterpart $A, B \in \{1, \dots, n_{\text{global}}\}$ with the number of degrees of freedom per element $n_{\text{dof}} = n_u + n_\varphi + n_\theta$, the number of global degrees of freedom n_{global} and the number of elements n_{el} . Here, the test functions η_i , ζ and ψ are approximated by the same set of polynomial ansatz functions as the solution variables. The variables n_u , n_φ and n_θ denote the number of displacement, electric potential and temperature degrees of freedom within an element.

The three semi-discretized Equations (A1)–(A3) can then be written in a more convenient matrix formulation

$$\begin{bmatrix} M_{uu} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} \ddot{u} \\ \ddot{\varphi} \\ \ddot{\theta} \end{bmatrix} + \begin{bmatrix} D_{uu} & 0 & 0 \\ 0 & 0 & 0 \\ D_{\theta u} & D_{\theta\varphi} & D_{\theta\theta} \end{bmatrix} \cdot \begin{bmatrix} \dot{u} \\ \dot{\varphi} \\ \dot{\theta} \end{bmatrix} + \begin{bmatrix} K_{uu} & K_{u\varphi} & K_{u\theta} \\ K_{\varphi u} & K_{\varphi\varphi} & K_{\varphi\theta} \\ 0 & 0 & K_{\theta\theta} \end{bmatrix} \cdot \begin{bmatrix} u \\ \varphi \\ \theta \end{bmatrix} = \begin{bmatrix} F_u \\ F_\varphi \\ F_\theta \end{bmatrix} \quad (A13)$$

which is also mentioned in Section 2.2. To account for Rayleigh-type damping, the submatrix D_{uu} was introduced with

$$D_{uu} = \alpha_R M_{uu} + \beta_R K_{uu}. \quad (A14)$$

The Rayleigh parameters α_R and β_R describe the frequency-dependent Lehr's damping ratio $D_i = \frac{1}{2} \left(\frac{\alpha_R}{\omega_i} + \beta_R \omega_i \right)$.

The coupling between the finite element structure and the electric circuit is then realized by means of the electric potential φ_{el} and the electric current $\dot{Q}_{\text{el}}$ where the existence of a grounded and a nongrounded electrode $\partial\mathcal{B}_0$ and $\partial\mathcal{B}_{\text{el}}$ is assumed, as indicated in Figure 1. The change in time in total charge at the upper electrode corresponds to the electric current $\dot{Q}_{\text{el}}$ where

$$\dot{Q}_{\text{el}} = \int_{\partial\mathcal{B}_{\text{el}}} \dot{\sigma}_f dA. \quad (A15)$$

This term is approximated in the FE simulation as

$$\dot{Q}_{el} \approx \sum_K^{\text{electrode nodes}} \dot{F}_\varphi^K \quad \text{with} \quad \dot{F}_\varphi^K = - \mathbf{A} \int_{\partial B_{el}^e} \hat{N}^k \dot{\sigma}_f dA. \quad (\text{A16})$$

The relationship between the current $\dot{Q}_{el}$ and the electric voltage φ_{el} is on the one hand determined by the piezoelectric structure but on the other hand simultaneously by the electric circuit in the form of a differential equation

$$\dot{Q}_{el} = \dot{Q}_{el}(\varphi_{el}, \dot{\varphi}_{el}, \ddot{\varphi}_{el}). \quad (\text{A17})$$

This relation is included in the FE simulation as a mixed boundary condition that defines the relationship between $\dot{F}_\varphi$ and the electric potential φ_{el} at the electrode. If the electric circuit consists, e.g., of a simple resistor with resistance R , relation (A17) becomes

$$\dot{Q}_{el} = \frac{1}{R} \varphi_{el}. \quad (\text{A18})$$

Since this relation is defined for $\dot{F}_\varphi$, as in Equation (A16), it can more easily be incorporated into the FE simulation by taking the time derivative of Equation (A2) [34,59]. The matrix formulation then results as

$$\underbrace{\begin{bmatrix} M_{uu} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_M \cdot \underbrace{\begin{bmatrix} \ddot{u} \\ \ddot{\varphi} \\ \ddot{\theta} \end{bmatrix}}_{\ddot{x}} + \underbrace{\begin{bmatrix} D_{uu} & 0 & 0 \\ K_{\varphi u} & K_{\varphi \varphi} & K_{\varphi \theta} \\ D_{\theta u} & D_{\theta \varphi} & D_{\theta \theta} \end{bmatrix}}_D \cdot \underbrace{\begin{bmatrix} \dot{u} \\ \dot{\varphi} \\ \dot{\theta} \end{bmatrix}}_{\dot{x}} + \underbrace{\begin{bmatrix} K_{uu} & K_{u\varphi} & K_{u\theta} \\ 0 & 0 & 0 \\ 0 & 0 & K_{\theta\theta} \end{bmatrix}}_K \cdot \underbrace{\begin{bmatrix} u \\ \varphi \\ \theta \end{bmatrix}}_x = \underbrace{\begin{bmatrix} F_u \\ \dot{F}_\varphi \\ F_\theta \end{bmatrix}}_F \quad (\text{A19})$$

and can be written in a more compact form as

$$M\ddot{x} + D\dot{x} + Kx = F. \quad (\text{A20})$$

The numerical solution of the transient Equation (A20) requires its discretization in time. A time period τ is discretized into a number of intervals $[t_n, t_{n+1}]$ with time step size $\Delta t = t_{n+1} - t_n > 0$ and $n = \{0, \dots, n_{\text{steps}} - 1\}$. In the following, the Bossak–Newmark integration scheme [60] is used. It solves Equation (A20) at time t_{n+1} coming from a previous known time step t_n

$$M[(1 + \alpha_B)\ddot{x}_{n+1} - \alpha_B\ddot{x}_n] + D\dot{x}_{n+1} + Kx_{n+1} = F_{n+1} \quad (\text{A21})$$

with the approximations of velocity and acceleration

$$\dot{x}_{n+1} = \frac{\gamma_B}{\beta_B \Delta t} (x_{n+1} - x_n) - \left(\frac{\gamma_B}{\beta_B} - 1 \right) \dot{x}_n - \left(\frac{\gamma_B}{2\beta_B} - 1 \right) \Delta t \ddot{x}_n \quad (\text{A22})$$

$$\ddot{x}_{n+1} = \frac{1}{\beta_B \Delta t^2} (x_{n+1} - x_n) - \frac{1}{\beta_B \Delta t} \dot{x}_n - \left(\frac{1}{2\beta_B} - 1 \right) \ddot{x}_n. \quad (\text{A23})$$

The Bossak parameter α_B can be chosen as $\alpha_B \in [0, 1]$. The Newmark parameters β_B and γ_B follow then as $\beta_B = \frac{1}{4}(1 + \alpha_B)^2$ and $\gamma_B = \frac{1}{2} + \alpha_B$. In the following we will set $\alpha_B = 0.5$ to introduce slight numerical damping and to obtain stability and second order accuracy $\beta_B = \frac{9}{16}$ and $\gamma_B = 1$. Inserting Equation (A22) and Equation (A23) into Equation (A21) results in

$$\begin{aligned}
 \left[\frac{1 + \alpha_B}{\beta_B \Delta t^2} \mathbf{M} + \frac{\gamma_B}{\beta_B \Delta t} \mathbf{D} + \mathbf{K} \right] \mathbf{x}_{n+1} = & \mathbf{F}_{n+1} + \alpha_B \mathbf{M} \dot{\mathbf{x}}_n \\
 & + \mathbf{M}(1 + \alpha_B) \left[\left(\frac{1}{2\beta_B} - 1 \right) \dot{\mathbf{x}}_n + \frac{1}{\beta_B \Delta t} \dot{\mathbf{x}}_n + \frac{1}{\beta_B \Delta t^2} \mathbf{x}_n \right] \\
 & + \mathbf{D} \left[\left(\frac{\gamma_B}{2\beta_B} - 1 \right) \Delta t \dot{\mathbf{x}}_n + \left(\frac{\gamma_B}{\beta_B} - 1 \right) \dot{\mathbf{x}}_n + \frac{\gamma_B}{\beta_B \Delta t} \mathbf{x}_n \right] \quad (\text{A24})
 \end{aligned}$$

which marks the final equation to calculate $\mathbf{x}_{n+1}$. Velocity $\dot{\mathbf{x}}_{n+1}$ and acceleration $\ddot{\mathbf{x}}_{n+1}$ follow again from Equations (A22) and (A23). After the solution of one time step, the harvested energy in this time step can be calculated by

$$\mathcal{E}_{n+1} = \mathcal{E}_n + \int_{t_n}^{t_{n+1}} \mathcal{P} \, dt = \mathcal{E}_n + \int_{t_n}^{t_{n+1}} \varphi_{\text{el}} \dot{Q}_{\text{el}} \, dt \quad (\text{A25})$$

which is numerically evaluated by means of the backward Euler method.

Appendix B. Implementation Verification

To verify the correct implementation of the linear pyroelectric equations, the benchmark example from Tauchert [42] is investigated. In [42], a five-layer plate under the assumption of a plane strain state was proposed; see Figure A1.

It consists of two outer piezoelectric layers, an isotropic layer in the center, and two orthotropic layers in between, whose orientations are shifted by 90 degrees around the z -axis. All layers have the same thickness, $\frac{t}{5} = 2 \text{ mm}$, with a width of $b = 50 \text{ mm}$. The length has been set to $l = 1 \text{ mm}$, but could be chosen arbitrarily as long as the plane strain condition is satisfied. The entire laminate is heated on its bottom surface $\partial\mathcal{B}_{\text{bo}}$ by a sinusoidal temperature distribution $\theta = \theta_0 \sin\left(\frac{\pi y}{b}\right)$ with $\theta_0 = 50 \text{ K}$, while the temperature at $\partial\mathcal{B}_l$ and $\partial\mathcal{B}_r$ is kept constant at $\theta = 0 \text{ K}$. The surfaces $\partial\mathcal{B}_l$ and $\partial\mathcal{B}_r$ are fixed in y -direction, with the edge $\mathcal{E}$ on the surface $\partial\mathcal{B}_l$ also fixed in z -direction to prevent rigid-body motions. To account for the plane strain state, the surfaces $\partial\mathcal{B}_f$ and $\partial\mathcal{B}_b$ are fixed in the x -direction. The electric potential is grounded at the inner surfaces $\partial\mathcal{B}_{\text{el}}^{\text{um}}$ and $\partial\mathcal{B}_{\text{el}}^{\text{lm}}$ between piezoelectric and orthotropic layers, as well as at the surfaces $\partial\mathcal{B}_l$ and $\partial\mathcal{B}_r$.

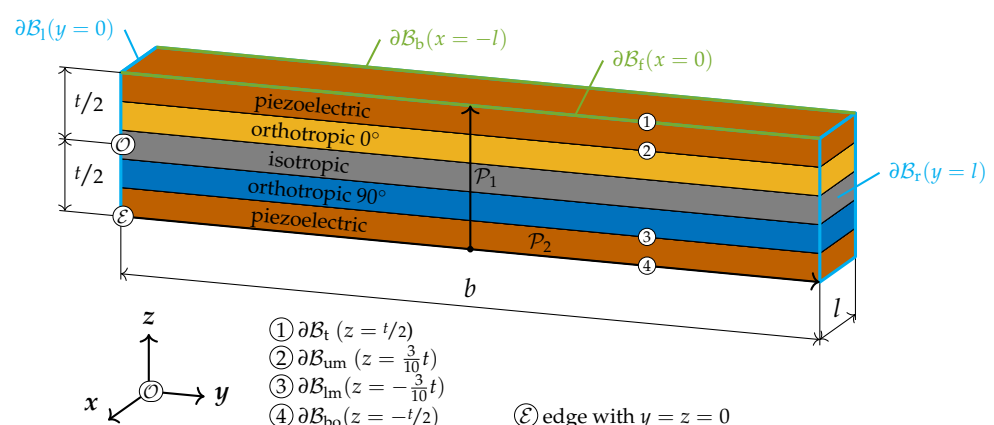


Figure A1. Geometry of the five-layer plate benchmark example from Tauchert [42] which is also discussed by Görndt and Gabbert [43].

For the given boundary conditions, Tauchert, in [42], derived an analytical solution for the resulting displacement u_z along the path $\mathcal{P}_1$ in the uncoupled case (without piezoelectric and pyroelectric effects). In [43], Görndt and Gabbert verified their implementation using Tauchert's solution and calculated the displacement u_z along the path $\mathcal{P}_1$ and the electric

potential along $\mathcal{P}_2$ numerically using the finite element method, for both the coupled and uncoupled cases. The temperature distribution along $\mathcal{P}_1$ is given in the work by Shang et al. [67].

To verify the implementation in this work, the geometry was discretized using $1 \times 20 \times 50$ elements with quadratic ansatz functions for the displacements u_i and linear ansatz functions for the electric potential φ and the temperature change θ . The number of elements was refined until no significant change in the solution variables could be detected (discretization error $< 1\%$). All material parameters used are specified in [43] and listed in Table A1. Figure A2a shows the resulting steady-state temperature distribution along the path $\mathcal{P}_1$. The dimensionless coordinate z^* was determined by normalizing to the total thickness t , i.e., $z^* = z/t$. There is a good agreement between the results of Görnandt and Gabbert and those of the present work. The temperature decreases from the maximum value $\theta_0 = 50$ K specified at the boundary $\partial\mathcal{B}_{\text{bo}}$ ($z^* = -0.5$) to $\theta = 0$ K specified at the boundary $\partial\mathcal{B}_t$ ($z^* = 0.5$). Figure A2b shows the dimensionless displacement $u_z^* = \frac{u_z t}{\alpha_0 \theta_0 b^2}$ which is compared with the results of Tauchert [42] and Görnandt and Gabbert [43] for the uncoupled case ($d_{ijk} = 0, p_i = 0$) and the coupled case ($d_{ijk} \neq 0, p_i \neq 0$). Again, a good agreement between the results is visible, with a deviation of $< 1\%$ for both cases. This also applies to the electric potential difference in Figure A2c along path $\mathcal{P}_2$. The y -coordinate is normalized by the width b with $y^* = y/b$. The results for u_z^* and φ also show that the pyroelectric effect can have a significant influence and should be taken into account in pyroelectric applications. Overall, the comparison of the results of this study with those of Tauchert and those of Görnandt and Gabbert shows excellent agreement and therefore confirms the correctness of the implementation used.

Table A1. Material parameters of the four different layer types in the five-layer laminate benchmark example by Tauchert [42] and Görnandt and Gabbert [43].

Basic Values			
$E_0 = 2 \text{ GPa}, \nu_0 = 0.25, \rho_0 = 7600 \text{ kg/m}^3$ $\epsilon_0 = 10^{-8} \text{ F/m}, d_0 = 2 \times 10^{-10} \text{ m/V}, p_0 = 0.25 \times 10^{-3} \text{ C/(m}^2 \text{ K)}$ $\alpha_0 = 10^{-5} \text{ 1/K}, k_0 = 1 \text{ W/(m K)}, c_{v0} = 420 \text{ J/(kg K)}$			
Piezoelectric	Orthotropic, 0°	Orthotropic, 90°	Isotropic
$E = E_0$	$E_1 = E_3 = 5E_0$ $E_2 = 90E_0$ $G_{12} = G_{23} = 4E_0$ $G_{13} = 1.5E_0$	$E_1 = 90E_0$ $E_2 = E_3 = 5E_0$ $G_{12} = G_{13} = 4E_0$ $G_{23} = 1.5E_0$	$E = E_0$
$\nu = \nu_0$ $\epsilon_1 = \epsilon_2 = \epsilon_0$ $\epsilon_3 = 10\epsilon_0$ $d_{31} = d_{32} = d_{24} = d_0$ $d_{33} = 1.4d_0$ $p_3 = p_0$ $\alpha = \alpha_0$	$\nu_{12} = \nu_{13} = \nu_{23} = \nu_0$ $\alpha_1 = \alpha_3 = 0.2\alpha_0$ $\alpha_2 = 0.0002\alpha_0$	$\nu_{12} = \nu_{13} = \nu_{23} = \nu_0$ $\alpha_1 = 0.0002\alpha_0$ $\alpha_2 = \alpha_3 = 0.2\alpha_0$	$\nu = \nu_0$
$k = k_0$	$k_1 = k_3 = k_0$ $k_2 = 100k_0$	$k_1 = 100k_0$ $k_2 = k_3 = k_0$	$k = k_0$
$\rho = \rho_0$ $c_v = c_{v0}$	$\rho = 0.2\rho_0$ $c_v = 3c_{v0}$	$\rho = 0.2\rho_0$ $c_v = 3c_{v0}$	$\rho = \rho_0$ $c_v = c_{v0}$

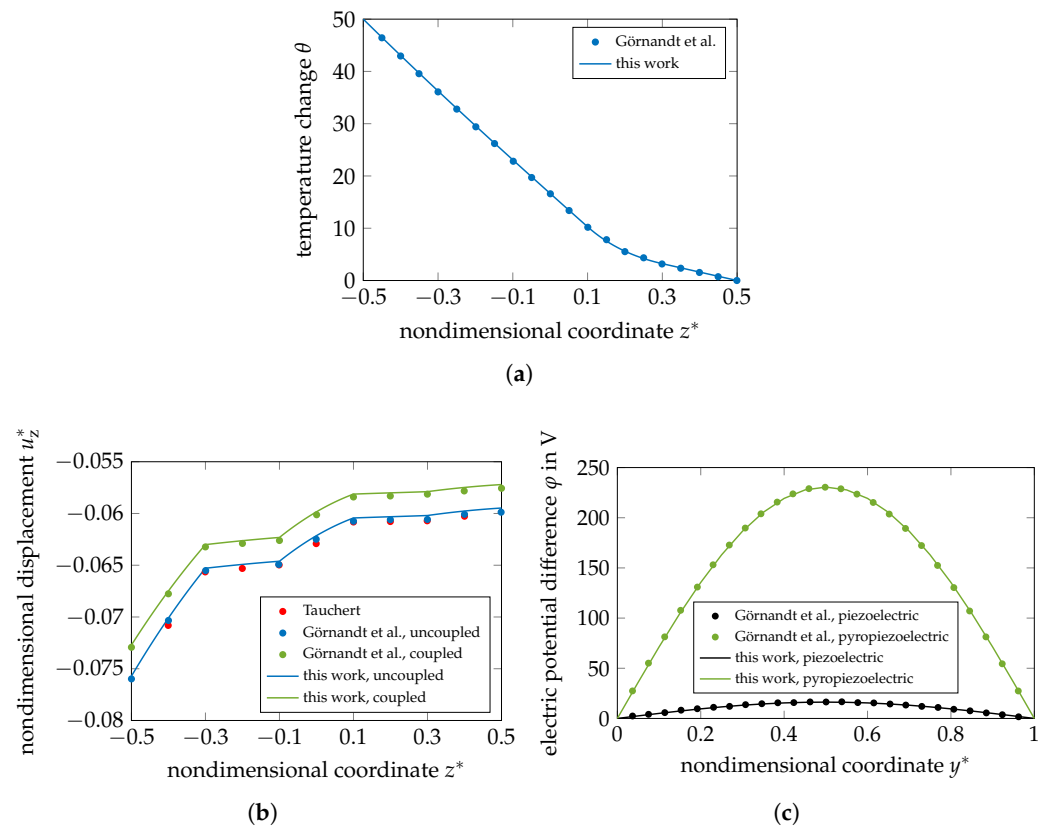


Figure A2. Comparison of the resulting quantities for the benchmark example proposed by Tauchert [42] and further discussed by Görnandt and Gabbert [43] and Shang et al. [67] with the implementation of this work: (a) Temperature change θ over the nondimensional coordinate z^* in the middle of the laminate along path $\mathcal{P}_1$. (b) Nondimensional displacement u_z^* over the nondimensional coordinate z^* in the middle of the laminate along path $\mathcal{P}_1$. (c) Electric potential difference φ over the nondimensional coordinate y^* on the bottom outer surface of the bottom piezoelectric laminate along path $\mathcal{P}_2$.

Appendix C. Material Parameters

The values for the unimorph (Figure 3) and bimorph (Figure 9) cantilever beam are listed in Table A2, while all parameters used for the simple cuboid (Figure 2a) and the bimetallic beam with attached PZT-5H patch from Kang and Yeatman [27] (Figure 12) are given in Table A3. The components of the elasticity tensor $\mathbf{C}$ and the piezoelectric coupling tensor $\mathbf{d}$ are written in Voigt notation according to the *IEEE Standard on Piezoelectricity* [56].

Table A2. Material parameters for the serial unimorph and bimorph.

PZT (C91) ¹	Phosphor Bronze ²	Unit
Mechanical		
$\alpha_R = 3.2782$		rad/s
$\beta_R = 1.2455 \times 10^{-5}$		s/rad
$\rho = 7750$	$\rho = 8780$	kg/m ³
$\underline{\mathbf{C}} = \begin{bmatrix} 118.27 & 75.52 & 73.64 & 0 & 0 & 0 \\ 75.52 & 118.27 & 73.64 & 0 & 0 & 0 \\ 73.64 & 73.64 & 109.97 & 0 & 0 & 0 \\ 0 & 0 & 0 & 24 & 0 & 0 \\ 0 & 0 & 0 & 0 & 24 & 0 \\ 0 & 0 & 0 & 0 & 0 & 21.38 \end{bmatrix}$	$E = 110$	GPa
	$\nu = 0.35$	/

Table A2. Cont.

PZT (C91) ¹	Phosphor Bronze ²	Unit
Electrical		
$\epsilon_{11} = \epsilon_{22} = 4400 \times 8.854 \times 10^{-12}$		F/m
$\epsilon_{33} = 5500 \times 8.854 \times 10^{-12}$		F/m
$\underline{d} = \begin{bmatrix} 0 & 0 & 0 & 0 & 820 & 0 \\ 0 & 0 & 0 & 820 & 0 & 0 \\ -330 & -330 & 640 & 0 & 0 & 0 \end{bmatrix} \times 10^{-12}$		C/N
Thermal		
$c_v = 440$	$c_v = 380$	J/(kg K)
$T_0 = 293.15$	$T_0 = 293.15$	K
$p_3 = -380 \times 10^{-6}$		C/(m ² K)
$k_{11} = k_{22} = k_{33} = 1.2$	$k = 50.0$	W/(m K)
$\alpha_{11} = \alpha_{22} = \alpha_{33} = 3.0 \times 10^{-6}$	$\alpha = 18.4 \times 10^{-6}$	1/K

Note: Only nonzero components of first- and second-order tensors are mentioned. ¹ Transversal isotropic material behavior with z-axis as axis of symmetry assumed with mechanical and electrical properties from *Fuji Ceramics Corporation* [68] and thermal properties from *Piezo.com* [69] and Bowen et al. [70]. ² Isotropic material behavior assumed with mechanical properties from Raghav et al. [71] and McCarthy et al. [72] and thermal properties based on Raghav et al. [71] and *Lake Shore Cryotronics Inc.* [73].

Table A3. Material parameters for the cuboid (only PZT-5H) and the bimetal beam from Kang and Yeatman [27] consisting of Ni-Fe and Ni-Cr-Fe with attached PZT-5H patch.

PZT-5H ¹	Ni-Fe (low CTE) ²	Ni-Cr-Fe (high CTE) ³	Unit
Mechanical			
$\alpha_R = 3.2782$			rad/s
$\beta_R = 1.2455 \times 10^{-5}$			s/rad
$\rho = 7500$	$\rho = 8050$	$\rho = 8100$	kg/m ³
$\underline{C} = \begin{bmatrix} 127.21 & 80.21 & 84.67 & 0 & 0 & 0 \\ 80.21 & 127.21 & 84.67 & 0 & 0 & 0 \\ 84.67 & 84.67 & 117.44 & 0 & 0 & 0 \\ 0 & 0 & 0 & 22.99 & 0 & 0 \\ 0 & 0 & 0 & 0 & 22.99 & 0 \\ 0 & 0 & 0 & 0 & 0 & 23.47 \end{bmatrix}$	$E = 145$ $\nu = 0.29$	$E = 210$ $\nu = 0.31$	GPa /
Electrical			
$\epsilon_{11} = \epsilon_{22} = 3130 \times 8.854 \times 10^{-12}$			F/m
$\epsilon_{33} = 3400 \times 8.854 \times 10^{-12}$			F/m
$\underline{d} = \begin{bmatrix} 0 & 0 & 0 & 0 & 741 & 0 \\ 0 & 0 & 0 & 741 & 0 & 0 \\ -274 & -274 & 593 & 0 & 0 & 0 \end{bmatrix} \times 10^{-12}$			C/N
Thermal			
$c_v = 440$	$c_v = 515$	$c_v = 445$	J/(kg K)
$T_0 = 298.15$	$T_0 = 298.15$	$T_0 = 298.15$	K
$p_3 = -380 \times 10^{-6}$			C/(m ² K)
$k_{11} = k_{22} = k_{33} = 1.2$	$k = 10.5$	$k = 12.0$	W/(m K)
$\alpha_{11} = \alpha_{22} = \alpha_{33} = 3.0 \times 10^{-6}$	$\alpha = 1.0 \times 10^{-6}$	$\alpha = 9.0 \times 10^{-6}$	1/K

Note: Only nonzero components of first- and second-order tensors are mentioned. ¹ Transversal isotropic material behavior with z-axis as axis of symmetry assumed with mechanical and electrical properties from *eFunda Inc.* [74] and thermal properties from *Piezo.com* [69] and Bowen et al. [70]. ² Isotropic material behavior assumed with mechanical and thermal properties estimated based on Kang and Yeatman [27] and *Lamineries Matthey* [75]. ³ Isotropic material behavior assumed with mechanical and thermal properties estimated based on Kang and Yeatman [27], *Special Metals* [76], Degnah et al. [77] and Wu et al. [78].

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