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A Topology Description Function Based Approach for Optimal Design of Piezoelectric Mass Sensors

Zheqi Lin[1], Xuansheng Wang[2]

[1] Research Institute of Sun Yat-sen University in Shenzhen, School of Information Science & Technology, Sun Yat-sen University, Shenzhen, 518057, China, linzheqi@gmail.com
[2] Research Institute of Sun Yat-sen University in Shenzhen, School of Information Science & Technology, Sun Yat-sen University, Shenzhen, 518057, China, wxs111111@163.com

1. Abstract
The mass sensors have attracted increased attention in the field of biomolecular and chemical detection. It has been found that the size, shape and geometry of the structure may affect the performance of the sensors. Based on this remark, in this paper, a topology optimization methodology for the design of plate-based sensors is proposed. The topology description function is used to describe the shape/topology of the structure. The design goal is to obtain the configuration of material that maximizes the mass detection sensitivity of the senor. On the basis of these formulations, an optimization algorithm is constructed using finite element method and the method of moving asymptotes (MMA). Two numerical examples are presented to demonstrate the validity of the proposed problem formulation. The results suggest that the performance of the sensors can be improved by using the proposed approach.

2. Keywords: topology optimization, mass detection sensitivity, finite element method, topology description function

3. Introduction
Mass sensors have attracted interest as a sensing platform for biomolecular and chemical detection. A great amount of research has been dedicated to the development of high performance mass sensors suitable for measuring masses down to molecular or atomic levels[1-3]. Mass sensing based on piezoelectric actuation is a powerful label-free technique that is receiving broad attention for many applications. In the detection, a piezoelectric mass sensor's resonance frequency shift is measured to quantify the small mass attached to the structural surface. Using this principle, a piezoelectric mass sensor was demonstrated for real-time in situ chemical or gas detection. Piezoelectric mass sensors have the advantages of using only electrical means for sensing avoiding the complex optical detection equipment in silicon-based sensors. Moreover, because it is highly piezoelectric, it can withstand damping in water and perform in situ biodetection and quantification in water, which is advantageous when compared to the commercially prevalent enzyme linked immuno sorbent assays which are less sensitive and require tedious labeling.

In view of their potential in biosensor development, it is important to examine how a piezoelectric mass sensor’s design affects its mass detection performance. The mass sensing behavior can be explained by the performance parameters, such as the mass detection sensitivity[4], the limit of detection or the minimum detectable mass[5], and the quality factor[6]. These parameters are of considerable importance when developing a high performance mass sensor. Many theoretical and experimental works are available on modeling and applications of piezoelectric mass sensor. In the work reported, the effect of geometric parameters (length, width, and thickness)[7] and material parameters (density and Young’s modulus)[8], or electrical properties (capacitance and dielectric permittivity)[9] on the performance of the piezoelectric mass sensor is examined. Based on this remark, we confirm that the structures can be configured in different ways to improve the performance of piezoelectric mass sensors.

Topology optimization is a powerful design technique that has been successfully applied to stiffness maximization problems[10], eigenfrequency problems[11], compliant mechanism design[12], piezoelectric transducer design[13] and so on. In this paper, a new approach for the design of piezoelectric mass sensors based on implicit topology description functions is proposed. The topology description function is used to describe the shape/topology of the structure, which is approximated in terms of its nodal values by finite element. The design goal is to obtain the configuration of material that maximizes the mass sensitivity of the senor. In the view of mass sensor development, the mass sensitivity is an important characteristic representing the sensor performance. A definition of mass sensitivity is the resonance frequency shift as a function of added mass on the sensing area. Numerical examples are presented to demonstrate the validity of the proposed problem formulation.

4. Problem formulation

In this section, problem formulation is presented for the design of piezoelectric mass sensors. First, a key performance parameter which explains the mass sensing behavior is introduced. Then, the optimization formulation that consists in distributing the material within a design domain to maximize the performance of piezoelectric mass sensors is proposed.

4.1. Mass sensing performance

As a powerful label-free technique, mass sensing based on piezoelectric actuation has received attention for many applications, ranging from biomedical, chemical, biosensors, and even atomic physics. In the view of mass sensor development, the mass detection sensitivity is a considerable characteristic representing the sensor performance. A definition of mass detection sensitivity is the variation in a measurable parameter as a function of adsorbed mass on the sensing area. The adsorption causes a change in the sensor's mass, which in turn causes a shift in the resonance frequency. The mechanical resonance is a measurable parameter commonly used for mass sensors operating in the resonant mode. The resonant frequency change $\triangle f$ of the sensor is proportional to the added mass $\triangle m$. Thus, the mass detection sensitivity S can be defined as resonance frequency shifts per unit mass change:

$$S = \frac{\Delta f}{\Delta m} \tag{1}$$

In mass detection, a piezoelectric sensor's resonance frequency shift is measured to quantify the small mass attached to its surface. The mass sensors with the higher mass detection sensitivity are highly desirable. In this paper, a topology optimization based method will be applied to design the configuration of the mass sensor with maximum mass detection sensitivity.

4.2. Topology optimization

When considering the design problem of determining the design domain Ω_d to minimize objective functions, the key idea of topology optimization is to introduce a fixed, extended design domain Ω that includes the original design domain Ω_d and the utilization of the following characteristic function:

$$\chi(x) = \begin{cases} 1, & x \in \Omega_d \\ 0, & x \in \Omega \setminus \Omega_d \end{cases} \tag{2}$$

where x denotes a position in the extended design domain Ω. Using this function, the original structural design problem is replaced by a material distribution problem. In practice, the topology optimization problem is treated by discretizing the design domain into n finite elements and requiring $\chi(x)$ to be constant in each element. Since this characteristic function can be discontinuous, some regularization techniques should be introduced. The solid isotropic material with penalization (SIMP) method is a popular method used in topology optimization. However, it also encounters some numerical instability problem, such as checkerboard patterns and mesh dependency. In this paper, a topology description function (TDF) based method is proposed to formulate the material distribution problem. The main idea of the TDF approach is to map a function T=$T(x)$ on the reference domain into a geometry using a cut-off level, as shown in Figure 1. A point x in the reference domain gets material assigned if the value of $T(x)$ exceeds the cut-off level, and otherwise the point is void. The characteristic function can be expressed as:

$$\chi(x) = H(T(x)) \tag{3}$$

Where, H is the Heaviside function. In this way, the geometry is determined by the topology description function which is considered as design parameter.

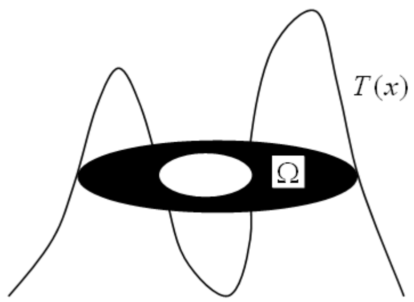


Figure 1: Topology description function

Typically, at each iteration of the topology optimization procedure a structural analysis has to be carried out, which is usually done using the finite element method. The interpolation scheme for topology description function is treated as the same with displacement field. That is, assuming the value of T at I^{th} node is T_I, in the whole design domain we have,

$$T^h = \sum_{I=1}^{n} N_I(x) T_I \tag{4}$$

where, $N_I(x)$ is the shape function for node I; n is the number of nodes in each element. Learn from the successful experience of RAMP for removing localized eigenmodes in low density areas, the material property is defined as,

$$C^e = C^0 \frac{\left(\sum_{i=1}^{m} H\left(T_i^h\right)\right) \Big/ m}{1 + q\left(1 - \left(\sum_{i=1}^{m} H\left(T_i^h\right)\right) \Big/ m\right)} \tag{5}$$

$$\rho^e = \rho^0 \left(\sum_{i=1}^{m} H\left(T_i^h\right)\right) \Big/ m \tag{6}$$

where, C^0 and ρ^0 denote the elasticity modulus and density of the material respectively; m is the number of gauss integral points in each element; q is a penalty parameter, which is chosen as 10 in this paper.

In mass detection, the adsorbed layer on the sensor is assumed to be uniformly distributed on the surface and no apparent rigidity. The distribution of adsorbed layer is depended on the configuration of the senor. Therefore, the mass perturbation in a senor can be considered as $\rho_a^e = \alpha \rho^e$, where α is a small number and chosen as 0.0001 here.

In numerical implementation, smooth processing should be applied to Heaviside function for its differential operation. The smooth form can be expressed as,

$$H(T) = \begin{cases} 0, & T < -\Delta \\ \dfrac{3}{4}\left(\dfrac{T}{\Delta} - \dfrac{T^3}{3\Delta^3}\right) + \dfrac{1}{2}, & -\Delta \le T < \Delta \\ 1, & T \ge \Delta \end{cases} \tag{7}$$

where, $\triangle > 0$ is a smoothing parameter.

4.3. Statement of Optimization Problem

In the considered topology optimization problem, the design objective is to maximize the mass detection sensitivity of a mass sensor. The design optimization problem for structural topology can be mathematically stated as

$$\begin{aligned} \underset{T(x)}{\text{maximize:}} \quad & S = \frac{f - f_a}{\Delta m} \\ \text{subject to:} \quad & K\phi = \lambda M \phi \\ & K_a \phi_a = \lambda_a M_a \phi_a \\ & V = \int H\left(T(x)\right) d\Omega \le \overline{V} \\ & -l \le T_i \le l \qquad i = 1, 2 \cdots, nd \end{aligned} \tag{8}$$

where, f_a and f is the resonance frequency of the mass senor with and without add mass respectively; $\triangle m$ is the added mass; K and M are stiffness matrix and mass matrix of the structure; ϕ is the eigenvector; λ is square of natural frequency; the subscript a indicates the structure with added mass; $\overline{V}$ is the upper bound of the material volume; l is the bound of topology description function; nd is the number of the node.

The design optimization problem described in Eq.(8) can be solved using a gradient-based mathematical programming approach. The method of moving asymptotes (MMA)[14], which is suitable for solving large-scale constrained optimization problems, is employed in this study.

4.4. Sensitivity analysis

The design sensitivity analysis of the concerned performance functional is necessary in the gradient-based optimization process. In what follows, the procedure for calculating the sensitivity of objective function and constraint with respect to the design variables will be described.

By taking the derivative of the objective function, we obtain

$$\frac{\partial S}{\partial T_I} = \frac{\Delta m\left(f^{'} - f_a^{'}\right) - \Delta m^{'}\left(f - f_a\right)}{\left(\Delta m\right)^2} \tag{9}$$

From Eq.(4)-(8), we have that,

$$\partial \lambda / \partial T_I = \sum_{e=1}^{ne} \frac{(1+q)}{\left(1+q\left(1-\left(\sum_{i=1}^{m} H\left(T_i^e\right)\right)\Big/ m\right)\right)^2} H^{'}\left(T_I\right)\left(\phi^e\right)^T k_0^e \phi^e - \lambda \sum_{e=1}^{ne} H^{'}\left(T_I\right)\left(\phi^e\right)^T m_0^e \phi^e \tag{10}$$

where, ne is the number of elements whose nodes include node I. The superscript e denotes these elements. Since $f = \sqrt{\lambda}/2\pi$, it is easy to obtain the derivatives of the f in relation to the design variables. To calculate the derivative of the sensitivity of the sensor, we therefore solve two systems of equations for the conditions with and without added mass.

The derivative of the added mass with respect to design variables can be expressed as:

$$\partial \Delta m / \partial T_I = \alpha \rho \int H^{'}\left(T^h(x)\right) N_I(x) \, d\Omega \tag{11}$$

The sensitivity of constraint function is similar to Eq.(11). It can be expressed as:

$$\partial V / \partial T_I = \int H^{'}\left(T^h(x)\right) N_I(x) \, d\Omega \tag{12}$$

5. Numerical example

In this section, two examples will be presented to illustrate the effectiveness of the proposed formulation and numerical techniques. The piezoelectric mass sensors are composed of a PZT layer attached to a stainless steel substrate (plate). The purpose of this paper is focused on the design of structures with maximum detection sensitivity. The properties of the PZT layer and stainless steel are listed in Table 1. The target values $\overline{V}$ is set to 0.4, i.e., material is allowed to fill 40% of the design domain.

Table 1: Material properties

	PZT	Stainless steel
Density (kg/m^3)	7500	7800
Young's modulus (N/m^2)	6.1×10^{10}	20×10^{10}
Poisson's ratio	0.3	0.3
Thickness (mm)	0.3	0.1

5.1. Optimal design of a cantilever sensor

Consider the design of a cantilever sensor, which has a dimension of 20×20 mm and is discretized with 40×40 finite elements. For simplicity in structural analysis, the effective Young's modulus and density of the sensor can be expressed as[7]:

$$E^0 = \frac{E_p^2 r_p^4 + E_s^2 r_s^4 + 2E_p E_s r_p r_s \left(2r_p^2 + 2r_s^2 + 3r_p r_s\right)}{E_p r_p + E_s r_s} \tag{13}$$

$$\rho^0 = \rho_p r_p + \rho_s r_s \tag{14}$$

where, $r_p = h_p/h$; $r_s = h_s/h$. The design task is to maximize the mass detection sensitivity of a sensor with adsorbed layer distributed on the surface.

In the initial design, we set the topology description function value of each node T_i=0.1 (i=1,2,…nd). The iteration history is plotted in Figure 2, from which a fairly steady increase of detection sensitivity can be observed. The optimization procedure converges after approximately 40 iteration steps. The topology optimization results are shown in Figure 3, which suggests a distinct black-and-white distribution of material.

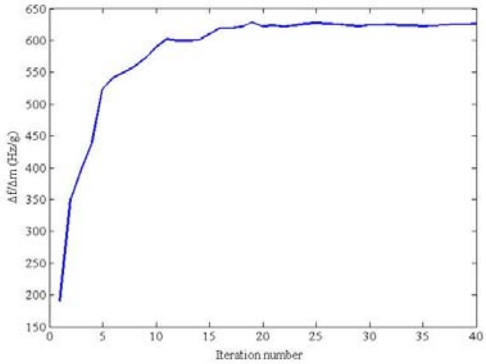
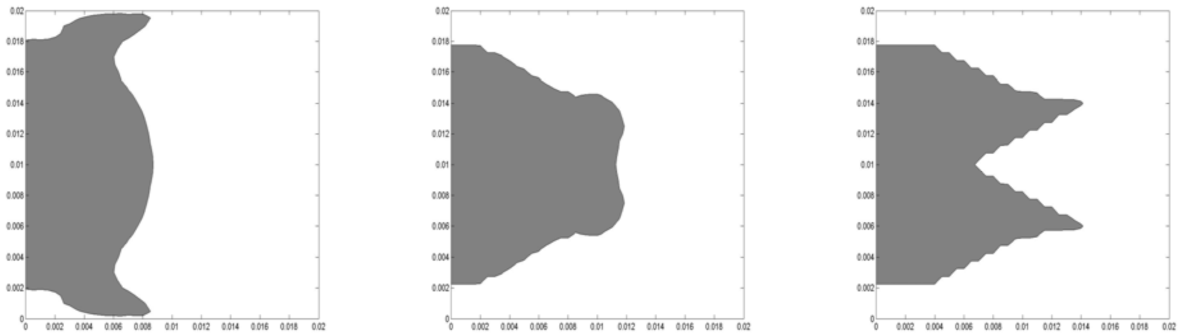


Figure 2: Iteration process



The 5th step | The 15th step | The final design

Figure 3: The intermediate and optimal topology of the sensor

5.2. Optimal design of a sensor with four edges clamped

Consider the optimal design of a sensor with four edges clamped, which has the same design domain with the first example. The iteration history is plotted in Figure 4. The optimization process converges after 35 iterations. The intermediate and optimal topology of the sensor are plotted in Figure 5. It can be seen that the layout of the whole structure is clear and suitable for manufacture.

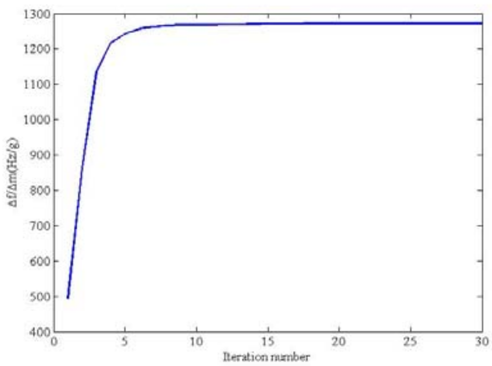
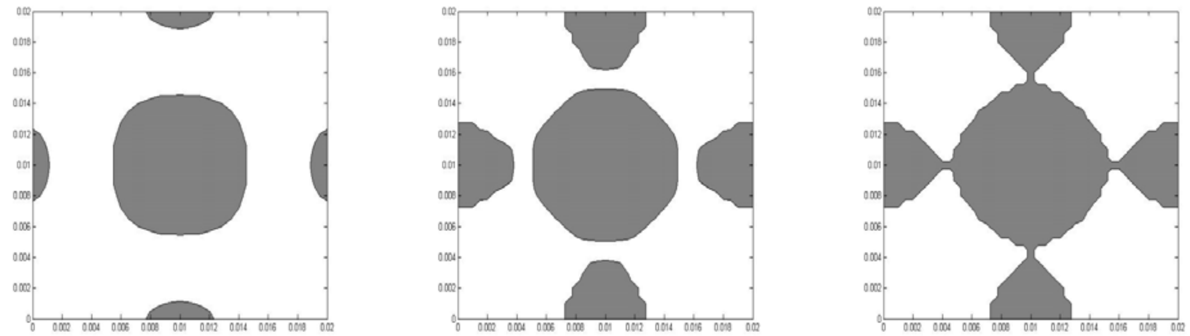


Figure 4: Iteration process



The 5th step The 15th step The final design

Figure 5: The intermediate and optimal topology of the sensor

6. Conclusion

This article presents a design optimization method for piezoelectric mass sensor. Both the structural layout is determined using topology optimization techniques for acquiring maximum mass detection sensitivity. The topology description function is used to describe the shape/topology of the structure. Numerical examples have confirmed that the proposed method is effective in presenting useful conceptual designs of piezoelectric mass sensors. Moreover, the obtained optimal structural layouts are relatively clear and easy for manufacturing.

7. Acknowledgements

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8. References

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