



Design and finite element simulation of metal-core piezoelectric fiber/epoxy matrix composites for virus detection

Yinli Wang^a, Yu Shi^b, Fumio Narita^{c,*}

^a Department of Materials Processing, Graduate School of Engineering, Tohoku University, Aoba-yama 6-6-02, Sendai, Japan

^b Department of Mechanical Engineering, University of Chester, Thornton Science Park, Pool Lane, Chester, CH2 4NU, UK

^c Department of Frontier Sciences for Advanced Environment, Graduate School of Environmental Studies, Tohoku University, Aoba-yama 6-6-02, Sendai, Japan

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ABSTRACT

Undoubtedly, the coronavirus disease 2019 (COVID-19) has received the greatest concern with a global impact, and this situation will continue for a long period of time. Looking back in history, airborne transmission diseases have caused huge casualties several times. COVID-19 as a typical airborne disease caught our attention and reminded us of the importance of preventing such diseases. Therefore, this study focuses on finding a new way to guard against the spread of these diseases such as COVID-19. This paper studies the dynamic electromechanical response of metal-core piezoelectric fiber/epoxy matrix composites, designed as mass load sensors for virus detection, by numerical modelling. The dynamic electromechanical response is simulated by applying an alternating current (AC) electric field to make the composite vibrate. Furthermore, both concentrated and distributed loads are considered to assess the sensitivity of the biosensor during modelling of the combination of both biomarker and viruses. The design parameters of this sensor, such as the resonant frequency, the position and size of the biomarker, will be studied and optimized as the key values to determine the sensitivity of detection. The novelty of this work is to propose functional composites that can detect the viruses from changes of the output voltage instead of the resonant frequency change using piezoelectric sensor and piezoelectric actuator. The contribution of this detection method will significantly shorten the detection time as it avoids fast Fourier transform (FFT) or discrete Fourier transform (DFT). The outcome of this research offers a reliable numerical model to optimize the design of the proposed biosensor for virus detection, which will contribute to the production of high-performance piezoelectric biosensors in the future.

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1. Introduction

The coronavirus disease pandemic 2019 (COVID-19) has significantly impacted global wellbeing. By now there have been tens of millions of people infected. COVID-19 has quickly run out of control and triggered outbreaks in almost every country on the earth due to this virus spreading through the respiratory route, both by droplets and aerosols. Social distancing and the wearing the face coverings such as cloth face masks, surgical masks, and respirators, has become a regular way to constrain the virus's further expansion, however, such controls might be less able to protect people from a long term infection risk as the respiratory droplets could evaporate into aerosols and hence remain suspended in the air for longer

periods of time causing airborne transmission [1]. There is plenty of data in the literature [2,3] which shows that airborne transmission of viruses has threatened human health and safety for a long while in this world. Therefore, there is an urgent demand for methods to tackle the challenge of accurately monitoring and detecting such viruses in the air, so assisting governments to control the pandemic and benefit all.

The quartz crystal microbalance (QCM) has been widely used for micro-mass detection based on the piezoelectric effect of quartz crystals. The QCMs utilize frequency shift as the determining element of an oscillator circuit where the resonant frequency is measured. Many studies have been conducted to verify their performance. A 150 MHz high fundamental frequency quartz crystal microbalance (HFF-QCM) sensor was designed for bio-sensing applications and validated by both experimental and the finite element method (FEM) [4]. The result showed that simulations of the proposed design were in good agreement with the electrical

* Corresponding author.

E-mail address: narita@material.tohoku.ac.jp (F. Narita).

characterization of the manufactured resonators, and the sensor was also validated for bio-sensing applications. Using a QCM sensor platform, a single functional bio-sensor would require at least two separate quartz crystals. This brings a lot of problems such as larger sensor size, increased price tag, and further measurement errors. To solve these problems, multichannel QCM (MQCM) have been devised, such as the 4-channel molecularly imprinted polymer (MIP) coated QCM biosensor array. The 4-channel MQCM has been demonstrated to be a suitable miniature sensor platform for MIP-based biosensors, and finite element analysis (FEA) is a very suitable and convenient tool in the search for improved crystal designs [5]. But MQCMs still have drawbacks as the mass absorbed on the surface of one channel results in frequency decreases of not only its own but also other channels. Although QCM techniques have improved in robustness and reliability and allow the measurement of molecular interactions in real-time, the lack of sensitivity to electrical properties still limits their application.

In the same manner, lead zirconate titanate (PZT) also has a great potential for application as a micro-mass detection sensor due to its outstanding piezoelectricity. PZT is a high-performance piezoelectric ceramic which is used in a number of practical applications such as sensors, actuators, and energy harvesters. Compared with other piezoelectric materials, PZT shows excellent piezoelectricity. However, its inherent mechanical brittleness impedes its strain resistance and prevents it from forming complex shapes [6]. To tackle the technical barrier of flexibility of piezoelectric ceramics, many strategies have been devised to overcome its weaknesses, such as three-dimensional (3D) printing technology. By this method, complex shapes of piezoelectric ceramics can be precisely produced with potential applications in various fields [7]. The most common way to improve the mechanical properties of piezoelectric ceramics is to fabricate them as composites. For example, polymethyl methacrylate (PMMA) based PZTs flexible composite films have been fabricated by a solvent evaporation technique, and the results showed that the composites are suitable, potential, and functional candidates for energy harvesting applications [8]. In our previous study, embedding a PZT hollow fiber into an aluminum matrix not only enhanced the mechanical performance, but also improved the piezoelectricity of the PZT composites due to the high residual stresses of the PZT fiber [9]. Many studies have proved that PZTs are prospective materials for building a dynamic detection system, and FEA is a potential method to further optimize the design of detecting viruses. A novel piezoelectric micro electromechanical system (MEMS) sensor for the detection of 100 nm size viruses has been designed, which mainly consists of a PZT-5A micro cantilever and biomarker [10]. The results showed a strong possibility of the sensor to be realized as a 100 nm virus detector. Further studies were implemented to confirm the dynamic electromechanical response of PZT under alternating current (AC) electric fields [11,12]. Therefore, in this research, the development of a piezoelectric composite sensor for real-time virus detection is proposed, for the benefit of global well-being.

Although the feasibility and promise have been demonstrated by the above literatures, the design of a biosensor, with optimized parameters for the detection of a specific virus with reliable accuracy, still needs to be addressed. Therefore, FEM could be an ideal technique to help numerically optimize the design with parametric studies and guide the experimental measurements under a shortened design cycle [13–15].

In this study, the PZT fibers are composed with an epoxy matrix. This is because polymer matrix composites have many advantages such as being lightweight, possess high stiffness, and have high strength along the direction of their reinforcements, which can not only improve the mechanical properties but also keep the high sensitivity of the piezoelectric ceramics. The commercial FEA package

ANSYS is used to numerically design and optimize the piezoelectric sensor system for virus detection. The design parameters of this system are studied and optimized with varying the resonant frequency, and the location and size of the biomarker to achieve a reliable sensitivity of virus detection. All of the results are presented graphically and discussed so as to judge the feasibility of this system.

2. Basic equations

Consider a piezoelectric material with no body force and free charge. The field equations in the Cartesian coordinates x_i ($i = 1, 2, 3$) are given by:

$$\sigma_{ji,j} = \rho u_{i,tt} \quad (1)$$

$$D_{i,i} = 0 \quad (2)$$

where σ_{ij} and D_i are the components of the stress tensor and electric displacement vector, respectively, u_i is the component of the displacement vector, and ρ is the mass density. A comma followed by an index denotes partial differentiation with respect to the space coordinates x_i or the time t , and the Einstein summation convention over repeated indices is used. The relation between the strain tensor component ε_{ij} and the displacement vector component u_i is given by:

$$\varepsilon_{ij} = \frac{1}{2}(u_{j,i} + u_{i,j}) \quad (3)$$

and the electric field intensity vector component E_i is:

$$E_i = -\phi_{,i} \quad (4)$$

where ϕ is the electric potential. Constitutive relations can be written as:

$$\varepsilon_{ij} = s_{ijkl}\sigma_{kl} + d_{kij}E_k \quad (5)$$

$$D_i = d_{ikl}\sigma_{kl} + \varepsilon_{ik}^T E_k \quad (6)$$

where s_{ijkl} , d_{kij} , ε_{ik}^T are the elastic compliance, piezoelectric coefficient, and permittivity at constant stress, respectively, which satisfy the following symmetry relations:

$$s_{ijkl} = s_{jikl} = s_{ijlk} = s_{klij}, d_{kij} = d_{kji}, \varepsilon_{ik}^T = \varepsilon_{ki}^T \quad (7)$$

The constitutive Eqs. (5) and (6) for piezoelectric material poled in the x_3 -direction are:

$$\begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{31} \\ 2\varepsilon_{12} \end{Bmatrix} = \begin{bmatrix} s_{11} & s_{12} & s_{13} & 0 & 0 & 0 \\ s_{12} & s_{11} & s_{13} & 0 & 0 & 0 \\ s_{13} & s_{13} & s_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{66} \end{bmatrix} \begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \end{Bmatrix} + \begin{bmatrix} 0 & 0 & d_{31} \\ 0 & 0 & d_{31} \\ 0 & 0 & d_{33} \\ 0 & d_{15} & 0 \\ d_{15} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} E_1 \\ E_2 \\ E_3 \end{Bmatrix} \quad (8)$$

$$\begin{Bmatrix} D_1 \\ D_2 \\ D_3 \end{Bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & 0 & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \end{Bmatrix} + \begin{bmatrix} \epsilon_{11}^T & 0 & 0 \\ 0 & \epsilon_{11}^T & 0 \\ 0 & 0 & \epsilon_{33}^T \end{bmatrix} \begin{Bmatrix} E_1 \\ E_2 \\ E_3 \end{Bmatrix} \quad (9)$$

where:

$$\sigma_{23} = \sigma_{32}, \sigma_{31} = \sigma_{13}, \sigma_{12} = \sigma_{21} \quad (10)$$

$$\epsilon_{23} = \epsilon_{32}, \epsilon_{31} = \epsilon_{13}, \epsilon_{12} = \epsilon_{21} \quad (11)$$

$$\begin{aligned} s_{11} &= s_{1111} \\ &= s_{2222}, \\ s_{12} &= s_{1122}, \\ s_{13} &= s_{1133} \\ &= s_{2233}, \\ s_{33} &= s_{3333}, \\ s_{44} &= 4s_{2323} \\ &= 4s_{3131}, \\ s_{66} &= 4s_{1212} \\ &= 2(s_{11} - s_{12}) \end{aligned} \quad (12)$$

$$d_{15} = 2d_{131} = 2d_{223}, d_{31} = d_{311} = d_{322}, d_{33} = d_{333} \quad (13)$$

In this study, the equation of motion (1) and Gauss's Eq. (2) are solved by the FEM. From Eqs. (8) and (9), the differential Eqs. (1) and (2) are coupled. Dynamic FEA was performed on the specific piezoelectric devices [11,16], and the validity of the theory was verified by comparison with the experimental results. In Ref. 16, the output voltage of the piezoelectric energy harvesting cantilever under vibration was analyzed, and it was numerically and experimentally shown that the resonant frequency f_0 decreases with the weight m of the proof mass at the tip of the cantilever. The principle of this piezoelectric energy harvesting device is equivalent to that of a virus detecting sensor. That is, the change in the mass loading of the piezoelectric sensor is translated into a resonant frequency change (see Fig. 1). For the simple thickness shear vibration mode, the shift of frequency f due to mass deposition on the active surface area A of the piezoelectric device is given by [17]:

$$\Delta f = -\frac{2f_0^2}{A\sqrt{\rho/s_{44}}} \Delta m \quad (14)$$

For the cantilever bending vibration mode, the relation between frequency shift and mass deposition can be described as [18,19]:

$$\left[\frac{1}{(f_0 - \Delta f)^2} - \frac{1}{f_0^2} \right] = \frac{4\pi^2}{k} \Delta m \quad (15)$$

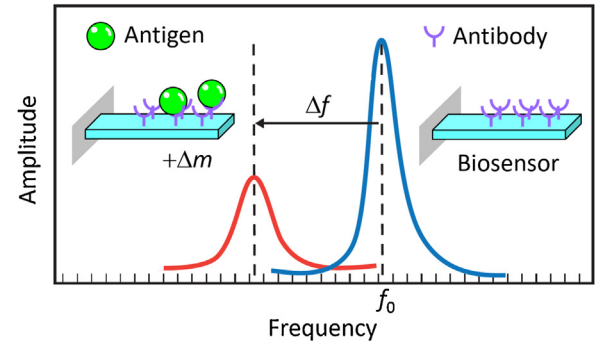


Fig. 1. Schematic illustration of the operation of the piezoelectric virus detecting sensor. Biomarker antibodies are fixed on the upper surface of the sensor. Antigen then binds with the antibodies and the mass change Δm on the surface leads to the frequency shift Δf .

Table 1
Dimensions of this composite.

Dimension	Value (mm)
Diameter of Pt (d_0)	0.05
Diameter of PZT (d_1)	0.2
Length of epoxy matrix (l)	10
Width of epoxy matrix (w)	1
Thickness of epoxy matrix (h)	0.3

where k is the spring constant. The constant k for the cantilever with microscale length (l), width (w), and nanoscale thickness (h) can be obtained as [20]:

$$k = \frac{h^3 w}{4s_{11} l^3} \quad (16)$$

In the case of the metal-core piezoelectric fiber/epoxy matrix composite, it is impossible to evaluate the frequency change using Eq. (14) or (15). Hence FEA is required. Here, the change in mass Δm is approximated by a concentrated or distributed load, as described later.

3. Finite element modelling

A numerical 3D finite element model has been developed to simulate and optimize the dynamic electromechanical response of the metal-core piezoelectric fiber/epoxy matrix composite material, illustrated by Fig. 2(a). Essentially, the virus sensor of this study is utilizing this composite as a mass load detection sensor. For this reason, the whole mass of this composite should keep it as low as possible; because the smaller it is, the higher sensitivity can be achieved. In this structure, platinum (PT) fibers are embedded in PZT hollow fiber as electrodes since platinum is very stable in high temperature when PZT ceramic was producing, and then the polarization direction of PZT fibers can be implemented radially. As a result, PZT fibers can maximize the electromechanical transformation of strains from every direction because the piezoelectricity of d_{33} that is the polarization direction of PZT is largest. The diameter of PZT fiber in this study is already closed to the market limit. In consideration of application, thinner fiber will not be taken into account here; additionally, symmetrical structure can make vibration more stable. Therefore, three PZT fibers are put into use. In order to avoid mutual interferences, the distance between each PZT fiber is also reserved. The shape of base material, where the PZT fibers are embedded, is cuboid because square geometry is convenient to cohere or embed in actual circumstances. In view of application, the ambient conditions are relatively simple and not too harsh, structure optimization for finding the perfect design is omitted. A rectangular cartesian coordinate system (x, y, z) is

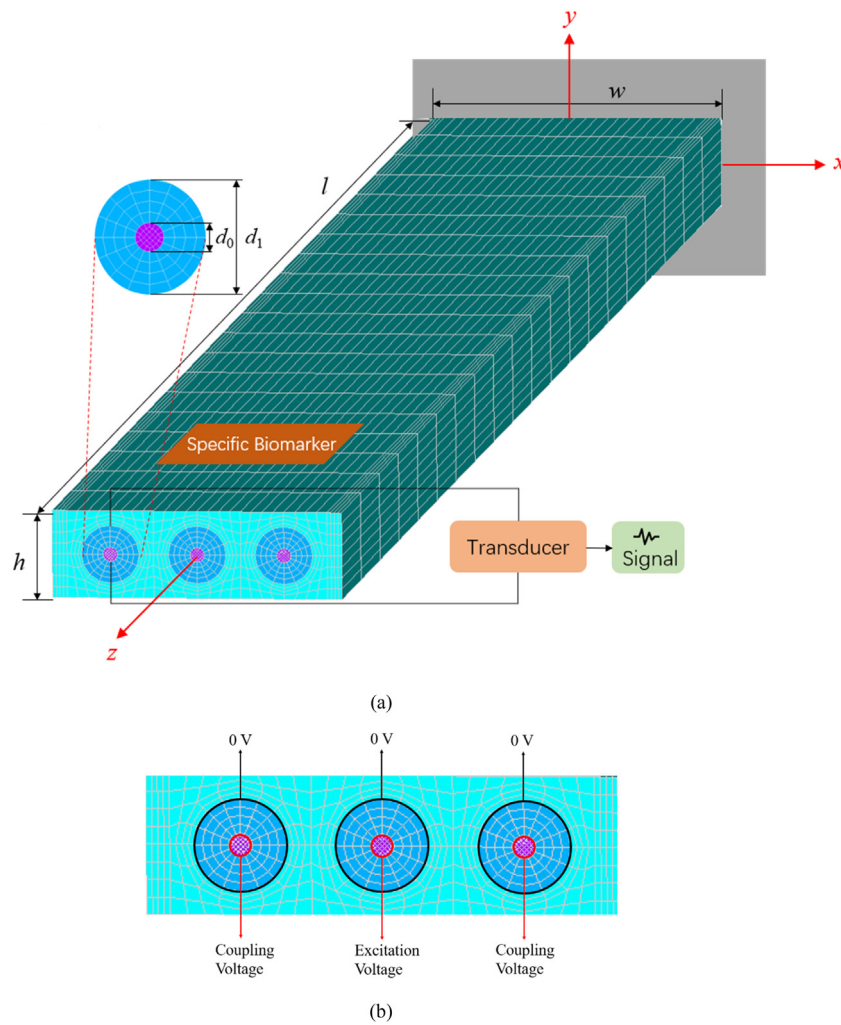


Fig. 2. (a) Schematic of Pt-core PZT fiber/epoxy matrix biosensor.

(b) Degrees of freedom of electric potential

Table 2
Material properties of PZT.

Elastic compliances ($\times 10^{-12}$ m ² /N)	
s_{11}	16.5
s_{33}	20.7
s_{44}	43.5
s_{12}	-4.78
s_{13}	-8.45
Piezoelectric coefficients ($\times 10^{-12}$ m/V)	
d_{31}	-274
d_{33}	593
d_{15}	741
Permittivity ($\times 10^{-10}$ C/Vm)	
ϵ_{11}^T	277
ϵ_{33}^T	301
Mass density (kg/m ³)	
ρ	7800

Table 3
Material properties of epoxy and Pt.

	Epoxy	Pt
Young's modulus ($\times 10^9$ N/m ²)		
E	3.23	168
Poisson's ratio		
ν	0.3	0.38
Mass density (kg/m ³) ρ	2000	21,450

used for modelling with coincidence between the z axis and the direction of the piezoelectric fiber. Meanwhile, the origin of the coordinate system coincides with the center of the back side in the composite material. All of the boundary conditions about the epoxy matrix are operated based on the cartesian coordinate system. In the traditional fabrication process of epoxy resin composites, the temperature and shrinkage during solidification are relatively low, so that the residual thermal stress which can be generated during working temperature is ignored. This model consists of a PT fiber (diameter d_0 , length l) embedded into a circular PZT tube (outer diameter d_1 , inner diameter d_0 and length l) and an epoxy plate (length l , width w and thickness h). Each of the PZT tubes is assumed to be perfectly bonded on the Pt surface and to the epoxy matrix. In order to apply proper boundary conditions on the PZT hollow fibers, the problem is also formulated using a three cylindrical coordinate system ($r_i, \theta_i, z_i, i = 1, 2, 3$), where the z_i is also in accordance with each longitudinal axis of the Pt fiber and 1, 2, 3 represent the left, center and right fibers, respectively. The dimensions of this composite with three metal-core piezoelectric fibers are shown in Table 1. The distance between the centers of two fibers is 0.3 mm so that the distance between adjacent fiber surfaces is equal to the fiber radius. The material properties of PZT, epoxy and Pt are listed in Table 2 and Table 3. The constitutive Eqs. (8) and (9) for piezoelectric material in a cylindrical coordinate system can be rewritten

as [21]

$$\begin{Bmatrix} \varepsilon_{rr} \\ \varepsilon_{\theta\theta} \\ \varepsilon_{zz} \\ \varepsilon_{r\theta} \\ \varepsilon_{\theta z} \\ \varepsilon_{rz} \end{Bmatrix} = \begin{bmatrix} s_{33} & s_{13} & s_{13} & 0 & 0 & 0 \\ s_{13} & s_{11} & s_{12} & 0 & 0 & 0 \\ s_{13} & s_{12} & s_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{44} \end{bmatrix} \begin{Bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{zz} \\ \sigma_{r\theta} \\ \sigma_{\theta z} \\ \sigma_{rz} \end{Bmatrix} + \begin{bmatrix} d_{33} & 0 & 0 \\ d_{31} & 0 & 0 \\ d_{31} & 0 & 0 \\ 0 & d_{15} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & d_{15} \end{bmatrix} \begin{Bmatrix} E_r \\ E_\theta \\ E_z \end{Bmatrix} \quad (17)$$

$$\begin{Bmatrix} D_r \\ D_\theta \\ D_z \end{Bmatrix} = \begin{bmatrix} d_{33} & d_{31} & d_{31} & 0 & 0 & 0 \\ 0 & 0 & 0 & d_{15} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{15} \end{bmatrix} \begin{Bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{zz} \\ \sigma_{r\theta} \\ \sigma_{\theta z} \\ \sigma_{rz} \end{Bmatrix} + \begin{bmatrix} \varepsilon_{33}^T & 0 & 0 \\ 0 & \varepsilon_{11}^T & 0 \\ 0 & 0 & \varepsilon_{11}^T \end{bmatrix} \begin{Bmatrix} E_r \\ E_\theta \\ E_z \end{Bmatrix} \quad (18)$$

This model was meshed using a twenty-node coupled field element. In total, 11,840 elements and 51,657 nodes were used. It should be noted that before carrying out simulations, a mesh sensitivity study was performed to ensure that the mesh was fine enough. Degrees of freedom (DOF) of this model's nodes include 3D displacements u_x , u_y , u_z and electric potential ϕ . In this study, the biosensor is considered to be implemented by fixing the back side ($z=0$ plane) as shown in Fig. 2(a), so the displacements of all nodes in the back side are set to zero, i.e., $u_x = u_y = u_z = 0$ ($-w/2 \leq x \leq w/2$, $-h/2 \leq y \leq h/2$, $z=0$). The middle PZT fiber is used for the actuator to make this composite sensor vibrate and generate an electric field. The excitation voltage amplitude applied to the middle fiber was chosen to be 1 V, which is applied by setting the electric potential of outer circle in the PZT tube as $\phi=0$ ($r_2=d_1/2$, $0 \leq \theta_2 \leq 2\pi$, $0 \leq z_2 \leq l$) and applying the excitation AC voltage $\phi_e = 1 \times \exp(i\omega t)$ ($r_2 = d_0/2$, $0 \leq \theta_2 \leq 2\pi$, $0 \leq z_2 \leq l$) on the Pt, where the Pt serves as an electrode, and $\omega = 2\pi f$ is the angular frequency. In the same manner, to evaluate the output voltage, the electric potentials of the left and right fibers are also set up. The details refer to Fig. 2(b). The electrical potential of each outer circle (black circles in Fig. 2(b)) in the PZT fiber is set as $\phi=0$ ($r_i=d_1/2$, $0 \leq \theta_i \leq 2\pi$, $0 \leq z_i \leq l$ ($i=1, 3$)), and the inner circle (red circles in Fig. 2(b)) of the left and right PZT fibers is similarly coupled respectively, where the Pt is set for measuring the generated output electrical voltage. Damping parameters were not included in the model for simplicity [11,22].

Here, we assumed that the change in mass due to the viruses is a concentrated or distributed load. So, we applied the concentrated load $P_y = -P_0$ at various locations on the top surface ($y = h/2$). We also applied the distributed load $p_y = -p_0$ at various areas on the top surface ($w' \leq x \leq w''$, $y = h/2$, $l' \leq z \leq l''$). In this case, the area

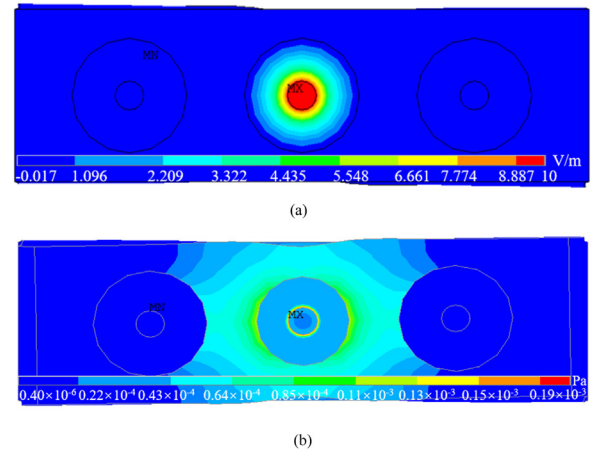


Fig. 3. Distribution of (a) electric field under applied 10V on middle PZT fiber and (b) von mises total mechanical strain.

of load mass was $(w'' - w')(l'' - l')$ and we assumed $p_0 = P_0 / (w'' - w')(l'' - l')$.

4. Results and discussion

4.1. Electromechanical response

The piezoelectric effect of this metal-core piezoelectric fiber/epoxy matrix composite was analyzed to prove its capacity as a biosensor application. After the input of direct current (DC) voltage (frequency $f=0$ Hz) is applied to the middle PZT fiber, the strain of the middle PZT fiber occurs due to the converse piezoelectric effect. The electric field E_r and the von mises total mechanical strain of this composite under 10 V on the middle PZT fiber, are shown in Fig. 3(a) and Fig. 3(b), respectively. The output voltage of the left and right PZT fibers are the same, at 0.017 V, on account of their symmetry. As depicted in Fig. 3(b), the von mises total mechanical strain was generated by applying the input voltage on the middle PZT fiber, which was transmitted to the edges of the left and right PZT fibers. This mechanical strain forced the left and right PZT fibers to generate an output voltage which was sufficient to be detected. Based on these results, it can be proved that the middle PZT fiber can be used as an actuator to force this composite to generate an output voltage. With this mechanism, this composite can be used as a sensor.

4.2. Harmonic analysis

Since the excitation voltage ϕ_e for the real-time detection system is an alternating current, which means the voltage will change periodically, the strains will also be changed as well as the excitation voltage. In order to understand the resonance behavior of this biosensor in detail, the frequency response was calculated. The harmonic analysis based on ANSYS was conducted to analyze the vibration characteristics of this composite. Theoretically, the electrical output attains a peak value if the vibration frequency of the environment matches the resonant frequency of the composite and dies out dramatically when it deviates from the resonant frequency. Fig. 4(a) shows the calculated frequency response of this composite from $f=0$ Hz to 1 MHz. As shown in Fig. 4(a), there are several peaks in this range of frequency where resonance occurred. Furthermore, in the range of about 0 Hz to 100 kHz, there is an obvious resonance peak which greatly enhanced the output voltage of the left PZT fiber. To get a more accurate result of this resonant frequency, the frequency from $f=0$ Hz to 100 kHz was also calculated, as shown in Fig. 4(b). As illustrated in this figure, the resonance peak

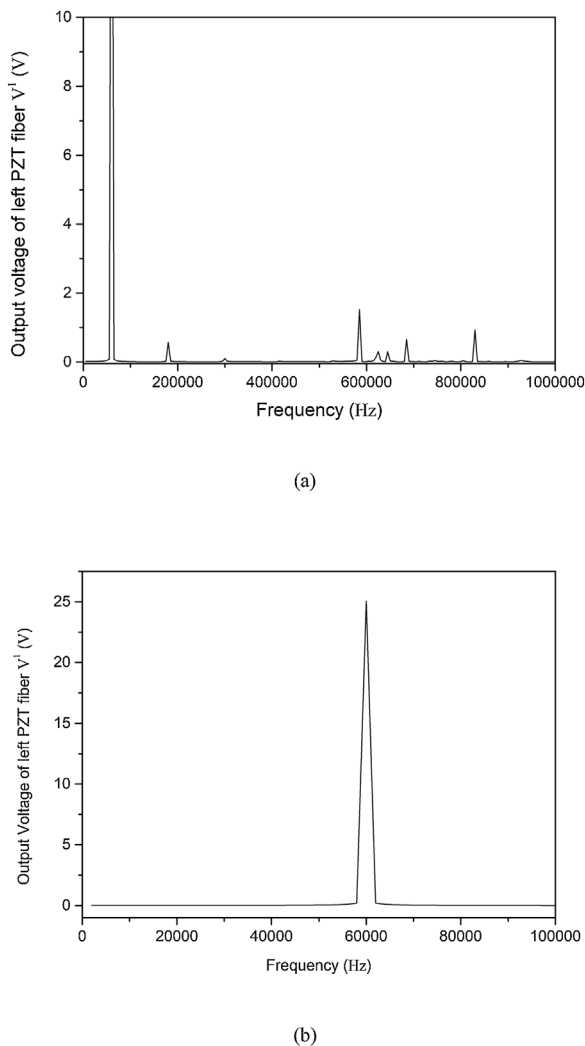


Fig. 4. Frequency response from (a) 0 Hz to 1000 kHz and (b) 0 Hz to 100 kHz.

at 60 kHz is the first resonant frequency for this composite. Moreover, the dynamic output voltage of this composite did not change much until it reached the resonant frequency. From both results, at the first resonant frequency of 60 kHz, this system produces the largest output voltage of this composite. Fig. 5 shows the electric potential distribution at $f = 60$ kHz of this composite. Besides the considerable augmentation of the output voltage, it was also found that the output voltages of the left fiber and right fibers were almost the same due to symmetry. Through harmonic analysis, the resonant frequency was clarified, and 60 kHz was selected to be applied in the virus detection system for the optimal performance of this composite.

4.3. Sensitivity analysis

When viruses are combined with a specific biomarker (see Fig. 2(a)), the mass load on this composite will vary with the progressive characteristic update of the vibration, such as resonant frequency and output voltage. The combination between the virus and the biomarker could be identified by migration of the resonant frequency. However, the mass of virus would be too small to influence the resonant frequency, while the detection of the resonant frequency is not easily carried out. Therefore, the change of output voltage was selected to detect the viruses as the change of electrical signal is easier to measure and compare. To stimulate the process of combination between viruses and antibodies of the biomarker, the mass load is used to represent mass change on the surface of the composite. However, because the position and size of the biomarker cannot be confirmed at the same time, the concentrated load is used to simply evaluate mass load change of this composite and where the mass load is applied to achieve the highest sensitivity. The position of the load where the electrical signals are best in the z and x -directions under $P_0 = 1 \mu\text{g}$ mass concentrated load is illustrated in Fig. 6(a) and Fig. 6(b). The detection ranges per milliliter of the piezoelectric biosensors for hepatitis B virus and dengue virus are 0.1 ng – $10 \mu\text{g}$ [23] and 0.01 – $10 \mu\text{g}$ [24], respectively. Here, an arbitrary value ($1 \mu\text{g}$) within these ranges was selected as an example. Considering the symmetry of this composite, only the left part was calculated. Since the locations of concentrated load in both the x and z -directions are unknown, at first, the offset distance in the x -direction was assumed as 0.3 mm (right above the left fiber) so as to find the best position in the z -direction, as illustrated in Fig. 6(a) which shows the output voltage change of the left PZT fiber $|\Delta V^1|$. Fig. 6(b) shows the output voltage change of the left PZT fiber $|\Delta V^1|$ as a function of the offset distance of the load position in the x -direction. As shown in the results of the z -direction, the peak of output voltage change $|\Delta V^1|$ of the left PZT fiber was found at an offset of 6 mm . After that, when the offset distance in the z -direction was 6 mm , the output voltage change of the left PZT fiber reached a maximum (most sensitive) when the offset of concentrated load was 0.5 mm , in other words, the load locates on the edge of the matrix. Hence, the best position of the concentrated load is where the offset of the x - and z -directions is 0.5 mm and 6 mm , respectively, as shown by the red point in Fig. 7. Moreover, it was found that the optimal location is independent of the magnitude of the load (no figure shown). After the position was confirmed, different values of the concentrated load were applied on that position to measure the sensitivity of biosensor system, as shown in Fig. 8. The relationship between the concentrated load and output voltage change is linear. Additionally, the output voltage changes of the left and right PZT fibers are almost the same. The subtle differences of output voltage change in this and next parts are owing to the mass loads which were above the left fiber.

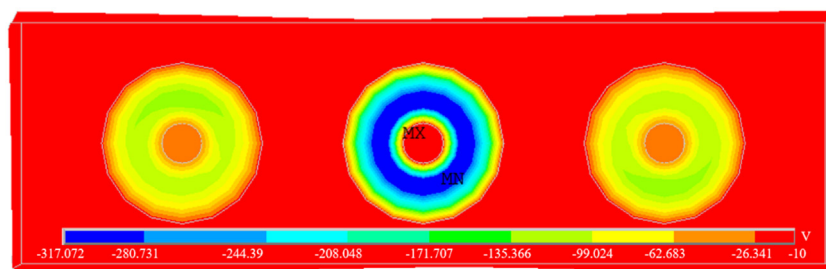
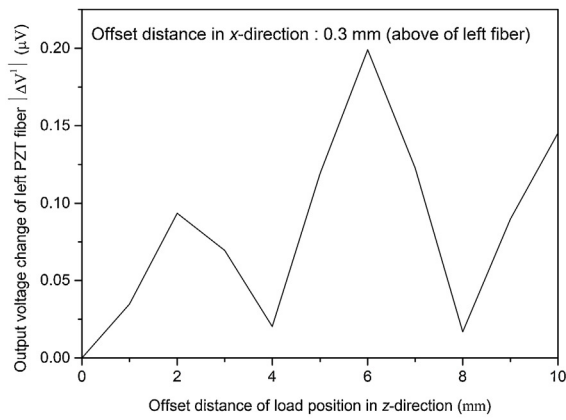
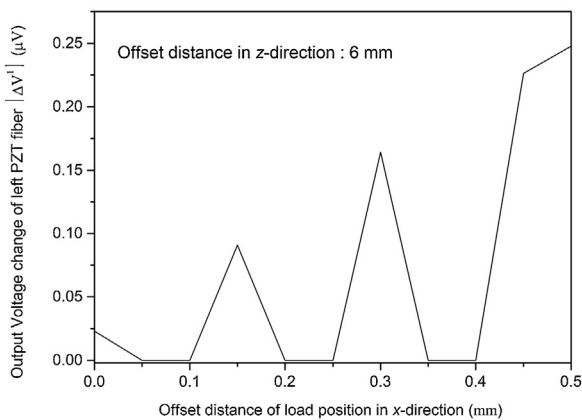


Fig. 5. Electric potential at 60 kHz.



(a)



(b)

Fig. 6. Output voltage change of left PZT fiber on range of (a) x-direction and (b) z-direction.

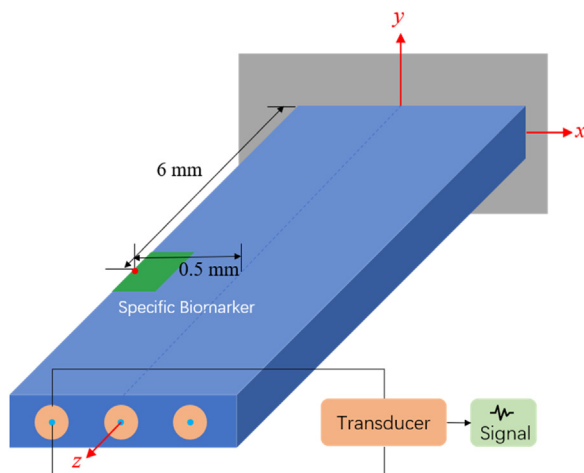


Fig. 7. Schematic of biomarker area.

4.4. Optimization of biomarker

The area of biomarker is also a factor point which will influence the sensitivity of this biosensor. If the surface area of biomarker is too small, the space where antibodies can be placed is insufficient. On the contrary, if it is too big, the large weight of the biomarker

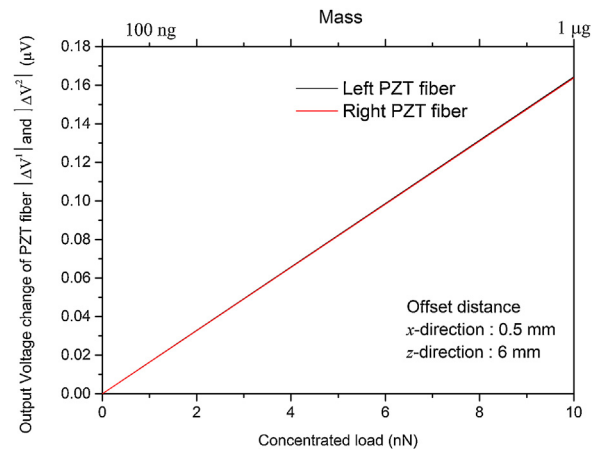
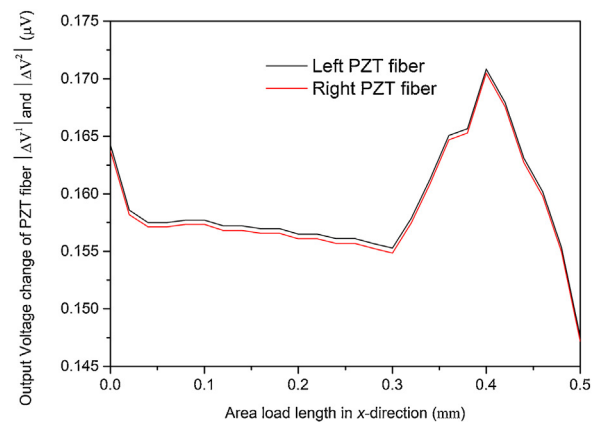
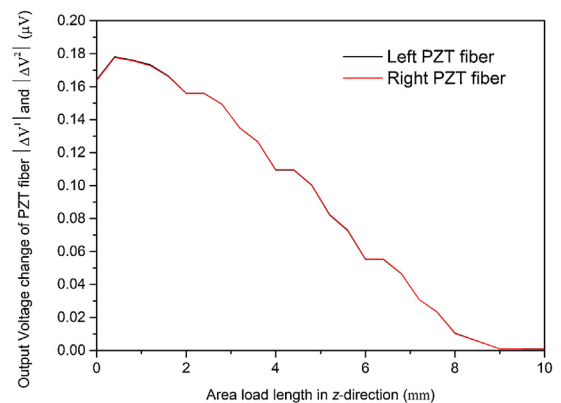


Fig. 8. Output voltage change of PZT fiber on point loads.



(a)



(b)

Fig. 9. Relationship between output voltage change and (a) side length in x-direction and (b) side length in z-direction.

will decrease the sensitivity of this biosensor. Therefore, in this section the concentrated load was exchanged for the distributed load to seek out the optimal size of the biomarker, as shown in Fig. 7. The total area load mass $(w'' - w')(l'' - l')p_0$ is the same as a concentrated load of $1 \mu\text{g}$. As the dimensions of the biomarker in both the x and z-directions will affect the sensitivity, they will be analyzed, respectively. The area of the distributed load is set on the side of the load area corresponding to the length edge of the

epoxy as Fig. 7, due to the optimal location of the concentrated load has been proved to be there. In the first place, the relationship between the side length in the x -direction and the output voltage change is numerically predicted to be where the length of side in the z -direction is a constant of 1 mm (see Fig. 9(a)). The maximum change of output voltage is found at 0.4 mm away from the edge. Similarly, the optimal change of output voltage is captured at the depth of 0.4 mm (z axis in Fig. 9(b)). After this analysis of the biomarker, we predict that the area of the biomarker should be $0.4\text{ mm} \times 0.4\text{ mm}$ for the optimal performance of this biosensor. By using such a $0.4\text{ mm} \times 0.4\text{ mm}$ size biomarker employing spike glycoprotein with engineered surfaces [25,26], it may be possible to detect the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) efficiently. The results of this simulation provide a basis for the systematic development of new biosensors, required to meet the needs of the COVID-19 pandemic.

In this paper, two piezoelectric sensors were considered, and it was shown that the same output voltages could be obtained in either side. That means viruses can be detected with a single piezoelectric fiber while the other piezoelectric fiber can be used to demonstrate other functionalities. For example, it could play the role as an energy harvesting fiber to power other two PZT fibers for virus detection. This is a challenging research area [27], and later some progress will be made.

5. Conclusion

In this study, a metal-core piezoelectric fiber/epoxy matrix composite was designed and optimized as a biosensor for virus detection by 3D FEM. The detection process was realized through monitoring the change of mass load via the piezoelectricity of PZT, which is similar to traditional virus detection sensors. Firstly, the piezoelectric effect of this composite was analyzed to determine whether it has potential as a biosensor. Then, the resonant frequency and output voltage of the sensor, excited by an AC electric field, were determined so as to obtain the optimal performance. From the results of these two parts, it was found that owing to the high piezoelectricity of PZT, this composite shows great potential as a biosensor. Thereafter, a load was applied on the surface of the composite to simulate the combination of biomarker and viruses. The simulation results showed that the change of output voltage under a mass load of $1\mu\text{g}$ was enough to be detected. Finally, the position and dimensions of the biomarker were also optimized to get the highest sensitivity. However, the design of a virus sensor is still a challenging topic and many factors influence the detection results and their application. A further research on optimization and development of such virus detection sensors will be therefore pursued with the improved performance and accuracy.

Author statement

Yinli Wang: Formal analysis, Investigation, Visualization, Writing - original draft

Yu Shi: Methodology, Writing - review & editing

Fumio Narita: Conceptualization, Supervision, Funding acquisition

Declaration of Competing Interest

The authors declare no conflict of interest.

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Biographies

Yinli Wang is a student in graduate school of Tohoku University, studying for materials science. Her major in undergraduate is computer science. Now she is doing research about piezoelectric materials. Since she has learned many knowledges about both computer and materials science. She is particularly interested in interdisciplinary research of computer and materials, such as simulation and application of artificial intelligence technology in materials science.

Yu Shi is a Research Professor and lead of Chester Smart Composite Group (CSCG) at University of Chester, UK. He has widely worked on the development of smart composite with design and integration of nano-functional materials for sensing, energy

harvesting, structural health monitoring, communication etc. for aerospace, automotive, renewable energies and healthcare sectors. He is also an expert on failure assessment of composite structures by both experimental and computational (FEA) approaches for both thermoset and thermoplastic composites, resulting from static and/or dynamic (e.g. Impact, Crash, Blast) loadings as well as processing such as cutting, milling and drilling and composite welding.

Fumio Narita is currently a Professor at the Department of Frontier Sciences for Advanced Environment at Tohoku University in Japan. He is engaged in research to design and develop piezoelectric/magnetostrictive materials and structures in energy harvesting and self-powered environmental monitoring. He is extensively using state-of-the-art electromagneto-mechanical characterization techniques in combination with computational multiscale modeling to understand the fundamental structure–property relations of complex multifunctional composite materials.