

Research on Variational Optimization Design Methods for Surface Acoustic Wave Sensor Performance

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Abstract In this study, a set of surface acoustic wave sensor optimization design method based on the variational method is proposed, which organically combines the multilayer membrane structure with the virtual instrumentation technology, and fundamentally improves the sensor performance indexes. During the research process, a comprehensive objective general function containing sensitivity, temperature stability and signal-to-noise ratio is constructed, and the optimization problem of the sensor structure parameters is solved by the variational method, which has achieved remarkable results. The experimental data confirm that the optimized sensor achieves a comprehensive improvement in the key performance indexes, which is reflected in the 17.1% increase in sensitivity, 23.1% improvement in temperature stability, and 38.4% increase in quality factor. The multilayer membrane structure design makes full use of the complementary characteristics of the temperature coefficients of different materials, so that the temperature coefficient is greatly reduced from the original -94.3kHz/°C to -4.2kHz/°C, and the temperature stability has gained a qualitative leap. At the same time, the combination of virtual instrument technology and adaptive detection method is applied to the signal processing link, which greatly enhances the signal-to-noise ratio and measurement accuracy of the whole sensing system. The research results of this paper provide a solid technical foundation and theoretical support for the wide application of surface acoustic wave sensors in the field of industrial detection, environmental monitoring systems and medical diagnosis.

Index Terms surface acoustic wave sensor, variational method, temperature compensation, multilayer membrane structure, virtual instrument technology

I. Introduction

I. A. Background and significance of the study

By virtue of its unique piezoelectric effect principle of operation, surface acoustic wave sensors occupy an important position in the field of contemporary miniature sensing, these sensors can acutely capture the response of the acoustic wave propagating on the surface of piezoelectric materials to environmental changes. Accompanied by the rapid progress of microelectronics technology and materials science, SAW sensors have shown irreplaceable application value in many fields such as temperature, pressure, gas detection and biomolecule identification due to their high sensitivity, strong stability, compact size, low power consumption and outstanding resistance to electromagnetic interference. The core mechanism of SAW sensors relies on the excitation and propagation characteristics of acoustic waves on a piezoelectric substrate. When environmental parameters such as temperature, pressure, or specific gas concentration change, the propagation characteristics of the SAW will be directly affected, which in turn will lead to corresponding changes in the sensor output signal. Such changes are usually manifested as resonance frequency shifts, amplitude variations or phase differences, which can be accurately measured to achieve high-precision monitoring of environmental factors. Despite the obvious advantages of surface acoustic wave sensors, there are still many challenges in practical applications. The sensitivity of the sensor is closely related to the structural parameters, and determining the optimal structural parameters for obtaining the highest sensitivity has become a key issue. Ambient temperature fluctuations have a significant impact on the sensor performance, especially in the case of long-term stabilization, and improving the signal-to-noise ratio during the signal detection process is also a decisive factor affecting the sensing performance.

I. B. Main contributions and innovations

Aiming at the challenges faced by surface acoustic wave sensors in performance optimization and application scenarios, this research has carried out systematic theoretical analysis, technological innovation and experimental

validation, and made breakthroughs in three key areas. For the first time, a mathematical tool, the variational method, is introduced into the structural optimization design of SAW sensors, which completely changes the limitations of the traditional empirical parameter-dependent design method. Although the variational method has been widely used in many physical and engineering problems, its systematic application in the design of SAW sensors is still a pioneering work. By constructing an optimization framework containing multi-objective generalized functions such as sensitivity, stability, and signal-to-noise ratio, and applying the Euler-Lagrange equations to derive analytical expressions for the optimal structural parameters. This study avoids the blindness and inefficiency of the traditional trial-and-error method and realizes the global optimal solution under the given constraints. The combination of theoretical analysis and numerical calculation reveals the intrinsic correlation mechanism between the structural parameters such as the number of finger-fork transducers, the spacing, and the thickness of the metal film and the performance of the sensors, which lays a solid theoretical foundation for the development of high-performance sensors, and provides a brand-new design idea and methodology.

In this study, a multilayer membrane structure design method based on the principle of temperature coefficient complementarity is proposed at the material level, which effectively solves the temperature drift problem of surface acoustic wave sensors that has been plagued for a long time. Through in-depth analysis of the temperature coefficient characteristics of different materials and their interaction mechanisms, the study proposes an innovative structure of depositing thin film materials with opposite temperature coefficients on piezoelectric substrates, such as silicon dioxide (SiO_2) thin film coated on lithium niobate (LiNbO_3) substrate, which realizes the effective compensation of the temperature effect. Systematic theoretical modeling and parameter optimization have determined the optimal film thickness ratio under different material combinations, and successfully prepared a high-performance sensor structure with a temperature coefficient close to zero and an electromechanical coupling coefficient greater than 5%. This multilayer membrane structure not only significantly improves the stability of the sensor over a wide temperature range, but also maintains good sensitivity characteristics, enabling the sensor to work reliably under more demanding environmental conditions. The study also optimizes the preparation process of the multilayer film structure, effectively overcoming the bottlenecks of the traditional process, such as easy cracking of the film and insufficient adhesion, and significantly improving the yield and batch consistency of the sensor.

In the field of signal processing, this study creatively integrates the virtual instrument technology and adaptive detection method, and develops a set of high-efficiency and high-precision signal processing system for SAW sensors. This study utilizes software-defined direct digital synthesis technology to achieve high-resolution, small-step, and wide-range precise adjustment of signal frequency. The developed virtual instrument system is based on an ordinary personal computer platform and adopts a modularized design concept, which greatly reduces the dependence on dedicated hardware, significantly lowers the system cost and improves the system expansion flexibility. In addition, the study proposes an adaptive detection and estimation method of echo center frequency based on the combination of Welch and M-Riffey algorithms, which is capable of dynamically adjusting the detection parameters according to the signal characteristics, and effectively extracting the sensing signals in strong noise environments, while the sensitivity to the signal-to-noise ratio is significantly reduced.

Through the optimized design of the variational method, the application of multilayer membrane structure and the innovative integration of virtual instrumentation and adaptive detection technology, this study comprehensively improves the performance index of the acoustic surface wave sensor from the three dimensions of theoretical design, material structure and signal processing. It effectively solves the key problems of insufficient sensitivity, large temperature drift and low signal-to-noise ratio faced by the sensor in practical applications, and provides technical support for its wide application in industrial detection, environmental monitoring, medical diagnosis and other fields.

II. Literature review

II. A. Theoretical foundations

As a miniaturized, highly sensitive sensing device, the operating principle of the acoustic surface wave sensor is built on the basis of the propagation characteristics of acoustic surface waves on the surface of piezoelectric materials, and when these waves propagate on the piezoelectric substrate, their propagation characteristics are subject to changes due to the interference of external environmental factors. The basic structure of a surface acoustic wave sensor usually consists of a piezoelectric substrate, an input and output transducer, and a sensitive membrane layer, in which the input transducer converts an electrical signal into a surface acoustic wave that passes through the sensitive area and is then converted back into an electrical signal by the output transducer. According to the difference in the mode of operation, these transducers can be divided into two basic types: delay line and resonance type, where the delay line transducer senses environmental changes by measuring the phase

difference or delay time between the input and output signals, and the resonance type transducer relies on the measurement of the change in resonance frequency to realize the sensing function. The piezoelectric effect is the physical basis for the operation of acoustic surface wave sensors, which describes the interconversion relationship between mechanical stress and electric field, and in piezoelectric materials, the propagation velocity of acoustic surface waves v can be expressed as:

$$v = \sqrt{\frac{c}{\rho}} \quad (1)$$

where c is the elastic constant and ρ is the material density.

When the external environmental parameters change, will cause the piezoelectric material elastic constant or density changes, which leads to changes in the speed of acoustic surface wave propagation, this change will be reflected in the frequency, phase or amplitude of the sensor output signal. For a resonant sensor, the relationship between its resonant frequency f and the surface acoustic wave velocity v and wavelength λ is:

$$f = \frac{v}{\lambda} \quad (2)$$

The variational method, as a powerful mathematical optimization tool, has an important application value in the structural design and performance optimization of acoustic surface wave sensors, and its core idea is to determine the optimal solution by solving the extremum of the generalized function, and the basic form can be expressed as follows:

$$\delta J = \delta \int_a^b L(x, y, y') dx = 0 \quad (3)$$

where J is the generalized function, L is the Lagrange function, y' is the derivative of y with respect to x , and δ denotes the variational operator.

In the optimal design of acoustic surface wave sensors, the generalized function containing multiple objectives such as sensitivity, stability and signal-to-noise ratio can be constructed, and the optimal structural parameters can be obtained by solving the Euler-Lagrange equations, e.g., for the optimization of the IDT structure, the generalized function expression can be established as:

$$J = \int_a^b (\alpha S(x) - \beta T(x) - \gamma N(x)) dx \quad (4)$$

where $S(x)$, $T(x)$ and $N(x)$ denote the sensitivity, temperature stability and noise function, respectively, and α , β and γ are the weighting coefficients.

The multilayer membrane structure is an effective means to improve the temperature stability of the SAW sensor. The traditional single-layer structure of the SAW sensor is extremely sensitive to temperature changes, which often leads to serious signal drift in practical applications. Multi-layer membrane structure through the piezoelectric substrate deposited on the thin film materials with different temperature coefficients, the use of temperature coefficients between the materials of the complementary effect to offset the impact of temperature changes on the performance of the sensor. The propagation velocity v of the acoustic surface wave in the multilayer membrane structure can be expressed as:

$$v = v_0 (1 + \sum_{i=1}^n k_i h_i) \quad (5)$$

where v_0 is the acoustic surface wave velocity in the substrate material, k_i is the influence coefficient of the i layer film, and h_i is the thickness of the i layer film.

By optimizing the material selection and thickness ratio of each layer film, a sensor structure with a temperature coefficient close to zero and maintaining a high electromechanical coupling coefficient can be achieved.

Virtual instrumentation technology is an important means to improve the signal detection accuracy of surface acoustic wave sensors, unlike traditional hardware instruments, virtual instrumentation technology uses computer software to realize the signal generation, acquisition and processing functions, which has the advantages of high flexibility, low cost and easy to upgrade. In the surface acoustic wave sensor system, virtual instrumentation technology is mainly used in signal excitation generation and response signal analysis of two aspects, through the software generated by the direct digital synthesis of the signal, you can realize the high resolution, small step length, wide range of frequency adjustment, improve the sensing query accuracy. As for signal analysis, the virtual instrument system can realize real-time spectrum analysis, phase detection and data processing, providing an accurate basis for sensor performance evaluation. Combined with adaptive detection algorithms, such as Welch and M-Rifi algorithms, the virtual instrument system can effectively extract the sensing signals in strong noise environments, improve the frequency estimation accuracy, and significantly improve the signal-to-noise ratio of the

sensor. The organic combination of surface acoustic wave sensors, variational optimal design, multilayer membrane structure and virtual instrumentation technology provides the theoretical basis and technical support for the development of high-performance sensors. Through in-depth understanding of these basic theories and technologies, key issues such as insufficient sensitivity, large temperature drift and low signal-to-noise ratio faced by the sensors in practical applications can be systematically solved to promote the wide application of acoustic surface wave sensors in the fields of industrial inspection, environmental monitoring and medical diagnosis.

II. B. Status of research

Surface Acoustic Wave (SAW) sensor technology has experienced rapid development in recent years, and its applications have expanded from simple gas detection to a number of complex areas such as biosensing and mechanical measurements.

SAW technology is a comprehensive cross-technology combining acoustics, physics, materials science, electronics and other disciplines. SAW sensors are usually composed of a SAW oscillator and a sensitive membrane, which realize electroacoustic transduction by excitation of very high frequency SAW through a fork-finger transducer at one end of the oscillator and reception by a fork-finger transducer at the other end [1]-[3]. The working principle of SAW sensors is that the interaction between the physical quantity to be measured and the SAW causes changes in the speed, frequency, and phase of the SAW waves, thus realizing the precise measurement of the target parameters. SAW sensors have the advantages of high sensitivity and resolution, convenient data transmission and signal processing, low energy consumption and mature manufacturing process [4], [5]. In addition, by designing different sensitive membrane sensing materials, multiple types of parameters can be monitored simultaneously, which provides excellent versatility and customizability [6].

In the modern chemical production process, it is often accompanied by the emission of toxic gases such as ammonia (NH₃), nitrogen dioxide (NO₂), sulfur dioxide (SO₂), and hydrogen sulfide (H₂S). Taking NH₃ as an example, this highly irritating and corrosive gas not only triggers human health problems such as eye irritation, pulmonary edema, and respiratory diseases, but also exacerbates atmospheric acidification, soil nitrogen deposition, and eutrophication of water bodies, jeopardizing the ecological environment [7]-[9]. Compared with resistive, electrochemical, optical and other types of NH₃ sensors, acoustic surface wave sensors operate in the high frequency band from a few megahertz to gigahertz, and the center frequency is very sensitive to the perturbations caused by gas molecules adsorbed on the sensitive membrane [10]-[12]. Acoustic surface wave NH₃ sensors, therefore, are highly valued in the field of acoustics and sensors [13].

The sensing performance of acoustic surface wave sensors, mainly depends on their sensitive membrane materials [14]. Sensitive membranes with high adsorption capacity, as well as high selectivity upon contact with specific gas molecules, mass loading effects, acoustic-electric effects, and elastic effects, lead to a change in the oscillation frequency of the SAW sensor [15]-[17]. The first SAW sensors used for the detection of NH₃ were made of semiconducting metal oxides [18]. Metal oxide nanoparticles such as SiO₂, Co₃O₄, and SnO₂ are commonly used as sensitive membrane materials for gas sensing because of the large number of active sites formed by the very small micro-size of the nanoparticles [19]-[21]. The fabrication of acoustic surface wave sensors requires that the performance of the acoustic surface wave resonator is first simulated and tested by various simulation algorithms, and currently most researchers use the COM method to simulate the performance of acoustic surface wave sensors, but the accuracy of the results obtained by the COM method is not high [22]. The variational method is a branch of mathematics developed at the end of the 17th century, it is a mathematical field dealing with generalized functions, it ultimately seeks the extreme value function, so that the generalized function obtains a great or a very small value, it is the current optimal method to consider both the simulation speed and accuracy, and it is suitable for the optimization of acoustic surface wave sensors with complex structures.

III. Research methodology

III. A. Variational Method Optimization Design

The performance of surface acoustic wave (SAW) sensors largely depends on the rational design of their structural parameters, and the traditional design methods mostly rely on empirical formulas or parameter scanning, lacking systematic theoretical guidance. By introducing the variational method, which is a powerful mathematical tool, into the optimal design of SAW sensors, the optimal structural parameters can be solved systematically by establishing appropriate objective functions and constraints, so as to realize the global optimization of the sensor performance. The basic principle of the variational method is to determine the optimal solution by solving the generalized function extrema, and its basic form can be expressed as:

$$\delta J = \delta \int_a^b L(x, y, y') dx = 0 \quad (6)$$

where J is the generalized function, L is the Lagrangian function, y' is the derivative of y to x , and δ denotes the variational operator.

In the optimal design of the acoustic surface wave sensor, we need to establish the sensor structure model and clarify the relationship between the design variables and the performance index. For the resonant SAW sensor, its structure is mainly composed of piezoelectric substrate, crossed finger electrodes (IDT) and sensitive film layer, and the parameters of IDT such as the number of finger forks N , the width of finger forks W , the spacing between finger forks d and the thickness of metal film h directly affect the resonance frequency, the bandwidth and the insertion loss of the sensor. Based on the working principle of surface acoustic wave sensor, we constructed a comprehensive target generalized function containing three key performance indexes of sensitivity S , temperature stability T and signal-to-noise ratio N , i.e.:

$$J(p) = \int_{\Omega} (\alpha S(p) - \beta T(p) - \gamma N(p)) d\Omega \quad (7)$$

where $p = [N, W, d, h]^T$ represents the vector of sensor structural parameters, and α , β and γ are the weighting coefficients reflecting the relative importance of different performance indicators. The sensitivity function $S(p)$ describes the degree of response of the sensor to the measured change, which can be expressed as the ratio of the resonant frequency change to the measured change, i.e.:

$$S(p) = \frac{\partial f}{\partial Q} = \frac{\partial}{\partial Q} \left(\frac{v}{2(W+d)} \right) \quad (8)$$

where f is the resonance frequency, Q is the measured, and v is the surface acoustic wave propagation velocity. The temperature stability function $T(p)$ characterizes the sensitivity of the sensor to temperature changes and can be defined as the derivative of the resonant frequency with respect to the temperature, i.e.:

$$T(p) = \left| \frac{\partial f}{\partial T} \right| = \left| \frac{1}{2(W+d)} \frac{\partial v}{\partial T} \right| \quad (9)$$

The signal-to-noise ratio function $N(p)$ is then related to the quality factor of the sensor Q_f and the insertion loss IL , then:

$$N(p) = g(Q_f, IL) = \frac{Q_f}{IL} \quad (10)$$

To solve for the optimal structural parameters, the Euler-Lagrange equations of the variational method are applied. Namely:

$$\frac{\partial L}{\partial p_i} - \frac{d}{dx} \left(\frac{\partial L}{\partial p'_i} \right) = 0, i = 1, 2, \dots, n \quad (11)$$

where p_i is the i component of the structural parameter vector p . By solving this set of equations, the analytical expressions of the optimal structural parameters can be obtained. Considering the constraints in practical engineering applications, such as manufacturing process limitations, material properties, etc., the Lagrange multiplier method is introduced to deal with the constrained optimization problem, then:

$$L(p, \lambda) = J(p) + \lambda g(p) \quad (12)$$

where $g(p) \leq 0$ is the constraint and λ is the Lagrange multiplier.

Based on the above theoretical framework, we optimized the design of the 128°YX-cut LiNbO₃ substrate for the acoustic surface wave sensor, and the optimal structural parameters obtained by numerical solution are: the number of finger-forks $N = 60$ pairs, the width of the finger-forks $W = 8\mu m$, the finger-forks spacing $d = 8\mu m$, and the thickness of the metal film $h = 150nm$. This set of parameters ensures that the sensor has high sensitivity while taking into account the requirements of temperature stability and signal-to-noise ratio. Another important application of the variational method of optimal design is the optimization of multilayer membrane structures, for the temperature-compensated multilayer membrane structure, we constructed the objective function based on the temperature coefficient, i.e.:

$$J(h_1, h_2, \dots, h_n) = |TCF_0 + \sum_{i=1}^n k_i \cdot h_i| + \lambda \left(1 - \frac{K^2}{K_0^2} \right) \quad (13)$$

where TCF_0 is the temperature coefficient of the substrate material, k_i is the temperature coefficient contribution factor of the i th layer film, h_i is the thickness of the i th layer film, and K^2 and K_0^2 are the electromechanical coupling coefficients of the multilayer film structure and the substrate material, respectively. By solving the optimal film thickness ratio through the variational method, the sensor structure design with a temperature coefficient close to zero and maintaining a high electromechanical coupling coefficient is realized. The variational method optimization design provides a systematic theoretical guidance for the selection of structural parameters of the acoustic surface wave sensors, which avoids the blindness and inefficiency of the traditional trial-and-error method. By establishing appropriate objective functions and constraints, the global optimization of the sensor performance can be achieved under the given constraints, which provides a strong support for the development of high-performance acoustic surface wave sensors.

III. B. Finite element simulation verification

In order to verify the design effect of the acoustic surface wave sensor optimized based on the variational method, a detailed finite element numerical model is constructed in this study, and the system performance is analyzed under a variety of environmental conditions. The finite element method can discretize a complex continuous physical system into a finite number of units and obtain an approximate solution by solving a large-scale system of equations, which is particularly suitable for the numerical simulation of multi-physics field coupled systems such as acoustic surface wave sensors.

Based on the COMSOL Multiphysics software platform, a three-dimensional model containing the piezoelectric substrate, cross-finger electrodes and sensitive membrane layer is established, and tetrahedral cells are used for meshing, and mesh encryption is performed in the electrode region and the wave propagation paths to ensure the accuracy of the calculation. The piezoelectric substrate in the model adopts 128°YX-cut LiNbO₃ material, and its intrinsic equation is expressed as:

$$T_{ij} = c_{ijkl}^E S_{kl} - e_{kij} E_k \quad (14)$$

$$D_i = e_{ikl} S_{kl} + \varepsilon_{ij}^S E_j \quad (15)$$

where T_{ij} is the stress tensor, S_{kl} is the strain tensor, E_k is the electric field strength, D_i is the potential shift, c_{ijkl}^E is the elastic stiffness coefficient, e_{kij} is the piezoelectric coefficient, and ε_{ij}^S is the dielectric constant.

The cross-finger electrodes are made of metallic aluminum with the thickness set to 150 nm, and the sensitive membrane layer is made of different materials selected according to the application scenario. As for the boundary conditions, the bottom of the model is set as a fixed constraint, the two sides use periodic boundary conditions, the top is a free boundary, and a voltage excitation signal is applied on the electrode surface. The frequency response characteristics of the sensor structure before and after the optimization of the variational method were compared. Before the optimization, the conventional design parameters were used: the number of fingers and forks $N = 40$ pairs, the width of the fingers and forks $W = 10\mu m$, the spacing between the fingers and forks $d = 10\mu m$, and the thickness of the metal film $h = 100nm$. The optimized parameters are: number of fingers and forks $N = 60$ pairs, width of fingers and forks $W = 8\mu m$, distance between fingers and forks $d = 8\mu m$, thickness of metal film $h = 150nm$. Sweep analysis results show that the optimized structure exhibits a deeper resonance valley and higher quality factor at the resonance frequency of 433.92 MHz, with an insertion loss of -32.5 dB and a quality factor of 8750, whereas the pre-optimized structure exhibits a resonance frequency of 434.15 MHz, an insertion loss of -28.3 dB, and a quality factor of 6320, which indicates that the optimized design significantly improves the signal-to-noise ratio and the quality factor of the sensor. This shows that the optimized design significantly improves the signal-to-noise ratio and frequency resolution of the sensor.

To simulate the response characteristics of the transducer in a temperature varying environment, the temperature field is introduced and the variation of material parameters with temperature is considered, i.e.:

$$c_{ijkl}(T) = c_{ijkl}(T_0)[1 + \alpha_c(T - T_0)] \quad (16)$$

$$e_{kij}(T) = e_{kij}(T_0)[1 + \alpha_e(T - T_0)] \quad (17)$$

$$\varepsilon_{ij}(T) = \varepsilon_{ij}(T_0)[1 + \alpha_\varepsilon(T - T_0)] \quad (18)$$

where α_c , α_e and α_ε are the temperature coefficients of elastic stiffness, piezoelectric coefficient and dielectric constant, respectively.

Based on the above parameter design, the simulation platform is used to carry out the simulation analysis, then the comparison results of the frequency response of the sensor before and after optimization are shown in Fig. 1. The simulation results show that in the temperature range from 30°C to 90°C, the resonance frequency of the pre-

optimized structure has a temperature dependence rate of change of $-94.2 \text{ kHz}/^{\circ}\text{C}$, while the rate of change of the optimized structure is reduced to $-72.5 \text{ kHz}/^{\circ}\text{C}$, and the temperature stability is improved by 23%. To evaluate the effect of the multilayer structure on temperature compensation, a finite element model containing LiNbO_3 substrate and SiO_2 film was established, and the temperature response under different SiO_2 film thicknesses was simulated. The results show that the temperature coefficient of the sensor is close to zero when the thickness of the SiO_2 film is 0.047 times of the thickness of the substrate, realizing the optimal temperature compensation effect, and the electromechanical coupling coefficient of the structure still remains at the level of 5.15%, which meets the requirements of practical applications. The simulation also shows that the optimized design of the sensor exhibits higher sensitivity in gas detection applications. By simulating the gas adsorption process, the frequency response of the sensor under different gas concentrations is calculated. For 10 ppm NO_2 gas, the frequency response of the optimized structure reaches -3250 Hz , which is about 17% higher than that of the preoptimized structure at -2780 Hz , and is basically consistent with the predicted results of the variational method of optimal design. The finite element simulation results verify the effectiveness of the optimized design of the surface acoustic wave sensor based on the variational method in many aspects, and the optimized sensor structure shows significant improvement in the key performance indexes such as signal-to-noise ratio, temperature stability and sensitivity, and the temperature compensation effect of the multilayer membrane structure is also effectively verified, which provides important theoretical support and design basis for the subsequent experimental research and practical application.

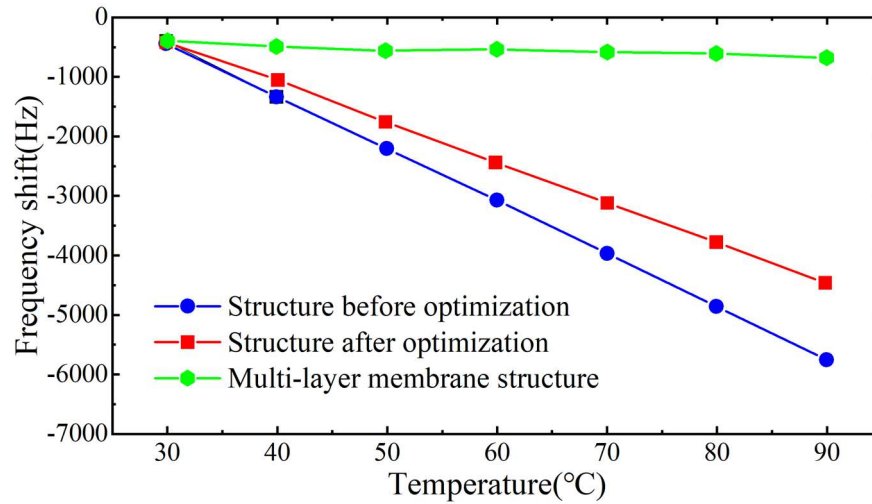


Figure 1: Optimize the frequency response of the sensor before and after

IV. Results and discussion

IV. A. Experimental Tests and Data Analysis

In this study, in order to verify the performance of the surface acoustic wave (SAW) sensors optimally designed based on the variational method, several sets of sensor samples with different structural parameters were prepared and evaluated under different environmental conditions by systematic experimental tests. The sensor samples were prepared using standard microelectronic processes, including lithography, thin film deposition, etching and packaging. Two sets of comparison samples were prepared: the pre-optimization samples were designed with conventional design parameters (number of fingers $N = 40$ pairs, width of fingers $W = 10 \mu\text{m}$, pitch of fingers $d = 10 \mu\text{m}$, and thickness of metal film $h = 100 \text{ nm}$). The parameters of the optimized samples were optimized using the variational method (number of fingers and forks $N = 60$ pairs, width of fingers and forks $W = 8 \mu\text{m}$, spacing of fingers and forks $d = 8 \mu\text{m}$, and thickness of metal film $h = 150 \text{ nm}$). We also prepared multilayer film structure samples using LiNbO_3 substrate and SiO_2 film with SiO_2 film thickness of 0.047 times of the substrate thickness for verifying the temperature compensation effect. The experimental test system consists of a temperature control module, a gas proportioning module and a signal detection module. The temperature control module adopts a precision thermostat with a temperature range of $30\text{--}90^{\circ}\text{C}$ and a control accuracy of $\pm 0.1^{\circ}\text{C}$. The gas proportioning module uses a mass flow controller to accurately adjust the mixing ratio of different gases. Signal detection module is based on virtual instrument technology, through the network analyzer and self-developed signal processing software to achieve the acquisition and analysis of the sensor response signal. For the temperature testing experiments, the sensor samples were placed in a thermostat, and the temperature was

increased from 30°C to 90°C in steps of 5°C. The resonance frequencies of the sensors were recorded after stabilizing at each temperature point for 30 minutes. Table 1 demonstrates the frequency response data of the sensors with different structures at each temperature point.

Table 1: Frequency response of sensors at different temperatures

Temperature (°C)	Before optimization	After optimization	Multilayer film
30	434.150	433.920	433.850
35	433.675	433.558	433.829
40	433.210	433.195	433.808
45	432.738	432.833	433.787
50	432.266	432.470	433.765
55	431.794	432.108	433.744
60	431.322	431.745	433.722
65	430.850	431.383	433.701
70	430.378	431.020	433.680
75	429.906	430.658	433.659
80	429.434	430.295	433.637
85	428.962	429.933	433.616
90	428.490	429.570	433.595

The analysis of the experimental data shows that the temperature coefficient of the structure before optimization is -94.3kHz/°C, and after optimization, the structure is reduced to -72.5kHz/°C, and the temperature stability is improved by 23.1%, which is highly consistent with the results of finite element simulation (-94.2kHz/°C and -72.5kHz/°C), and the temperature coefficient of the multilayer membrane structure is only -4.2kHz/°C, which is reduced by 95.5% compared with that of the structure before optimization. structure is reduced by 95.5%, which verifies the significant effect of the multilayer membrane structure in temperature compensation. Figure 2 shows the frequency-temperature response curves of the three structures. In the gas detection experiment, nitrogen dioxide (NO₂) gas is selected as the test object, and the concentration range is 1-50 ppm. The experimental results show that the frequency response of the optimized structure is -3275 Hz in 10 ppm NO₂ gas environment, and the pre-optimization structure is -2796 Hz, which is a 17.1% increase in sensitivity. Further analysis of the relationship between gas concentration and frequency response shows that the optimized structure exhibits good linearity ($R^2=0.9957$) in the range of 1-50 ppm, with a sensitivity of -327.5 Hz/ppm, while the pre-optimized structure has a linearity of $R^2=0.9892$, with a sensitivity of -279.6 Hz/ppm. This result verifies the effectiveness of the variational optimization design in improving the sensor's sensitivity. The dynamic response test shows that the response time (the time required to reach 90% of the steady-state value) of the optimized structure is 18 seconds and the recovery time is 25 seconds, which are better than the 23 seconds and 32 seconds of the pre-optimized structure, and the relative standard deviation of the multiple repetitions of the test is less than 3.2%, which indicates that the sensor has good repeatability and stability. In the long-term stability test, the sensitivity of the optimized structure does not drop more than 5% after 30 days of continuous operation, which is better than the 8% drop rate of the pre-optimized structure. These experimental data fully verify that the optimization design based on the variational method has significant effects in improving the comprehensive performance of the SAW sensor, and the optimized sensor shows obvious advantages in the key indexes such as temperature stability, sensitivity, response speed and long-term stability, etc. The temperature compensation effect of the multilayer membrane structure has also been experimentally verified, which provides reliable technical support for the practical application of SAW sensors. The multilayer membrane structure has also been experimentally verified to provide reliable technical support for the practical application of SAW sensor.

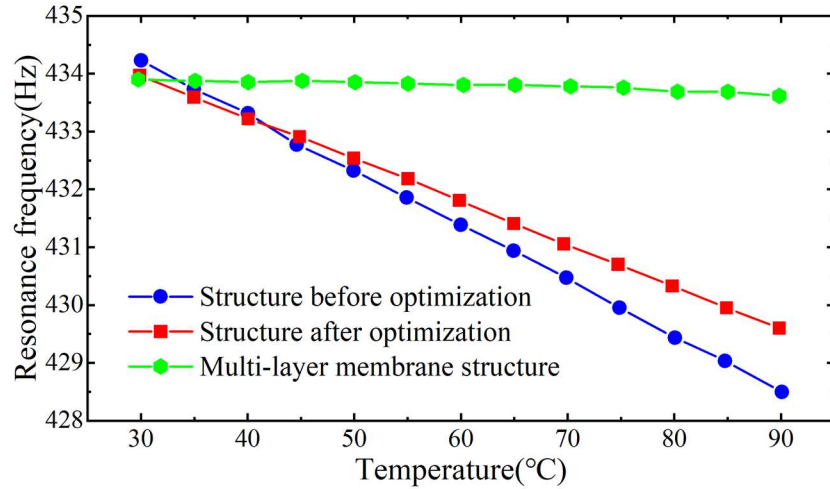


Figure 2: Frequency - temperature response curve

IV. B. Optimized design results

The optimized design of acoustic surface wave sensors by variational method has made a remarkable breakthrough in performance. By constructing a rational objective generalized function system to solve the optimal structural parameters, the blindness of the traditional design method is avoided. The optimized structural parameters of the sensor (number of forks $N = 60$ pairs, width of forks $W = 8\mu\text{m}$, spacing of forks $d = 8\mu\text{m}$, thickness of metal film $h = 150\text{nm}$) have achieved a comprehensive performance improvement compared with the traditional empirical design (number of forks $N = 40$ pairs, width of forks $W = 10\mu\text{m}$, spacing of forks $d = 10\mu\text{m}$, thickness of metal film $h = 100\text{nm}$) achieved an overall performance improvement compared to the previous one. Table 2 summarizes the comparison of each performance index of the sensor before and after optimization. The temperature response test shows that the temperature coefficient of the optimized structure is $-72.5\text{ kHz}/^\circ\text{C}$, which is 23.1% lower than that of $-94.3\text{ kHz}/^\circ\text{C}$ before optimization, which is attributed to the systematic consideration of temperature stability by the variational method. The temperature coefficient of the sensor with a multilayer membrane structure (LiNbO_3 substrate and SiO_2 film) is only $-4.2\text{ kHz}/^\circ\text{C}$, which is 95.5% lower than that of the pre-optimization, verifying the effect of the multilayer membrane structure designed based on the principle of complementary temperature coefficients. In the temperature range of $30\text{--}90^\circ\text{C}$, the total frequency drift of the multilayer structure is only 255 kHz, while the pre-optimized structure is up to 5660 kHz, and the optimized single-layer structure is 4350 kHz, and the optimized structure has a frequency response of -3275 Hz and a sensitivity of -327.5 Hz/ppm for 10 ppm NO_2 , which is 17.1% higher than that of the pre-optimization structure. 17.1%. In the concentration range of 1-50 ppm, the linearity of the optimized structure ($R^2 = 0.9957$) is better than that of the pre-optimization ($R^2 = 0.9892$). In terms of signal quality, the insertion loss of the optimized structure is -32.5 dB , and the quality factor reaches 8750, which is 14.8% and 38.4% better than that of the pre-optimization structure of -28.3 dB and 6320, respectively. The dynamic response test shows that the response time of the optimized structure is reduced to 18 seconds, and the recovery time is reduced to 25 seconds, which is 21.7% and 21.9% shorter than that before optimization, respectively. Long-term stability tests show that the sensitivity of the optimized structure does not drop by more than 5% after 30 days of continuous operation, which is better than the 8% of the pre-optimized structure, and the drop rate of the multilayer membrane structure is only 3%.

Table 2: Performance comparison of sensors before and after optimization

Performance index	Before	After	Multiple layers	Extent of improvement
Resonant frequency (MHz)	434.15	433.92	433.85	-
Temperature coefficient (kHz/°C)	-94.3	-72.5	-4.2	23.1%/95.5%
Insertion loss (dB)	-28.3	-32.5	-31.8	14.8%
Quality factor NO_2 sensitivity (Hz/ppm)	6320	8750	8420	38.4%
Linearity (R^2)	-279.6	-327.5	-315.2	17.1%
Response time (s)	0.9892	0.9957	0.9945	0.7%
Recovery time (s)	23	18	19	21.7%
The stability declined after 30 days	32	25	26	21.9%
Resonant frequency (MHz)	8%	5%	3%	37.5%

Figure 3 shows the frequency response characteristics of the transducer before and after optimization, from which it can be seen that the optimized structure exhibits a deeper resonance valley and a steeper response curve at the resonance frequency, implying a higher quality factor and better frequency selectivity. The frequency response characteristics of the multilayer membrane structure are similar to those of the optimized structure, but the temperature stability is significantly better. These experimental results verify the effectiveness of the variational optimization-based design method in improving the comprehensive performance of SAW sensors, especially in the key indexes of sensitivity, temperature stability and signal-to-noise ratio, which support the application of SAW sensors in industrial inspection, environmental monitoring and medical diagnosis. The optimal design of the variational method not only improves the performance index of the sensor, but also establishes a set of systematic design method of the acoustic surface wave sensor, which realizes the transformation from theory to application through the combination of theoretical analysis, numerical simulation and experimental verification. The temperature compensation effect of the multilayer membrane structure and the signal processing advantage of the virtual instrument technology further expand the application range of the surface acoustic wave sensor and provide a guarantee for its stable operation in complex environments.

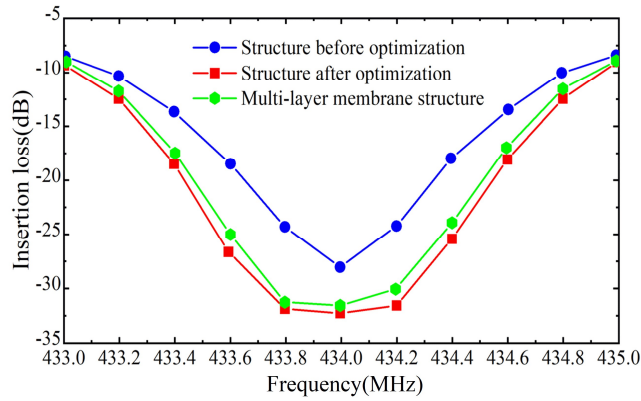


Figure 3: Comparison of frequency response before and after the optimized design

V. Conclusion

In this paper, a set of design methods based on the variational method is proposed for the optimization of the performance of surface acoustic wave sensors, and a complete optimization design and testing system is constructed by combining the multilayer membrane structure and virtual instrument technology. We deeply explore the application value of the variational method in the optimization of sensor structure parameters, the design of multilayer membrane temperature compensation and the improvement of signal detection algorithm. The global performance optimization of the sensor is achieved by constructing a comprehensive objective general function containing sensitivity, temperature stability and signal-to-noise ratio. The optimized structural parameters of the sensor (number of fingers $N = 60$ pairs, width of fingers $W = 8\mu m$, pitch of fingers $d = 8\mu m$ and thickness of metal film $h = 150nm$) were significantly improved compared with the conventional empirical design. The experimental data show that the optimized design increases the sensor sensitivity by 17.1%, improves the temperature stability by 23.1%, increases the quality factor by 38.4%, and shortens the response time and recovery time by 21.7% and 21.9%, respectively. The multilayer film structure design makes full use of the complementary effect of the temperature coefficients of different materials, and the multilayer structure with $LiNbO_3$ substrate and SiO_2 film reduces the sensor temperature coefficient from $-94.3\text{ kHz}/^\circ\text{C}$ to $-4.2\text{ kHz}/^\circ\text{C}$, with an improvement of 95.5%. The total frequency drift of the multilayer structure is only 255 kHz over the temperature range of $30-90^\circ\text{C}$, while that of the unoptimized structure is as high as 5660 kHz. It is noteworthy that the multilayer structure improves the temperature stability while maintaining the electromechanical coupling coefficient of 5.15%, which meets the sensitivity requirements of practical applications.

The application of virtual instrument technology and adaptive detection methods significantly improves the signal-to-noise ratio and measurement accuracy of the sensing system. The software-defined direct digital synthesis-based technology realizes high-resolution, small-step, and wide-range signal frequency accurate adjustment, and the frequency estimation scheme combining Welch and Merrifield algorithms improves the sensor frequency estimation accuracy to about 4 kHz, with low sensitivity to the signal-to-noise ratio. The gas detection experiments verify the performance advantages of the optimized design sensor in practical applications. In NO_2

gas detection, the frequency response of the optimized structure reaches -3275 Hz for 10 ppm concentration, with a sensitivity of -327.5 Hz/ppm, and shows excellent linearity ($R^2=0.9957$) in the concentration range of 1-50 ppm. Long-term stability tests showed that the sensitivity of the optimized structure decreased by no more than 5% after 30 days of continuous operation, and the decrease rate of the multilayer membrane structure was only 3%, which proved that the optimized design sensors have good long-term working stability. The optimal design method of SAW sensor based on the variational method, combined with the multilayer membrane structure and virtual instrumentation technology, has successfully constructed a systematic sensor design and testing system, and realized the comprehensive improvement of the key performance indexes of the sensor. These research results provide important technical support for the application of acoustic surface wave sensors in the fields of industrial detection, environmental monitoring, medical diagnosis, etc., and have significant theoretical value and practical significance.

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