



OPEN Enhancement and optimization of a graphene-based biosensing platform using machine learning for precise breast cancer detection

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In this study, we introduce a machine learning optimized graphene-based biosensor tailored for the early and accurate detection of breast cancer, aiming to elevate diagnostic reliability and clinical efficacy. The device employs a multilayer Ag–SiO₂–Ag architecture to amplify optical response, achieving a peak sensitivity of 1785 nm/RIU. Machine learning models are used to optimize structural parameters, enabling systematic refinement of detection accuracy and reproducibility. The optimized design demonstrates superior sensitivity compared with conventional biosensor configurations, underscoring its effectiveness in bioanalytical applications. The proposed platform offers a precise and robust solution for breast cancer screening and monitoring, with strong potential for clinical translation. To further refine sensor efficacy, a comprehensive parametric optimization approach is employed, strategically enhancing its sensitivity metrics. The sensor's heightened precision and responsiveness position it as a promising tool in biomedical diagnostics, particularly for early-stage breast cancer screening and monitoring.

Keywords Enhancement, Optimization, Breast cancer, Graphene, Surface Plasmon Resonance (SPR), Metasurface, Biosensor

Breast cancer remains a significant health concern, impacting countless lives globally. However, advancements in early detection have dramatically improved survival rates. Recognizing the importance of proactive healthcare is crucial. Early detection primarily relies on screening methods like mammograms, which can identify tumors before they become palpable. Regular self-exams also play a vital role, empowering individuals to become familiar with their bodies and notice any changes. It's important to note that any changes noticed should be brought to the attention of a medical professional. Factors such as family history, genetic predispositions, and lifestyle choices can influence breast cancer risk¹. Understanding these factors allows for personalized screening schedules and risk-reduction strategies. Medical professionals can provide guidance on appropriate screening frequencies and address individual concerns. Increased awareness and access to screening are essential in the fight against breast cancer². By prioritizing early detection, we can significantly improve outcomes and save lives. Methods such as mammography, ultrasound, and MRI help identify tumors before symptoms appear. Self-examinations and regular screenings increase the chances of detecting cancer at an early stage. Emerging technologies, including AI-driven imaging and biomarker-based blood tests, further enhance accuracy. Lifestyle changes, genetic testing, and awareness programs also play vital roles in prevention and early diagnosis. Detecting breast cancer early enables timely sensing and fast diagnosis^{3–5}.

Biosensors are used for detecting cancerous cells. The biosensors are designed using different materials to improve their sensitivity of the biosensors. Biosensors can be designed for various applications, including blood

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tests, urine analysis, and tissue biopsies⁶. This technology aims to revolutionize cancer diagnosis by facilitating earlier detection. Ongoing research focuses on developing more portable, affordable, and user-friendly biosensors. Biosensors are emerging as powerful tools for early breast cancer detection⁷. This technology aims to detect breast cancer at its earliest stages, when treatment is most effective. Researchers are developing biosensors with increased sensitivity and specificity to improve accuracy and reduce false positives. Portable and affordable biosensors could enable widespread screening, even in resource-limited settings, ultimately leading to earlier diagnoses and improved survival rates for breast cancer patients.

Graphene-based biosensors hold immense promise for revolutionizing early cancer detection, leveraging graphene's exceptional electrical conductivity and large surface area to detect minute biomarker concentrations⁸. Their high sensitivity enables the identification of cancer at its early stages, allowing for more effective treatment interventions. This versatility allows for the detection of a wide range of cancer-related biomarkers, from DNA fragments to proteins. Researchers are actively developing portable and cost-effective graphene biosensors, aiming to facilitate point-of-care diagnostics and expand access to screening in diverse settings. With the potential for improved accuracy and reduced false positives, these biosensors are poised to transform cancer diagnostics^{9,10}. By manipulating light, sound, or other waves, sensors can detect cancer biomarkers at extremely low concentrations, leading to earlier diagnosis. Their ability to focus and amplify signals can improve imaging techniques like MRI and optical detection methods, offering non-invasive and highly accurate results. Additionally, these materials can be tailored for specific types of cancer, improving detection across different stages. With advancements in nanotechnology and biophotonics, metamaterials could pave the way for compact, cost-effective, and efficient sensors, transforming early cancer diagnostics¹¹.

In medical diagnostics, graphene-based sensors can identify diseases at an early stage by detecting specific proteins or DNA sequences. Additionally, their flexibility and cost-effectiveness make them ideal for portable and wearable health monitoring devices. By integrating graphene oxide, these sensors achieve higher precision, efficiency, and reliability in detection¹². Graphene-based technology enhances breast cancer detection by significantly improving sensitivity. Its exceptional electrical and mechanical properties enable precise biomarker detection, leading to early diagnosis. The high surface area and conductivity of graphene improve signal accuracy, ensuring more reliable results. This advancement offers a promising, efficient, and accurate method for breast cancer screening¹³. The systematic review presented in¹⁴ explores the application of graphene-based materials in cancer detection, highlighting their exceptional sensitivity and accuracy. Graphene's unique electrical, mechanical, and optical properties enhance biomarker identification, enabling early diagnosis. The review examines advancements, challenges, and future prospects, emphasizing graphene's potential in revolutionizing cancer diagnostics through innovative, efficient, and highly precise detection techniques. A sensor featuring graphene/ is designed for detecting cancer. This innovative structure boosts detection efficiency by improving the quality factor and figure of merit. Its exceptional properties enable precise, reliable, and advanced disease diagnostics with superior sensitivity and performance^{15,16}. Graphene-based sensors offer wearable technology for real-time health monitoring. Their flexibility, lightweight nature, and high conductivity enable seamless integration into smart fabrics and medical devices. These sensors provide continuous data on vital signs, disease biomarkers, and environmental factors, revolutionizing personalized healthcare with enhanced accuracy, comfort, and efficiency¹⁷.

The ZnO–MWCNT nanostructure-based biosensor can serve as a promising pathway toward reliable, practical, and scalable applications in food safety and beyond¹⁸. The dominant and most reproducible sensing mechanism in carbon nanotube transistors, offering a reliable foundation for their advancement as robust platforms for biomolecular detection¹⁹. Schottky-to-Ohmic reversible biosensor provides a versatile and effective strategy for multifunctional, high-sensitivity detection, paving the way for next-generation biosensors and advanced electronic devices²⁰. SOI-DG TFET with low-k gate oxide demonstrates superior DC, AC, and RF performance, establishing it as a highly efficient candidate for low-power, high-speed, and diversified next-generation electronic applications²¹. Pocket-doped hetero-source SOI-TFET with an L-shaped gate demonstrates superior ON current, ultra-steep subthreshold swing, excellent Ion/Ioff ratio, and strong resistance to short-channel effects, highlighting its potential as an efficient device for future low-power and high-performance applications²². Machine learning on a ZnO nanoflower-based paper biosensor overcomes calibration limitations, achieves exceptional accuracy in troponin detection, and offers a broadly translatable strategy for next-generation biosensing applications²³. The SnS₂–MWCNT composite biosensor integrated with the OVSA-enabled explainable ML framework achieves ultra-sensitive and rapid troponin-I detection, positioning it as a highly promising platform for next-generation cardiac diagnostics and clinical translation²⁴.

The existing literature reveals a significant gap in the development of highly efficient sensors for the early detection of breast cancer. While various technologies have been explored, many lack the sensitivity, specificity, and real-time detection capabilities necessary for accurate diagnosis. Current methods often face limitations in detecting cancer at its initial stages, reducing the chances of timely intervention. Advanced materials, such as graphene-based sensors, have shown promise but remain underexplored. Addressing these shortcomings requires innovative approaches to enhance detection accuracy, reliability, and accessibility. Future research should focus on developing cutting-edge biosensors that enable early, precise, and non-invasive diagnosis. Our graphene-based sensor is designed for highly effective, early breast cancer detection, offering superior sensitivity, accuracy, and rapid diagnostic capabilities. The following section presents an in-depth study, including comprehensive modelling, experimental results, and conclusive findings derived from the research analysis. The following are the novelties of the current graphene-based sensor that distinguish it from other similar works.

- This study presents a machine learning–optimized graphene-based biosensor for early breast cancer detection.

- The sensor employs a multilayer Ag–SiO₂–Ag architecture, enabling enhanced plasmonic interaction and achieving a peak sensitivity of 1785 nm/RIU.
- Machine learning algorithms are applied to systematically optimize structural parameters, resulting in improved precision and reproducibility compared with conventional designs.
- Parametric optimization further refines resonance behavior, enhancing detection robustness.
- The proposed device demonstrates high sensitivity and stability, establishing its potential as a reliable platform for clinical breast cancer diagnostics.

Design and modelling

The designed biosensor employs a Metal–Insulator–Metal (MIM) configuration, which significantly boosts its efficiency and detection sensitivity. This layered structure strengthens the interaction between light and the sensing medium, resulting in heightened responsiveness. Maximizing the electromagnetic field confinement within the active region ensures precise signal capture. This advancement greatly contributes to the reliability of biomedical diagnostics, especially for early-stage breast cancer identification. The MIM-based architecture is tailored to deliver superior performance by reducing signal losses and enhancing resonance effects, making it a promising platform for high-accuracy clinical detection in healthcare and diagnostic applications. The MIM configuration enables superior electromagnetic field confinement, boosting the sensor's efficiency in identifying biomolecular changes. By incorporating this advanced technique, the biosensor achieves higher sensitivity, rapid response, and reliable detection capabilities. The MIM-based design also ensures better signal enhancement, making it a promising tool for early cancer screening. This innovative structure contributes to improved biosensing technologies, advancing medical diagnostics and patient care outcomes effectively. The proposed structure is illustrated in Fig. 1. In the designed MIM configuration, silver (Ag) is utilized as the metal layer, while silicon dioxide (SiO₂) serves as the insulating layer. This combination is chosen due to its excellent optical and electrical properties, which enhance the sensor's overall performance. The Ag layer provides superior conductivity and plasmonic effects, facilitating efficient light interaction for improved sensitivity. Meanwhile, the SiO₂ layer acts as a dielectric, ensuring optimal field confinement and minimizing signal loss. This strategic

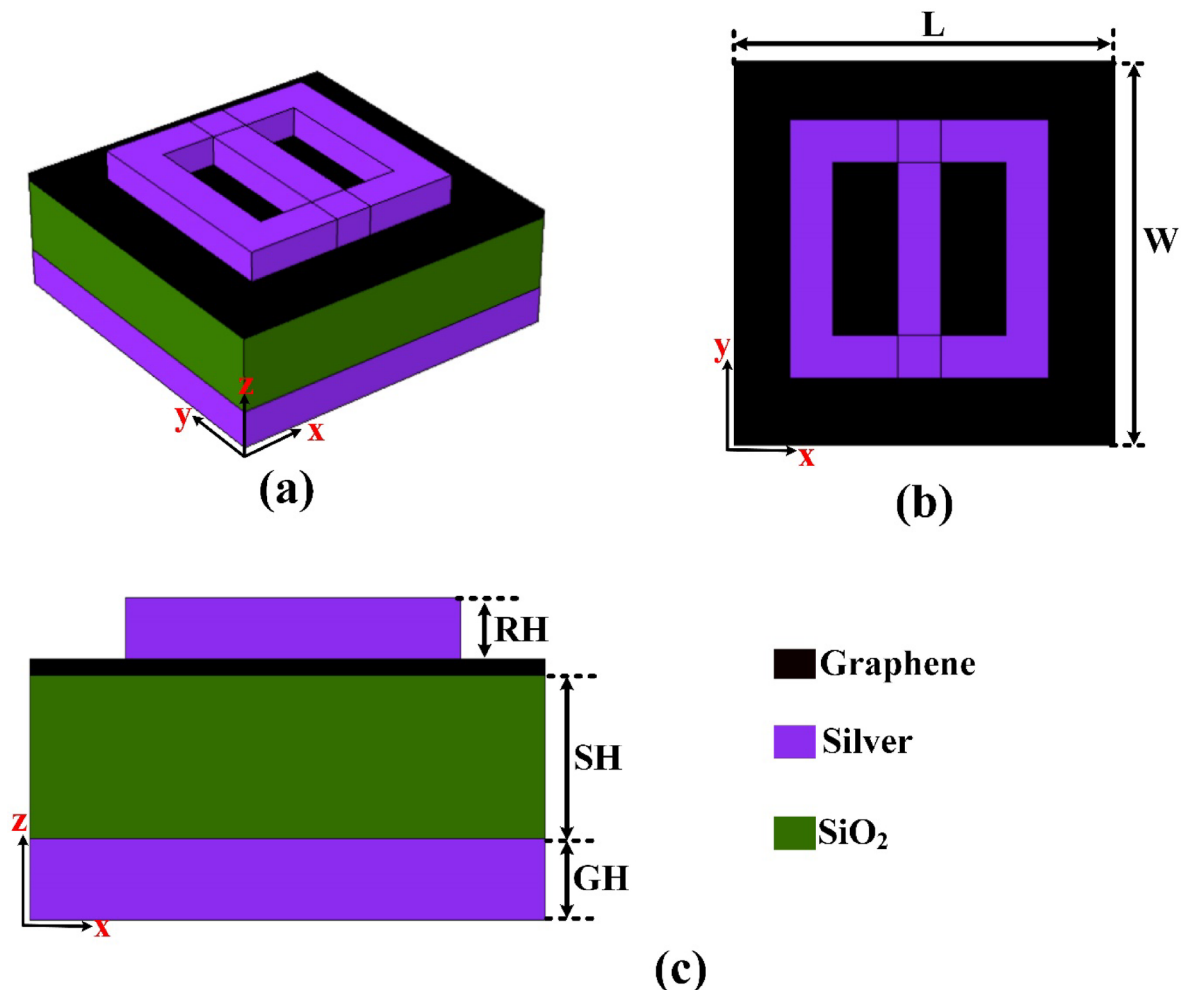


Fig. 1. (a–c) Three different views of the Sensor design.

selection of materials significantly boosts detection accuracy, making the biosensor ready for fast and early detection.

A graphene spacer is incorporated between the resonator and the substrate to enhance the sensor's sensitivity and overall performance. This addition optimizes electromagnetic field distribution, leading to improved signal detection and stronger plasmonic resonance effects. Graphene's exceptional electrical and optical properties contribute to better confinement of light waves, reducing energy loss and increasing interaction efficiency. By strategically positioning the graphene spacer, the sensor achieves higher sensitivity, making it more effective for biomedical applications. This structural enhancement plays a crucial role in detecting minute biomolecular changes, ensuring precise and early breast cancer diagnosis with greater accuracy and reliability.

The fabrication method for the MIM layers and graphene spacer is detailed in Fig. 2. This process involves precise deposition techniques to ensure optimal structural integrity and performance. The metal–insulator–metal (MIM) configuration is carefully developed using advanced layering methods, enhancing the sensor's efficiency. Additionally, the graphene spacer is integrated with high accuracy to improve electromagnetic field confinement, boosting sensitivity. This fabrication approach ensures minimal energy loss, superior detection capability, and enhanced plasmonic resonance. By following this structured methodology, the biosensor achieves reliable performance, making it extremely suitable for medical applications, mainly in early breast cancer detection and diagnosis.

The deposition of layers is carefully executed, followed by the application of a lithography technique to etch the resonator shape with high precision. This process ensures accurate structural formation, enhancing the sensor's performance and sensitivity. Thin-film deposition methods are employed to create uniform metal and insulator layers, optimizing plasmonic resonance effects. Lithography allows for intricate patterning, defining the resonator's geometry with nanoscale accuracy. This fabrication approach minimizes defects and improves electromagnetic field confinement, leading to superior detection capabilities. The combination of precise layer deposition and advanced etching techniques makes the sensor highly effective for biomedical applications, particularly breast cancer detection.

The incorporation of metal–insulator–metal (MIM) layers significantly enhances the sensitivity of the biosensor, ensuring precise and efficient detection. This layered structure optimizes electromagnetic field confinement, leading to stronger plasmonic resonance and improved signal strength. The metal layers, particularly silver (Ag), provide excellent conductivity, while the insulator layer, silicon dioxide (SiO_2), facilitates effective light-matter interactions. By minimizing signal loss and maximizing energy concentration, the MIM configuration boosts detection accuracy. This enhanced sensitivity is crucial for biomedical applications, particularly in early breast cancer diagnosis, where detecting minute biomolecular changes can lead to timely medical intervention and improved patient outcomes.

Graphene and its conductivity

Graphene plays a crucial role in biosensor design, particularly its conductivity, which varies with changes in potential. This unique characteristic allows graphene to enhance sensitivity by responding dynamically to external stimuli. Its high electron mobility and tunable Fermi level improve charge transfer efficiency, optimizing plasmonic interactions within the biosensor. Additionally, graphene's atomic thickness ensures minimal

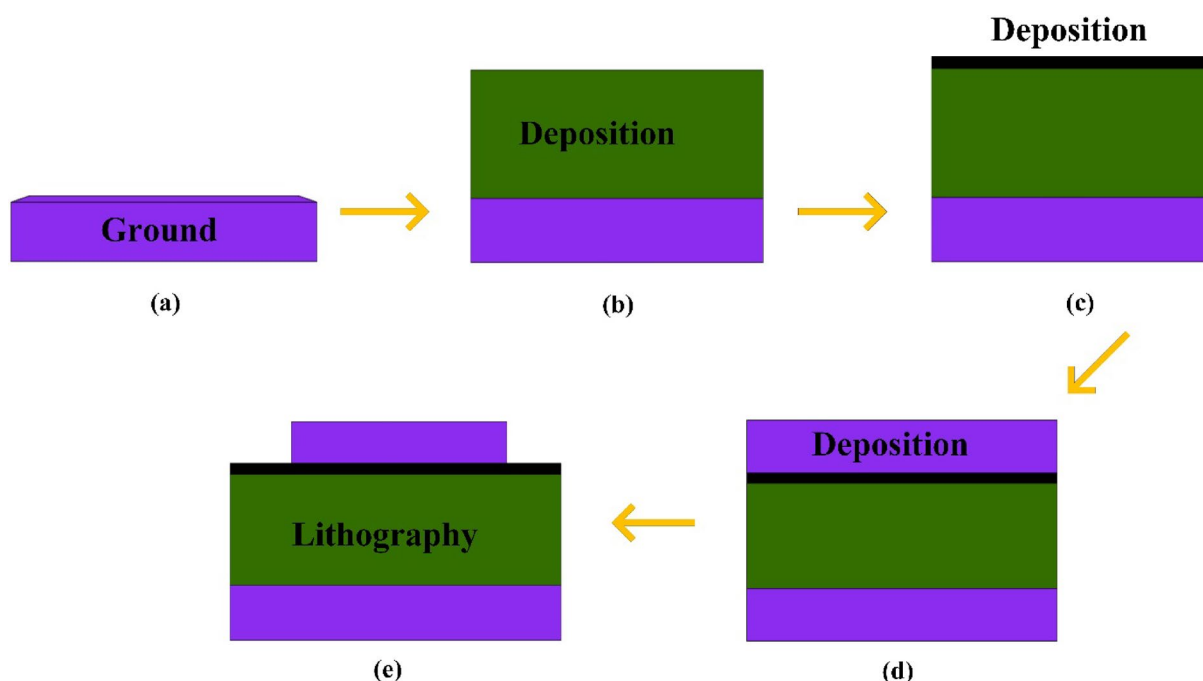


Fig. 2. (a–e) Fabrication approach of the sensor design.

interference while maintaining strong signal integrity. By incorporating graphene, the sensor achieves superior performance in detecting biomolecular variations. The equations show the relevance²⁵.

$$\varepsilon(\omega) = 1 + \frac{\sigma_s}{\varepsilon_0 \omega \nabla} \quad (1)$$

$$\sigma_{intra} = \frac{-je^2 k_B T}{\pi \hbar^2 (\omega - j2\Gamma)} \left(\frac{\mu_c}{k_B T} + 2 \ln \left(e^{\frac{\mu_c}{k_B T}} + 1 \right) \right) \quad (2)$$

$$\sigma_{inetr} = \frac{-je^2}{4\pi \hbar} \ln \left(\frac{2|\mu_c| - (\omega - j2\Gamma) \hbar}{2|\mu_c| + (\omega - j2\Gamma) \hbar} \right) \quad (3)$$

$$\sigma_s = \sigma_{intra} + \sigma_{inetr} \quad (4)$$

Sensitivity

Sensitivity, FOM, Q- factor, and DL are key performance metrics for evaluating a biosensor's efficiency. Sensitivity measures the sensor's response to changes in the refractive index, typically expressed in GHz/RIU, indicating how effectively it detects biomolecular interactions. FOM assessing detection precision. Q factor represents the intelligence of resonance peaks, with higher values signifying improved signal quality. Detection limit defines the smallest detectable refractive index change, determining the sensor's capability for early disease diagnosis. Optimizing these parameters ensures high-performance biomedical detection. All these parameters are presented in Eqs. (5–8)²⁶.

$$S = \frac{\Delta\lambda}{\Delta n} \quad (5)$$

$$FOM = \frac{S}{FWHM} \quad (6)$$

$$Q = \frac{\lambda r}{FWHM} \quad (7)$$

$$DL = \left(\frac{\Delta n}{1.5} \right) \times \left(\frac{FWHM}{\Delta\lambda} \right)^{1.25} \quad (8)$$

Results and discussions

The findings were derived through simulations conducted using the COMSOL Multiphysics software, which provided detailed insights into the system's performance. This advanced simulation tool enabled precise modeling and analysis, ensuring accurate evaluation of the proposed design's effectiveness in real-world applications. The results validate the system's feasibility and optimization potential. The results are presented in terms of absorbance, as illustrated in Fig. 3, for both breast cancer and normal cells. This analysis provides a comparative assessment of the absorption characteristics of the proposed system when interacting with different biological samples. By examining the absorbance variations, the distinction between cancerous and healthy cells can be effectively observed. The figure highlights the differences in absorption spectra, demonstrating the potential of the system in identifying breast cancer cells. These findings contribute to the understanding of terahertz metasurface interactions with biological tissues, reinforcing the biosensor's capability for non-invasive cancer detection and diagnosis.

The red-colored line plot represents the response of a normal cell with a refractive index of 1.385, while the green-colored line plot corresponds to the response of a breast cancer cell with a refractive index of 1.399. A clear spectral shift is observed between the two responses, indicating differences in their optical properties. The wavelength difference between the two absorption peaks is measured at 25 nm, as illustrated in Fig. 3. This shift highlights the sensitivity of the system in distinguishing between normal and cancerous cells, demonstrating its potential application in early breast cancer detection using terahertz metasurface biosensing technology. The sensitivity is 1785 nm/RIU. FOM, Q-factor and DL are 178 RIU⁻¹, 293, 0.00293 RIU respectively.

Parametric optimization

Parametric optimization is performed to enhance sensor performance by systematically adjusting key physical parameters, including thickness, length, and width. By fine-tuning these structural attributes, the sensor's sensitivity and efficiency can be maximized for precise detection. Optimization involves evaluating how variations in these parameters influence the device's absorbance, resonance shifts, and overall response. Advanced computational techniques, such as machine learning algorithms or simulation-based analyses, are employed to determine the ideal configurations. This process ensures the development of a highly optimized biosensor with superior accuracy, making it suitable for real-world applications such as non-invasive disease detection and biomedical diagnostics.

The resonator and substrate thickness were varied, and their corresponding results are presented in Figs. 4 and 5, respectively, highlighting their impact on the sensor's performance and response characteristics. By varying the resonator thickness from 0.5 to 1 μm, a noticeable shift in the resonance peak is observed for different thickness values. The thinner resonator, represented by the red-colored line plot, exhibits a sharper resonance peak, indicating improved sensitivity and performance. Additionally, selecting the lower thickness not only enhances the sensor's detection capabilities but also contributes to reducing the overall size of the

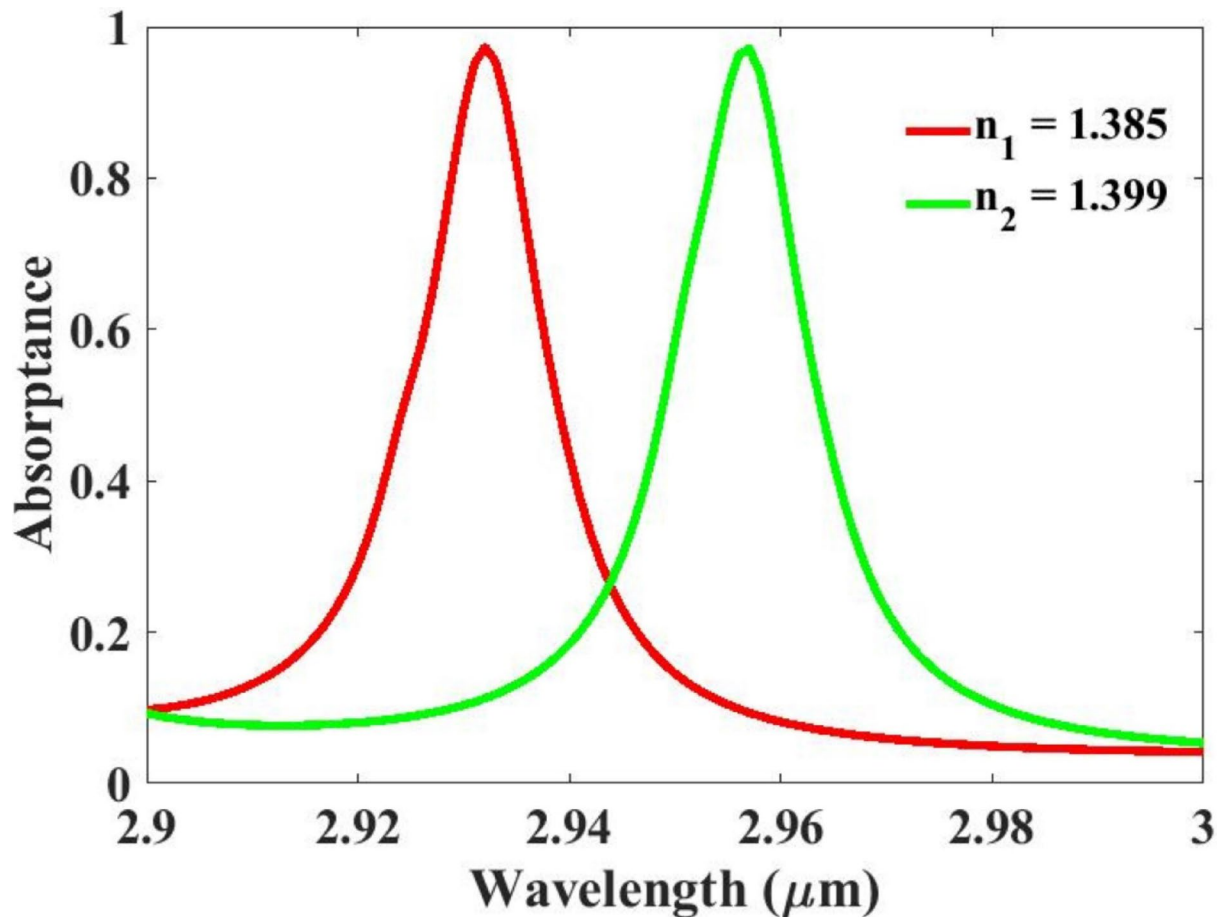


Fig. 3. Biosensor response in terms of absorbance. The two peaks are visible for normal and cancer cell.

structure, making it more compact and efficient. This optimization ensures that the biosensor remains highly effective for applications requiring precise detection while maintaining a minimal footprint, making it suitable for biomedical and biosensing applications.

The substrate thickness was varied from 1 to 1.5 μm , revealing that at lower thickness values, sharp resonance peaks are distinctly visible, demonstrating strong tuning behavior. However, as the substrate thickness increases, a reduction in absorption is observed, leading to diminished performance. The initial lower thickness provides better resonance characteristics and enhanced absorption, making it the preferred choice. Therefore, a substrate thickness of 1 μm is selected to optimize sensor efficiency while maintaining superior absorption properties. This selection ensures improved device sensitivity and performance, making it suitable for precise detection applications in biomedical and biosensing technologies.

The sensor structure's length and width are adjusted between 4.6 and 5.1 μm , as illustrated in Figs. 6 and 7, respectively, to analyze their impact on performance and resonance behavior. The substrate length is adjusted from 4.6 to 5.1 μm , and the corresponding response is depicted in Fig. 6. The results indicate a clear shift in resonance peaks for different length values. At the shortest length, a single resonance peak appears, represented by the red-colored line plot. However, for a length of 4.7 μm , two distinct resonance peaks are observed, suggesting a change in resonance behavior. Based on these findings, the lower length is chosen as the optimized value, ensuring improved performance and stability. This selection enhances the sensor's efficiency while maintaining a compact and effective structural design.

The structure's width is adjusted between 4.6 μm and 5.1 μm , as depicted in Fig. 7. This variation influences the resonance peak, causing it to shift toward the right as the width increases. To achieve the desired resonance behavior, the narrower width of 4.6 μm is chosen. The selection is based on optimizing performance by maintaining the resonance peak within the required spectral range. The effect of width variation on resonance behavior highlights the sensitivity of the structure to dimensional changes. Consequently, the reduced width of 4.6 μm .

Variations in graphene potential directly influence the resonance of the sensor, leading to observable tuning effects at different potential levels as shown in Fig. 8. This phenomenon demonstrates the sensor's sensitivity to electrical modulation. By adjusting the graphene potential, the resonance frequency shifts accordingly, enabling precise control over sensor performance. This tunability makes the device highly versatile for applications requiring adaptive sensing. The ability to fine-tune resonance through potential variation highlights the sensor's

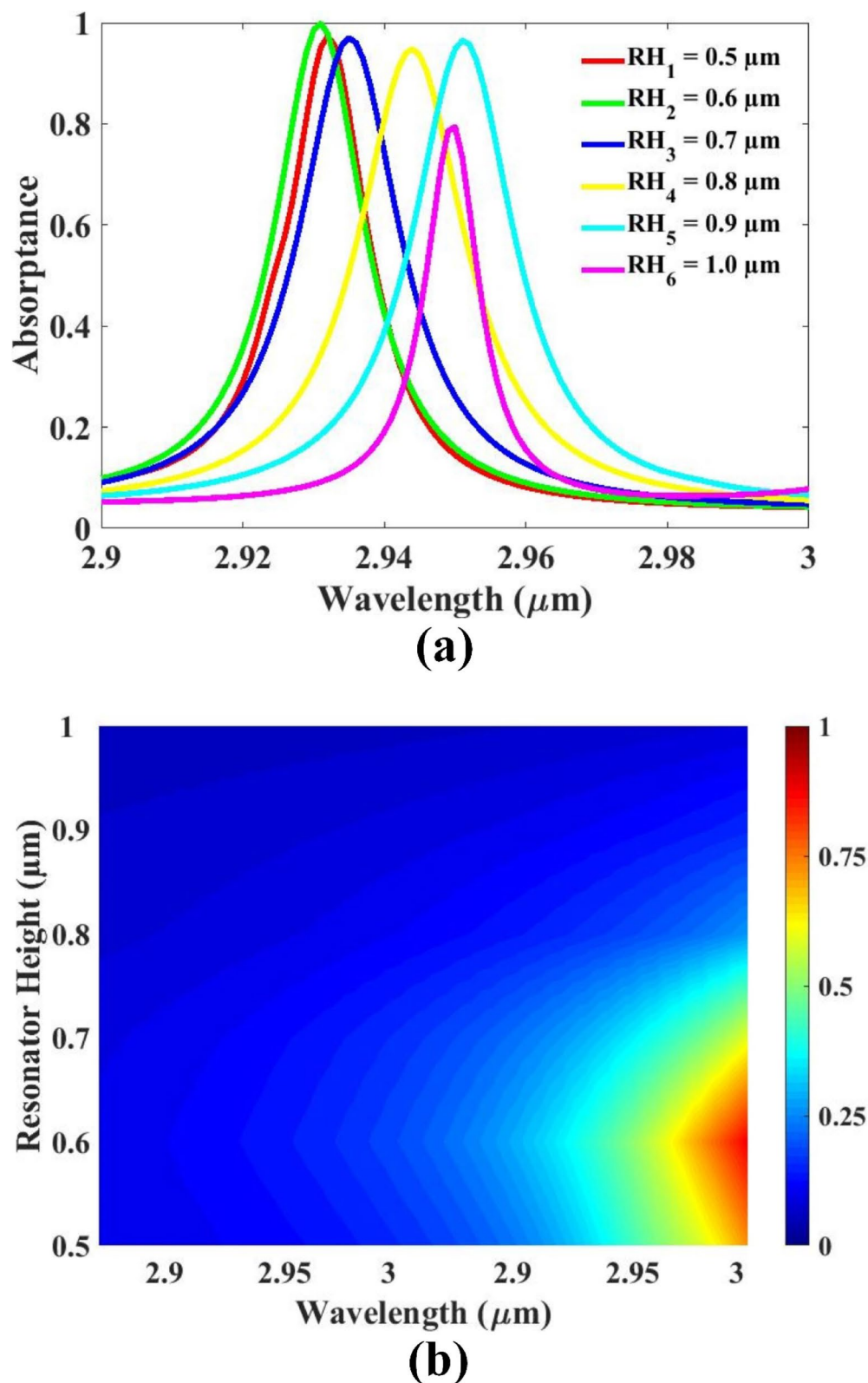


Fig. 4. (a,b) Resonator thickness variation from 0.5 to 1 μm .

dynamic nature. As a result, the device functions as a tunable sensor, capable of responding to external electrical changes, enhancing its usability in diverse sensing environments and advanced technological applications.

The electric field intensity is analyzed at two distinct wavelengths, 2.932 μm and 2.957 μm , to examine field variations at different spectral positions. This comparison helps in understanding the impact of wavelength on

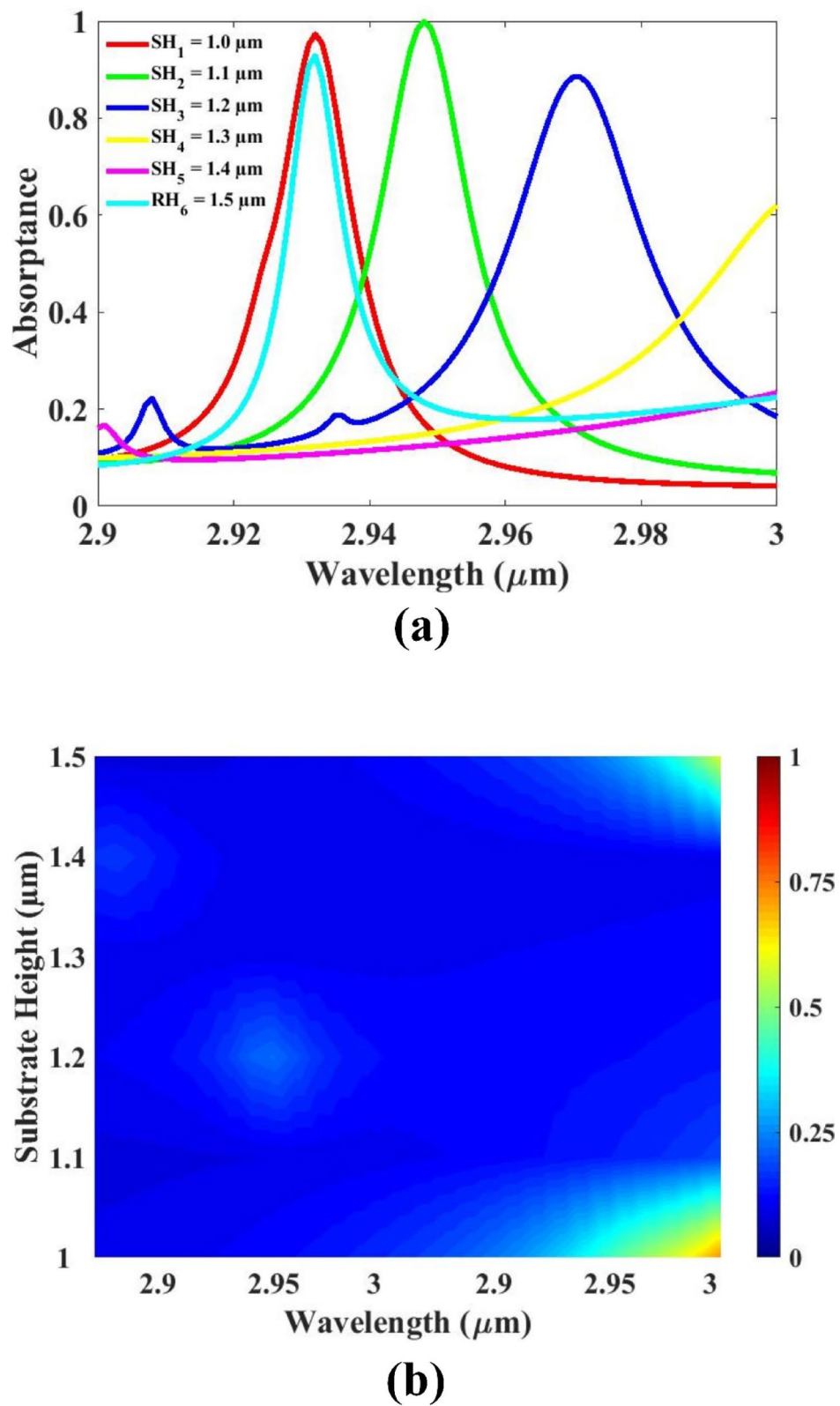


Fig. 5. (a,b) Substrate thickness variation from 1 to 1.5 μm .

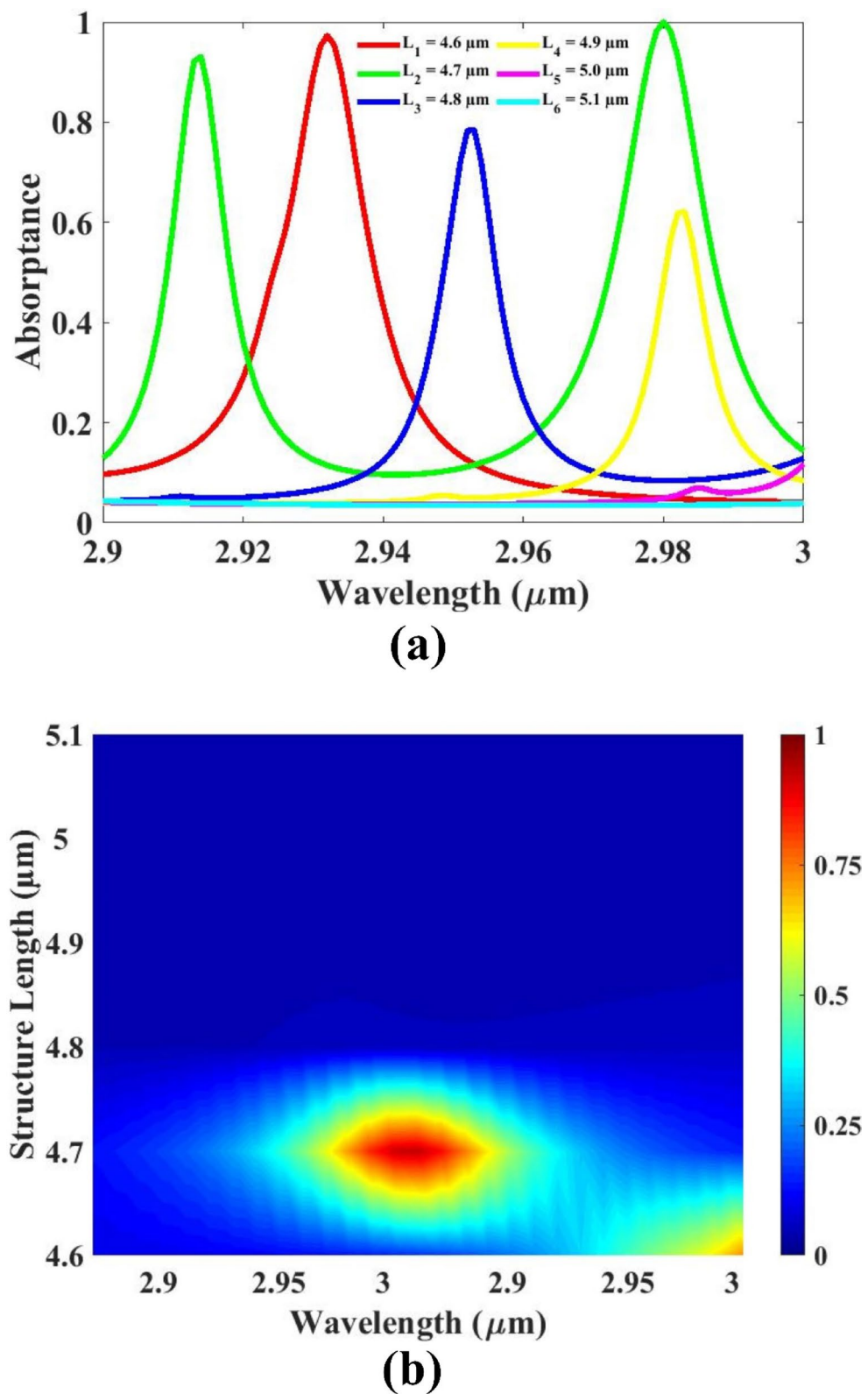


Fig. 6. (a,b) Substrate length variation from 4.6 to 5.1 μm .

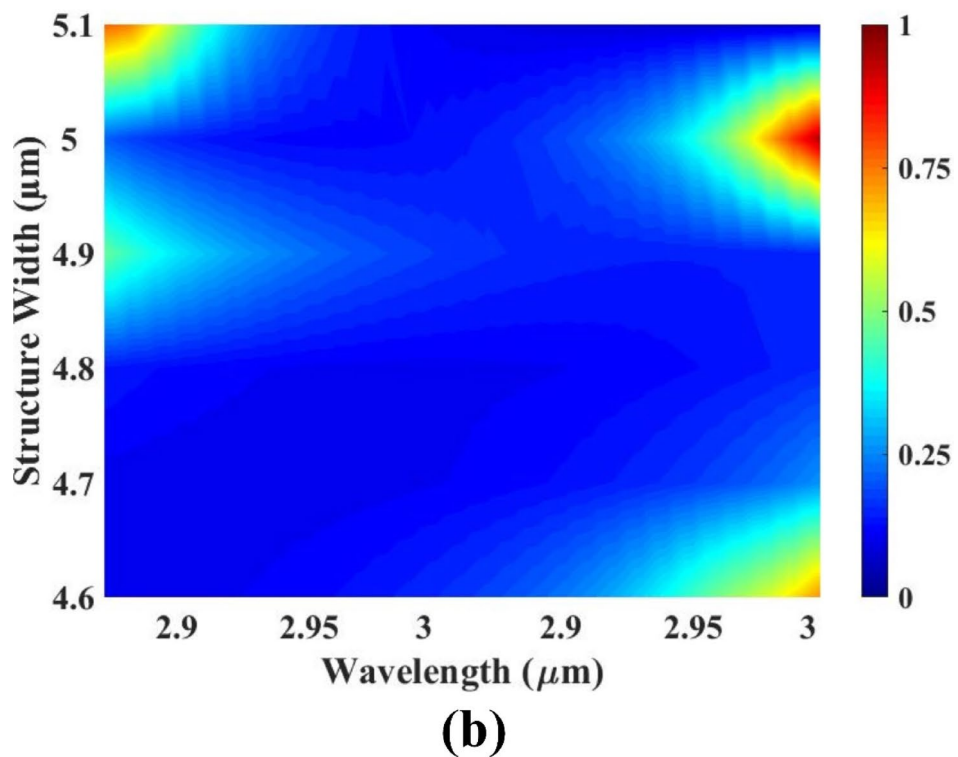
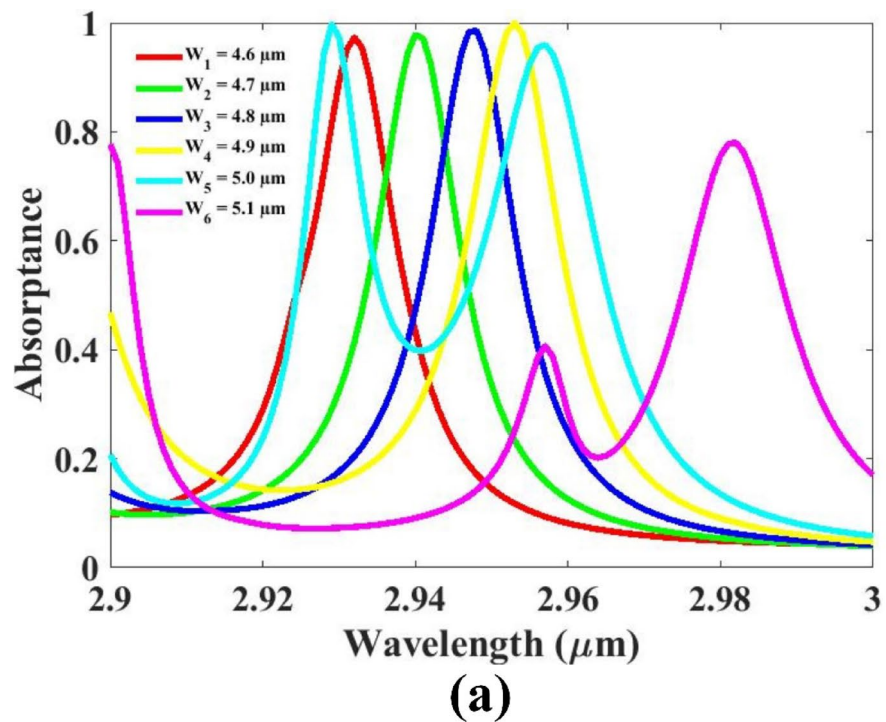


Fig. 7. (a,b) Substrate width variation from 4.6 to 5.1 μm .

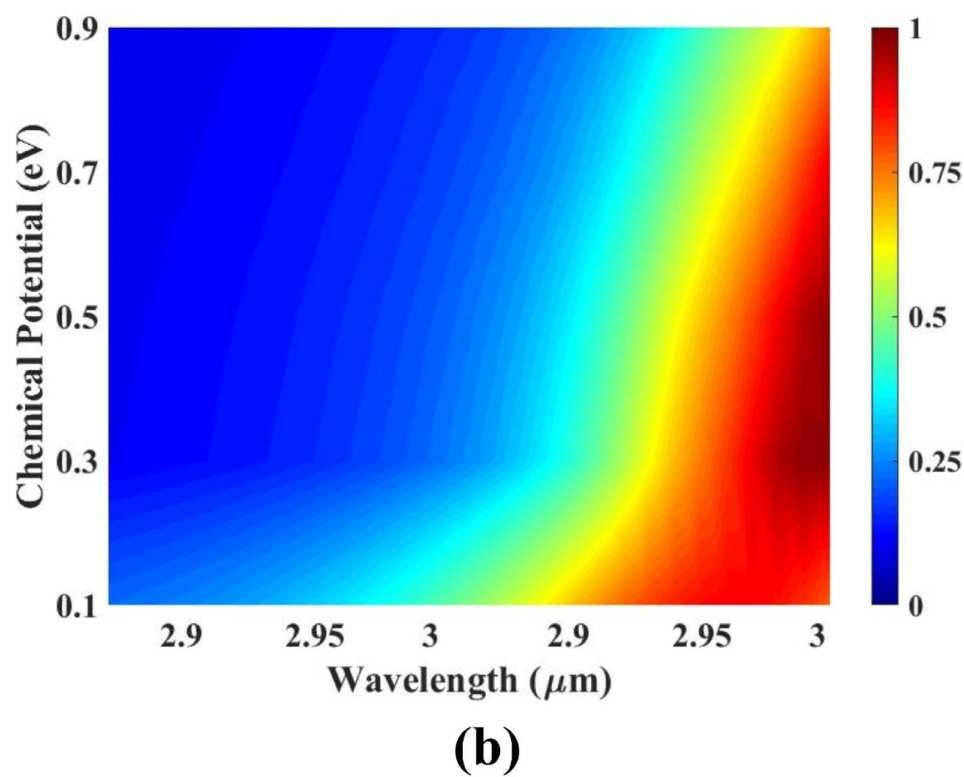
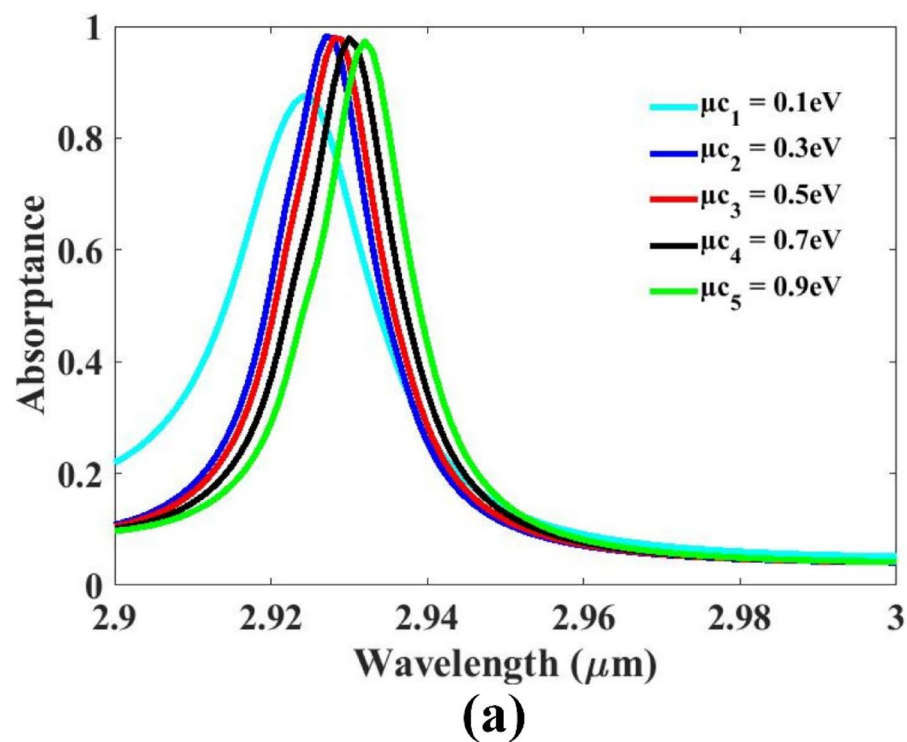


Fig. 8. (a,b) Graphene potential variation from 0.1 to 0.9 eV.

field distribution. By evaluating these specific wavelengths, the study investigates how the electric field responds across the spectrum. The analysis provides insight into spectral field behavior, offering valuable information on resonance characteristics. The observed results, depicted in Fig. 9, illustrate the field's behavior at these wavelengths. This assessment enhances understanding of the interaction between wavelength and field intensity, aiding in optimizing device performance and functionality.

A comparative analysis assesses various methods or devices by examining their advantages, limitations, and overall performance to identify the optimal solution. Table 1 presents one such evaluation.

Machine learning optimization

The explored figure mentions the machine learning section, where the sensor resonator height was varied from 0.5 to 1.0 μm using the linear regression method with a test size of 0.25. The machine learning outputs for the sensor resonator height yielded R^2 values of 0.99, 0.997, 0.994, 0.979, 0.937, and 0.802, with a mean square error of $0.869298951 \times 10^{-4}$ (Fig. 10).

Conclusion

A highly efficient sensor design is explored for breast cancer detection. Utilizing graphene enhances sensitivity while also enabling tunability. This material's properties improve detection accuracy and adaptability, making the sensor more effective. The combination of high sensitivity and tuning capability ensures optimized performance for precise and reliable breast cancer diagnostics. Parametric optimization enhances the structure's efficiency by refining its key dimensions, including length, width, and thickness. The optimized substrate parameters are determined as 4.6 μm for both length and width, with a thickness of 1 μm . Additionally, the resonator thickness is precisely optimized to 0.5 μm , ensuring improved performance. These optimized values contribute to better resonance characteristics, structural stability, and overall sensor efficiency. By fine-tuning these parameters, the device achieves superior functionality, making it more effective for its intended application in high-precision sensing and detection technologies. The sensor attains a maximum sensitivity of 1785 nm/RIU, ensuring enhanced detection accuracy and superior performance in sensing applications.

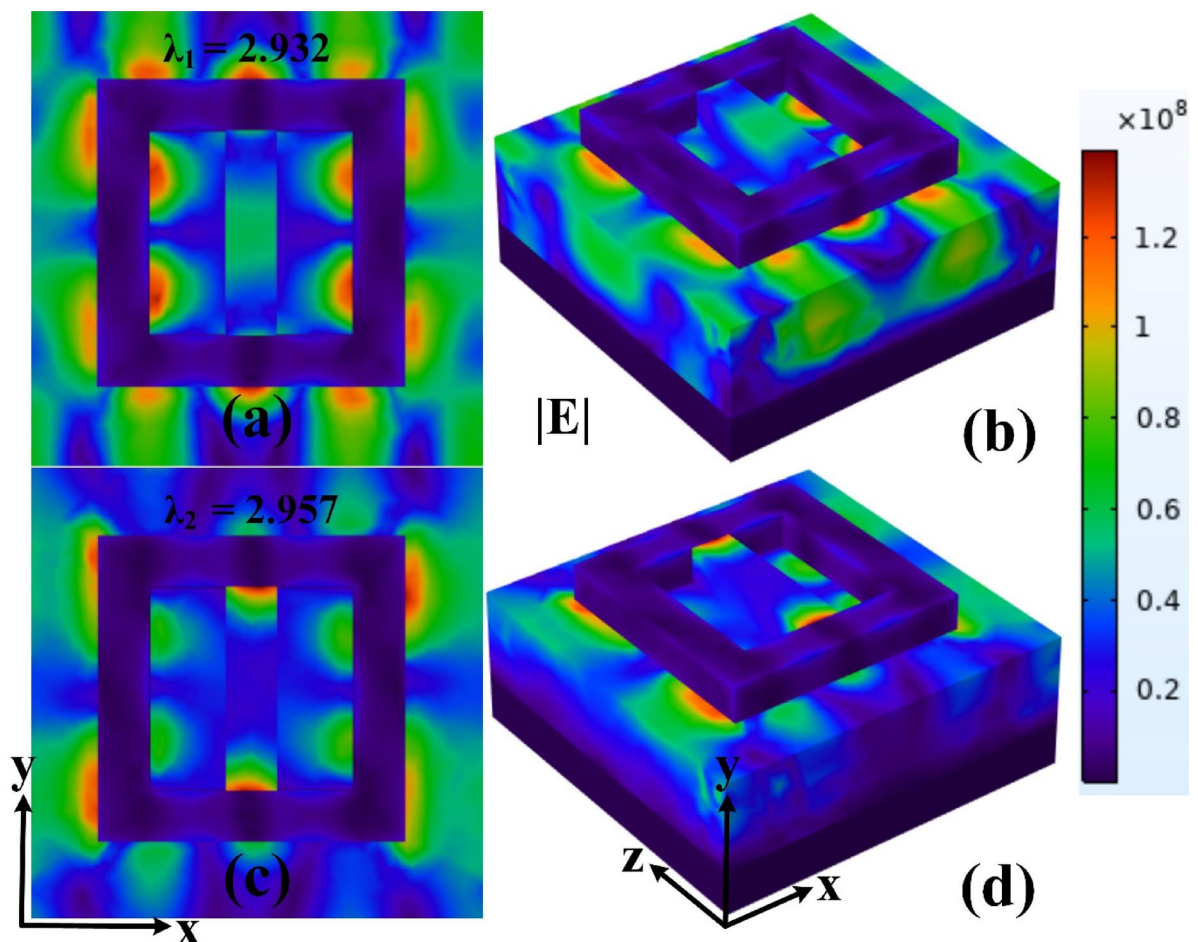


Fig. 9. (a–d) E-Field variation for two wavelengths 2.932 μm and 2.957 μm .

Design	Sensitivity (nm/RIU)	Quality factor (Q)	Figure of merit (FOM)	Detection limit (DL)
27	443	6630	–	–
28	1100	–	3.832	0.391
29	1000	5166	2.94	0.04
30	484	–	–	–
31	500	–	–	–
32	1000	–	–	–
33	1000	–	–	–
34	200	3493	222	–
35	690	2500	1400	–
36	1400	–	–	–
37	72	19	–	–
38	–	262	–	0.002
39	546.72	2066.44	–	1.44
40	306.25	5000	103	–
41	900	190	105	0.00001
42	74.5	19.82	–	–
Our research	1785	293	178	0.00293

Table 1. Comparative tabular approach of sensor designs.

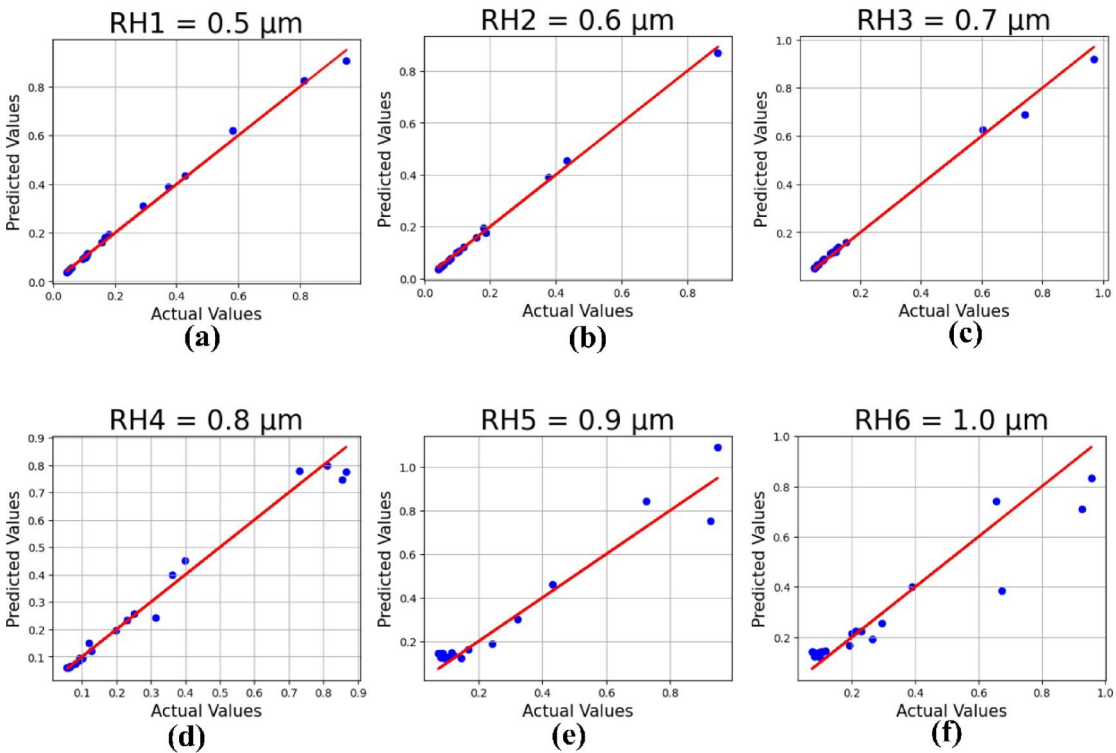


Fig. 10. Machine learning results for the resonator height with varying parameter values (μm): (a) 0.5, (b) 0.6, (c) 0.7, (d) 0.8, (e) 0.9, and (f) 1.0.

Data availability

The data will be made available on a reasonable request to the corresponding author.

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Declarations

Competing interests

The authors declare no competing interests.

Ethical approval

Not applicable.

Additional information

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