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Hybrid FEM–ANN Framework for Multi-Mass Detection on Graphene Nanoresonators

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Abstract

Graphene's remarkable stiffness, extremely low density, and large surface-to-mass ratio make it highly responsive to minute mass variations, even down to the zeptogram scale. Although most prior studies have concentrated on single-particle adsorption, practical scenarios often involve multiple particles randomly distributed on the surface, leading to complex nonlinear vibration behaviors. In this work, a hybrid FEM–ANN framework is developed that integrates high-fidelity finite element simulations with a deep-learning neural network to analyze the vibrational response of graphene sheets under multi-mass loading. The dataset generated from simulations—incorporating variations in aspect ratio, sheet dimensions, number of particles, and their random distribution—is used to train and validate the neural network. The trained model accurately predicts nonlinear frequency shifts with substantially reduced computational cost compared to full numerical simulations. This hybrid approach provides a reliable and efficient tool for rapid multi-mass detection in graphene nanoresonators, with potential applications in biosensing and environmental monitoring.

Keywords: graphene; Frequency response; Finite element modeling; mass sensing.

1. Introduction

Graphene, a single layer of carbon atoms arranged in a hexagonal lattice, is known for its exceptional mechanical strength, high electron mobility, and remarkable thermal stability [1–3]. Its combination of ultralow mass and high stiffness allows graphene resonators to achieve very high resonant frequencies, making them extremely sensitive to tiny mass changes [4,5]. This sensitivity enables the detection of mass variations down to the zeptogram scale, highlighting graphene's potential in ultra-sensitive nanoelectromechanical systems (NEMS) applications [6,7]. The core sensing mechanism relies on shifts in the resonance frequency caused by adsorbed particles, which has been extensively explored in graphene-based devices [8,9]. Various modeling approaches have been employed to study the vibrational behavior of graphene under added mass. Atomistic methods such as molecular dynamics (MD) and density functional theory (DFT) provide detailed insights into

local deformations and adsorption effects but are computationally demanding for large systems [10,11]. Continuum mechanics and nonlocal elasticity models offer a more efficient alternative by incorporating nanoscale effects through scale-dependent parameters [12–14]. Hybrid multiscale techniques have also been proposed to combine the accuracy of atomistic models with the efficiency of continuum approaches [15,16].

A significant challenge arises when multiple particles are randomly distributed on the graphene surface, leading to highly nonlinear shifts in resonant frequencies. Solving the inverse problem—determining the mass or distribution from measured frequencies—becomes increasingly difficult as the number of unknowns grows [17–19]. Recently, machine learning, particularly artificial neural networks (ANNs), has shown great promise in addressing this problem. ANNs can capture complex nonlinear relationships between system parameters and vibrational responses, offering rapid predictions once trained [20–25]. Finite element analysis (FEA) remains essential for generating accurate datasets for training these models. It allows detailed investigation of how geometry, boundary conditions, and particle placement affect resonance behavior [26]. In this study, we present a hybrid FEA–ANN framework to predict the vibrational response of single-layer graphene under multi-particle loading. A comprehensive dataset is generated by varying geometrical parameters and particle distributions, and an ANN is trained to predict natural frequencies as well as absolute and relative frequency shifts. The model is validated against FEA simulations, demonstrating both accuracy and efficiency. This framework offers a practical approach for rapid modeling and design of high-sensitivity graphene-based mass sensors.

2. Finite element method

In this study, a single-layer graphene sheet (SLGS) is modeled as a thin plate. Its fundamental mechanical and geometrical properties are summarized in Table 1. To simulate multi-mass loading, a predefined number of nanoparticles are randomly placed on the graphene surface (Fig.1).

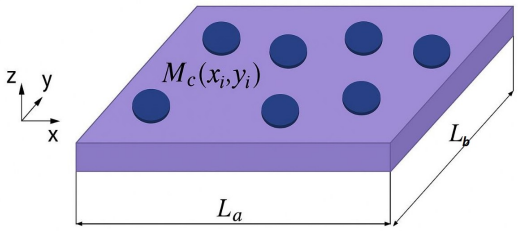


Figure 1: Schematic of a SLGS with N randomly distributed nanoparticles.

The sheet is discretized using an 8-node quadrilateral shell element, which provides high accuracy in capturing bending and stretching behavior. Simply supported boundary condition is applied along the edges.

Table 1. Mechanical and geometrical properties of SLGS (adapted from [27].)

Property	Value
Young's modulus (TPa)	**1.0**
Poisson's ratio	**0.149**
Mass density (kg/m³)	**2300**
Thickness (nm)	**0.345**

The dynamic behavior of the SLGS under multi-mass loading is analyzed using the finite element method (FEM). The governing equation of motion is:

$$[M]\{\ddot{q}\} + [K]\{q\} = 0 \quad (1)$$

where [M] and [K] are the global mass and stiffness matrices, {q} is the vector of nodal displacements, and {q̈} is the vector of nodal accelerations. Assuming harmonic vibration, $\{q\} = \bar{q}_i e^{j\omega_i t}$, the equation reduces to the eigenvalue problem:

$$[K]\bar{q}_i = {\omega_i}^2[M]\bar{q}_i \quad (2)$$

Here, ω_i is the ith natural frequency and $\bar{q}_i$ represents the corresponding mode shape.

The frequency shift caused by the attached nanoparticles is calculated as:

$$\Delta f_i = f_{0i} - f_i \quad (3)$$

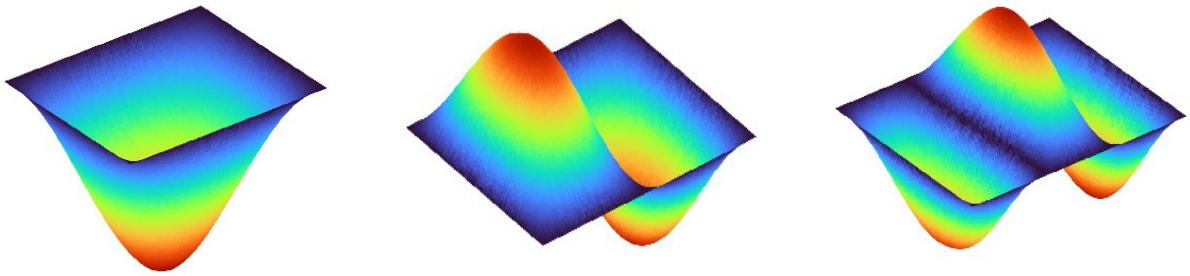
where f_{0i} and f_i are the natural frequencies of the unloaded and loaded SLGS, respectively, with:

$$f_i = \frac{\omega_i}{2\pi} \quad (4)$$

The relative frequency shift, a common metric to evaluate sensor sensitivity, is defined as:

$$f_{relative} = \frac{\Delta f_i}{f_{0i}} \times 100 \quad (5)$$

Simulations were repeated 10 times to account for statistical variations due to random particle placement. The results reported correspond to the average values across all repetitions.



(a) Mode 1 (b) Mode 2 (c) Mode 3

Figure 2. Mode shapes of SLGS under simply supported boundary conditions Simulation parameters: α = 2, L_a = 100 nm, m = 100 Zg, M_n = 100.

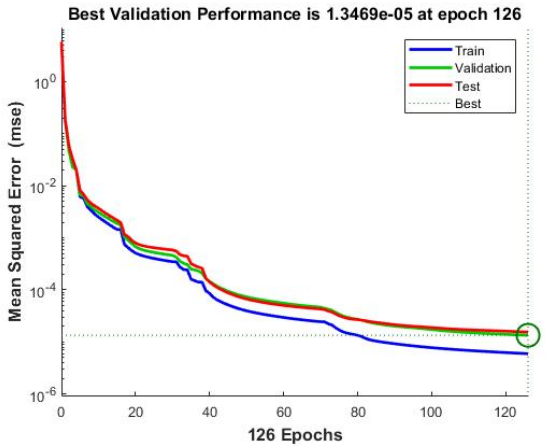
This FEM framework provides a reliable baseline for predicting vibrational behavior of graphene sheets with multi-particle loading. The generated data can be further used to train machine learning models, enabling fast prediction of frequency shifts and sensor performance for various geometries and mass distributions.

3. Artificial Neural Network (ANN)

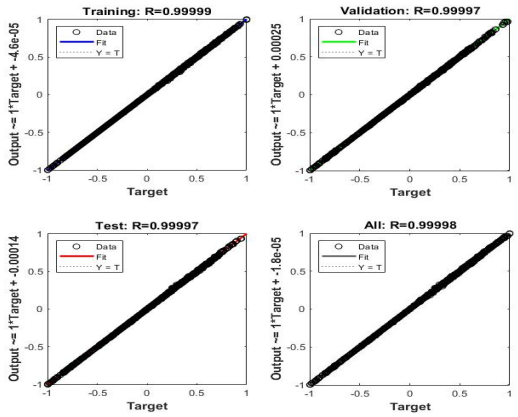
An artificial neural network (ANN) was developed to predict the vibration frequencies of single-layer graphene sheets (SLGSs) based on finite element simulations in ANSYS APDL. In this study, only simply supported boundary conditions were considered. The ANN architecture is a feed-forward multilayer perceptron (MLP) with two hidden layers containing 50 and 30 neurons, respectively. The hidden layers use the tansig activation function, and the output layer employs purelin to predict continuous frequency values. The network was trained using the Levenberg–Marquardt (trainlm) backpropagation algorithm with mean squared error (MSE) as the loss function.

The dataset was divided randomly into training, validation, and test subsets. The network's performance was evaluated using statistical metrics including MSE, RMSE, and the correlation coefficient (R). Results show excellent agreement between ANN predictions and FEM target values, confirming the network's ability to generalize and accurately capture the nonlinear relationship between the input parameters and the vibrational response

Fig. 3 illustrates the ANN performance. Fig. 3(a) shows the convergence of MSE during training, validation, and testing, while Fig. 3(b) presents regression plots comparing ANN predictions with FEM results. These results confirm that the ANN provides a robust and efficient tool for predicting the natural frequencies of SLGSs under simply supported boundary conditions.



(a) MSE convergence during training, validation, and testing.



(b) Regression plots comparing ANN predictions with FEM target values

Figure 3. Training performance and prediction accuracy of the ANN model

4. Results and Discussion

This section presents the results of finite element simulations and ANN-based predictions for single-layer graphene sheets (SLGSs) under simply supported boundary conditions. The influence of key parameters—including the number of attached masses, sheet length, aspect ratio, and mass distribution—on the fundamental frequency, frequency shift, and relative frequency shift of the SLGS is analyzed.

Fig. 4 shows the impact of aspect ratio (α = 1–5) on sensor characteristics under varying attached masses. As the mass increases, the fundamental frequency decreases due to added inertia. Higher aspect ratios exhibit larger initial frequencies because of geometric stiffening. The frequency shift increases at low mass values and gradually saturates for larger masses, reflecting nonlinear behavior. Relative frequency follows a similar trend, with higher aspect ratios providing enhanced sensitivity for minimal mass detection. ANN predictions closely match FEM results, confirming the reliability of the AI model.

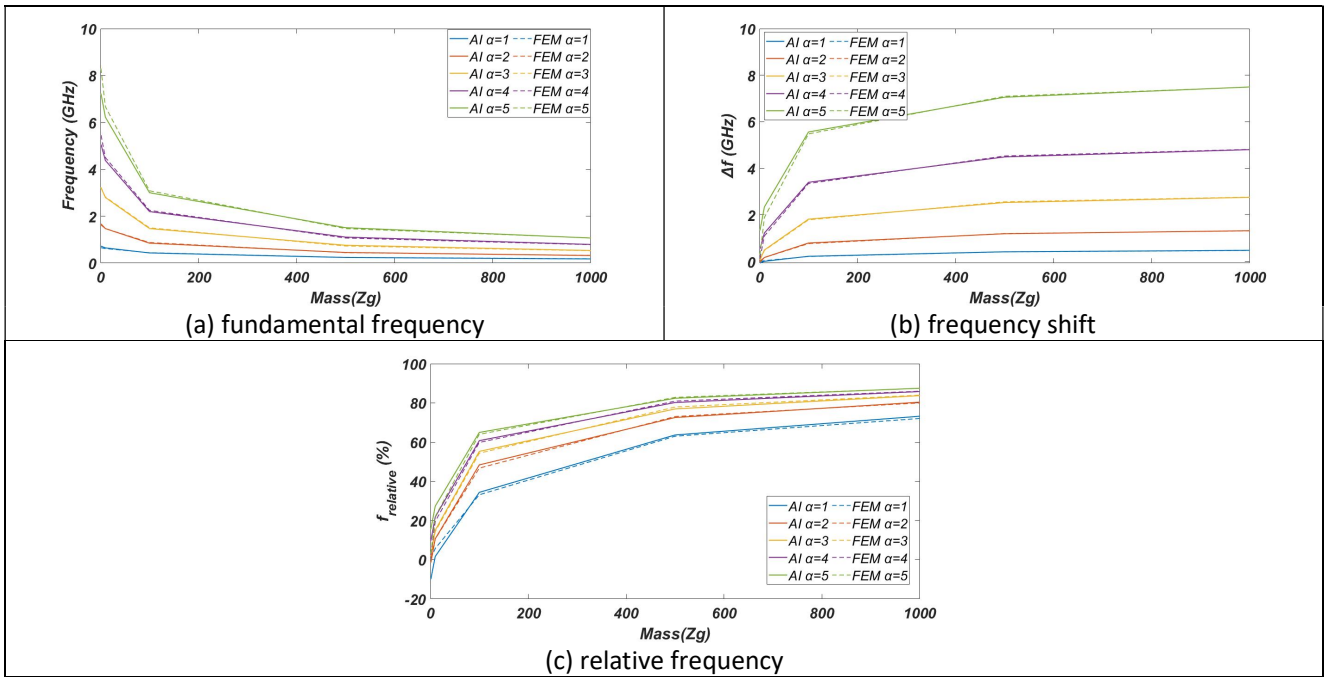


Figure 4. The effect of aspect ratio variation on the sensor characteristics is examined for different attached masses. In the simulations, the aspect ratio ranges from 1 to 5, the effective length is 100 nm, and the attached mass is 100 Zg.

The influence of varying the number of attached particles on the SLGS performance is illustrated in Fig. 5. As the number of particles increases, the fundamental frequency decreases steadily, while both Δf and relative frequency rise, initially sharply and then leveling off at higher counts. Higher aspect ratios consistently result in larger shifts, indicating increased sensitivity for slender sheets. The ANN accurately captures these trends, providing a fast and reliable surrogate for FEM simulations.

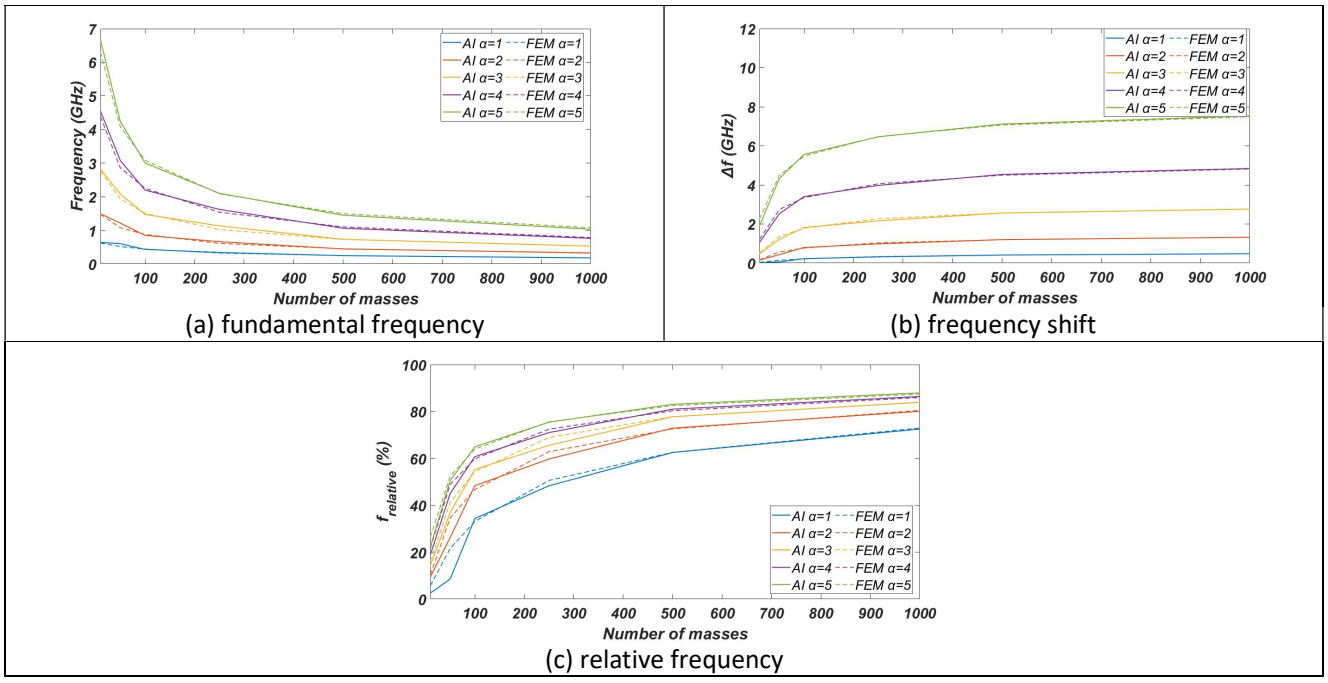
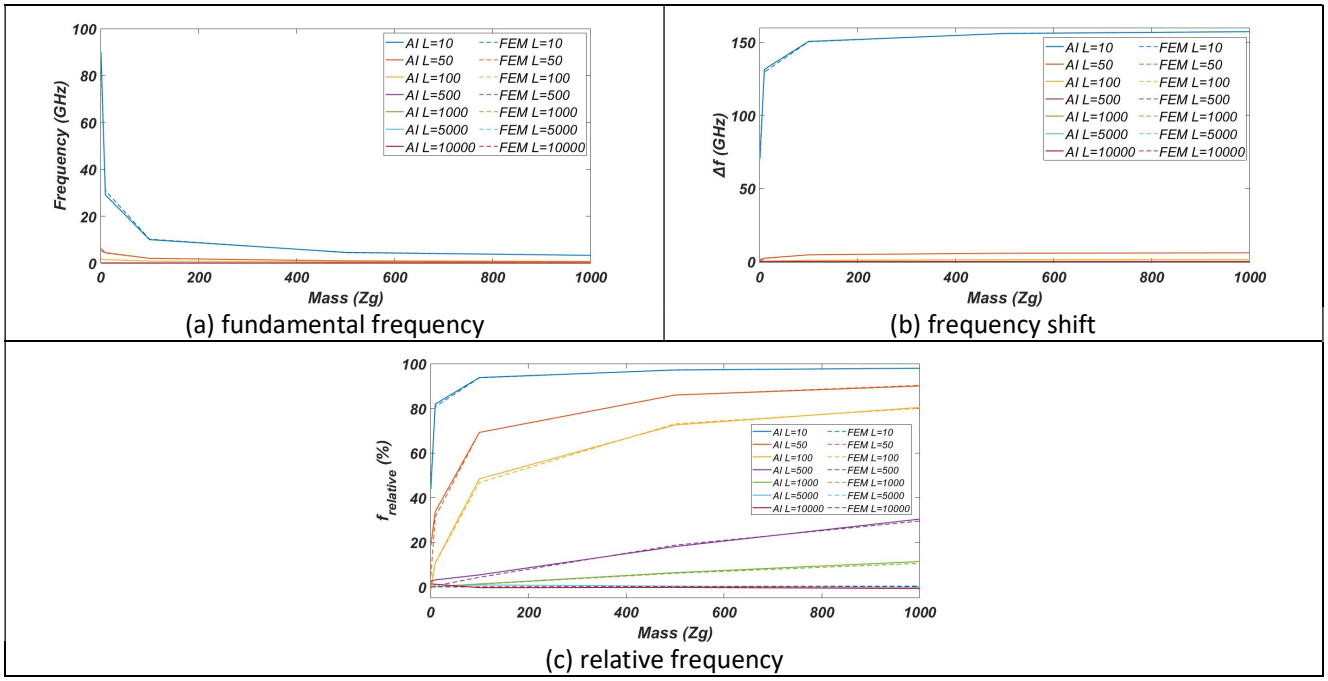


Figure 5. Effect of aspect ratio (α) variation on the sensor characteristics under increasing mass. In the simulations, the aspect ratio varies from 1 to 5, the effective length is 100 nm, and the attached mass is 100 Zg.

Fig. 6 examines how SLGS length affects vibration characteristics. Longer sheets have higher initial frequencies but show sharper declines when mass is added, indicating they are more sensitive. Shorter sheets start with lower frequencies and change more gradually. Both the frequency shift and the relative frequency increase as the sheet lengthens, emphasizing the importance of SLGS geometry in sensor performance. ANN results match well with FEM data, showing the model's ability to predict across a wide range of lengths.

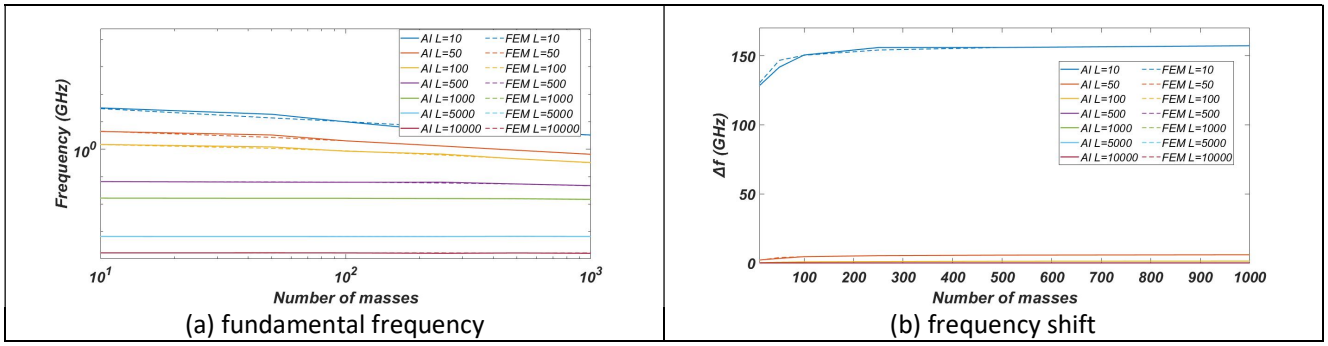


(a) fundamental frequency (b) frequency shift

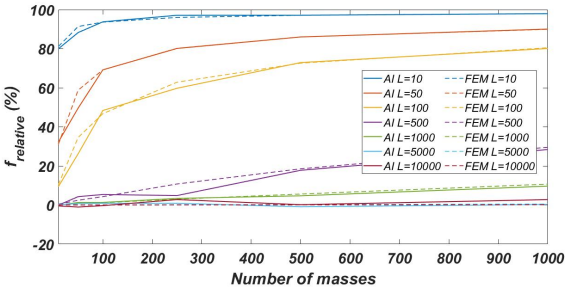
(c) relative frequency

Figure 6. Effect of attached mass on the sensor characteristics for different SLGS lengths. In the simulations, the aspect ratio is 2, the effective length is 100 nm, and the attached mass is 100 zg.

Fig. 7 depicts the variation of resonance characteristics under different attached masses. As expected, the fundamental frequency decreases with increasing mass, while Δf and relative frequency increase, initially rapidly and then saturating for larger values. These results demonstrate the nonlinear dynamic behavior of the system and the ANN's ability to predict it accurately.



(a) fundamental frequency (b) frequency shift



(c) relative frequency

Figure 7. Effect of aspect ratio on the sensor characteristics. In the simulations, the effective length is 100 nm, the attached mass is 100 zg, and the number of particles is 100.

Overall, the study confirms that the fundamental frequency, frequency shift, and relative frequency are strongly influenced by sheet geometry (length and aspect ratio) and the amount of attached mass. Higher aspect ratios and longer sheets enhance sensitivity, making them preferable for ultra-sensitive mass sensing applications. The ANN-based model provides excellent agreement with FEM results, capturing the nonlinear relationships efficiently and offering a robust tool for rapid performance prediction under simply supported boundary conditions.

5. Conclusion

This study presented a detailed investigation of the vibrational behavior of single-layer graphene sheets (SLGSs) under mass-loading conditions using a hybrid AI-based framework. An artificial neural network (ANN) was developed and validated against finite element method (FEM) simulations, showing excellent agreement across a range of geometrical parameters and loading scenarios.

Key findings are summarized as follows:

1. Model validation: The ANN accurately predicted fundamental frequency, frequency shift (Δf), and relative frequency (f_relative) with negligible deviation from FEM results, demonstrating its reliability as a fast and computationally efficient alternative to conventional simulations.
2. Mass detection capability: The resonance frequency decreased with increasing attached mass, while both Δf and f_relative increased, confirming the SLGS's suitability for ultra-sensitive mass sensing. The ANN effectively captured these trends for varying numbers of particles and mass values.
3. Geometrical influence: Sensitivity depends strongly on sheet aspect ratio and length. Higher aspect ratios and longer sheets produced larger frequency shifts, enhancing detection performance.
4. Design implications: The ANN framework enables rapid exploration of parameter spaces and sensor optimization without the computational cost of full FEM simulations, facilitating real-time analysis and design of graphene-based nanosensors.

In conclusion, the proposed AI-based approach provides a robust, accurate, and efficient tool for modeling, designing, and optimizing high-performance SLGS-based nanosensors, matching FEM-based accuracy while significantly reducing computational effort.

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