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Mechanical and Vibrational Behavior Analysis of Boron Nitride Nano Mass Sensor

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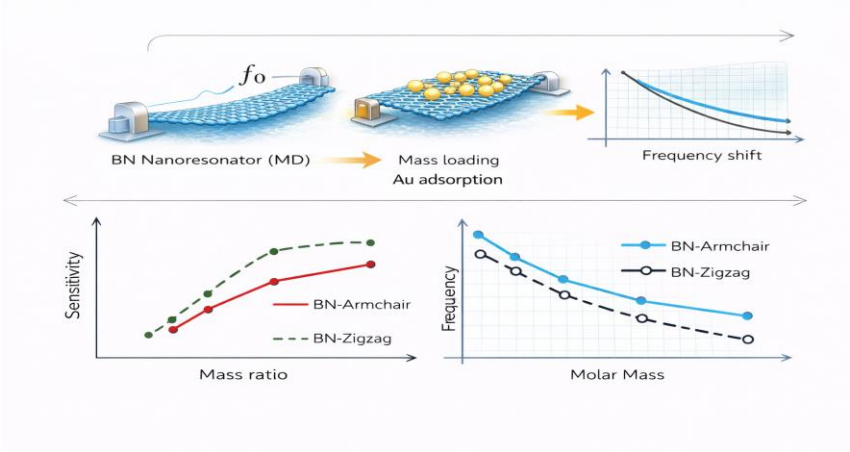
HIGHLIGHTS

- Single-layer BN nanosheets exhibit lower first natural frequency than graphene due to reduced modulus.
- Natural frequency decreases as sheet dimensions increase, showing size-dependent behavior.
- Adsorption of gold atoms significantly reduces natural frequency and enhances mass sensitivity.
- Zigzag BN sheets show higher frequency sensitivity than armchair, ideal for mass sensing.

GRAPHICAL ABSTRACT



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ABSTRACT

Two-dimensional nanostructures have recently gained significant importance in various scientific fields. Investigating the potential of materials to serve as nanomechanical sensors is among the newest topics in nanotechnology. This paper employs molecular dynamics simulations to explore this capability for single-layer boron nitride (BN) nanosheets, while also examining their mechanical and vibrational properties. BN sheets were modeled in various dimensions and geometries (square and rectangular) with both armchair and zigzag configurations. Tensile and vibrational tests were conducted to assess the mechanical and vibrational properties of the nanosheets. The vibrational tests were performed under two conditions: the sheet alone and the sheet with external particles attached to its surface. Stress-strain diagrams were used to analyze mechanical properties, and the system's natural frequencies and mode shapes were extracted using frequency decomposition methods to study vibrational behavior. Finally, to evaluate mass-sensing capability, the process was repeated in the presence of gold particles. The effect of these particles on the frequencies was examined, and the frequency sensitivity of sheets with varying dimensions and different numbers of external particles was calculated. The results indicate that increasing the number of gold particles and the sheet dimensions leads to a reduction in the system's natural frequency. Furthermore, the sensitivity analysis reveals that for sheets with identical nominal dimensions, the zigzag configuration exhibits higher frequency sensitivity to added mass compared to the armchair orientation. Specifically, sensitivity values increase significantly with the added mass ratio, highlighting the potential of optimized BN nanosheets for high-precision mass sensing applications.

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1- Introduction

Two-dimensional nanostructures have attracted considerable attention due to their structural characteristics and potential applications. The significant progress in graphene research has spurred scientists to explore other two-dimensional materials. Hexagonal boron nitride (H-BN), with its structural and lattice similarities to graphene, is often referred to as "white graphene" [1]. Its most stable form is the hexagonal crystalline structure, also known as H-BN, α-BN, or g-BN (graphitic boron nitride). H-BN features a layered structure similar to graphite, where boron and nitrogen atoms are bound by strong covalent bonds within each layer, while the layers themselves are held together by weak van der Waals forces.

Boron nitride is a chemically inert material with high transparency, exceptional mechanical strength, a high melting point, and superior thermal conductivity compared to graphene. Recent optical spectroscopy studies have also reported highly accurate refractive index and loss data for H-BN across ultraviolet to near-infrared wavelengths. These insights not only support BN's known transparency but also open up possibilities for its integration in photonic and optoelectronic Nano systems where precise dielectric behavior is critical [2]. H-BN not only exhibits Young's modulus and hardness comparable to graphene but also demonstrates strong oxidation resistance and thermal stability. It is a semiconductor with a bandgap of 5.3–5.9 eV, which can be modified through hydrogenation. Hexagonal boron nitride sheets, or "white graphene," share many properties with graphene, including exceptional mechanical strength and thermal conductivity. However, a key difference lies in their electrical conductivity: graphene is a conductor, while BN is an insulator.

H-BN is also known for its extremely low friction coefficient, making it useful in lubricants and cosmetics. BN lubricants are particularly advantageous where the electrical conductivity or chemical reactivity of graphite (an alternative lubricant) is problematic. Unlike graphite, BN does not require water or gas molecules between layers for lubrication, allowing its use in vacuum environments, such as space applications.

This vacuum compatibility has recently been leveraged in optoelectronic applications; for instance, H-BN nanosheets have shown excellent performance in vacuum ultraviolet (VUV) photodetectors, providing ultralow dark current and strong photo response stability. These properties further highlight H-BN's potential for high-sensitivity detection platforms operating in extreme environments [3].

BN is a unique material capable of solving problems that other compounds, like aluminum oxide or silicon carbide, cannot. It withstands temperatures exceeding 2000°C and provides a dielectric strength of approximately 1000 V/mm. Through hydrolysis, BN can be easily machined into rods, plates, or custom shapes. These exceptional properties make BN suitable for sintering and ceramic applications in induction, vacuum, and atmospheric furnaces.

The use of two-dimensional materials like BN in sensor fabrication is a novel and rapidly growing field. Due to its unique mass, structure, and properties, BN is particularly suitable for mass-sensing applications.

H-BN, with its small atomic size and low density, is highly functional for Nanosensors, especially in nanoelectromechanical systems (NEMS) and nanomechanical resonators. NEMS sensors can detect physical quantities such as molecular mass, temperature fluctuations, rotation, quantum states, and biochemical reactions with high sensitivity. Recent advancements in electrically tunable nanomechanical resonators, particularly those based on graphene, have significantly expanded the application range of NEMS devices. These systems offer dynamic frequency control through electrostatic tuning, enabling precise sensing across variable conditions and opening pathways to applications in quantum sensing and signal processing [4]. Rapid and reliable detection, particularly for specific diseases, makes NEMS sensors promising tools for early diagnosis, such as cancer detection. While some biosensors lack the required precision, nanomechanical sensors perform the same tasks with higher accuracy and speed, such as in protein identification and disease diagnosis [5].

Nanosensors have diverse applications depending on their type, including flow, pressure, temperature, mass, acoustic wave, and strain sensors [6]. A critical factor in evaluating Nanomass sensors is the change in resonant frequency relative to the number and mass of attached nanoparticles [7].

Yi et al. [8]studied the vibrational behavior of single-layer H-BN using molecular dynamics (MD) simulations and continuum plate models. They calculated the bending stiffness and Poisson's ratio of BN in armchair and zigzag directions, finding that BN is softer than graphene and its natural frequency decreases with increasing sheet dimensions. They reported bending stiffness of 1.42×10^{19} and a Poisson's ratio of 0.3.

Ein Alipour et al. [9] used MD simulations to examine the mechanical properties of hybrid graphene-BN sheets with various defects. By comparing stress-strain diagrams of pristine BN and graphene in armchair and zigzag directions, they showed that the presence of holes reduces fracture strength, strain, and Young's modulus. Circular holes were found to have a less severe impact on mechanical properties than square holes.

Mortazavi and Ramond [10] employed classical MD simulations with the Tersoff potential to study the thermal conductivity and tensile response of single-layer BN sheets. Axial stress simulations predicted that the elastic modulus of BN sheets is close to that of BN nanotubes, ranging between 0.8 and 0.85 TPa, depending on chirality.

Nguyen et al. [11]investigated the free transverse vibrations of single-layer graphene, BN, and silicon carbide using finite element methods (FEM). They analyzed the natural frequencies and mode shapes of these sheets under various boundary conditions and aspect ratios.

Panchal et al. [12] explored the feasibility of BN nanotubes as nanomechanical sensors using continuum mechanics and FEM. Panchal and Desai [13] analyzed the wavy atomic structures of BN nanotubes by modeling sinusoidal vibrations. Thomas et al. [14] used classical MD simulations with the Tersoff potential to study the mechanical and elastic properties of two-dimensional H-BN.

Peng et al. [15] employed density functional theory (DFT) to investigate the mechanical properties of single-layer H-BN. Sevik et al. [16] systematically studied the thermal transport properties of BN nanostructures using MD simulations with the Tersoff interatomic potential. Falin et al. [17] examined the mechanical properties of various BN nanosheets, demonstrating that BN is one of the strongest electrical insulators. Ein Alipour et al. [18] studied the effect of interface structure on the mechanical properties of graphene/BN hybrids.

Thomas et al. [19] investigated the thermodynamic and structural properties of pristine and defective H-BN sheets over a wide temperature range using atomic simulations and the Tersoff potential. Zhao and Chu [20] used MD simulations to analyze the mechanical properties of graphene-BN hybrid sheets with varying BN content (0% to 100%).

Slawman and Fazelino [21] compared the structural properties of single-layer H-BN and graphene using MD. Kinaci et al. [22]studied the thermal conductivity variations in graphene/BN hybrid nanostructures. Jalali and Naei [23] explored the application of single-layer graphene as a resonant sensor for nanoparticle detection using MD and nonlocal elasticity theory.

In parallel with advances in individual nanomechanical sensors, the concept of using coupled resonator arrays has emerged as a powerful strategy to enhance mass sensitivity, selectivity, and signal processing capabilities. These systems, particularly those based on graphene, exploit modal interactions and inter-resonator coupling to detect even subtler variations in mass and force fields. Although this technique has not yet been widely applied to BN-based devices, its extension to BN nanosheets presents an exciting direction for future Nano-sensors development [24].

Recent studies suggest that BN is a promising material for mass sensors, necessitating a thorough understanding of its mechanical and vibrational behavior. However, despite extensive research on the thermal and mechanical properties of H-BN, a systematic investigation into its mass-sensing capabilities—specifically

regarding the influence of chirality and sheet dimensions on sensitivity to atomic-scale mass loading—remains largely unexplored. Consequently, this paper aims to fill this gap by investigating the mechanical properties, vibrational behavior, and detection sensitivity limits of BN nano mass sensors.

2. Molecular Dynamics Method and Governing Equations

Figure 1 illustrates the zigzag and armchair orientations as well as the atomic configuration in a hexagonal boron nitride (H-BN) monolayer honeycomb lattice [8].

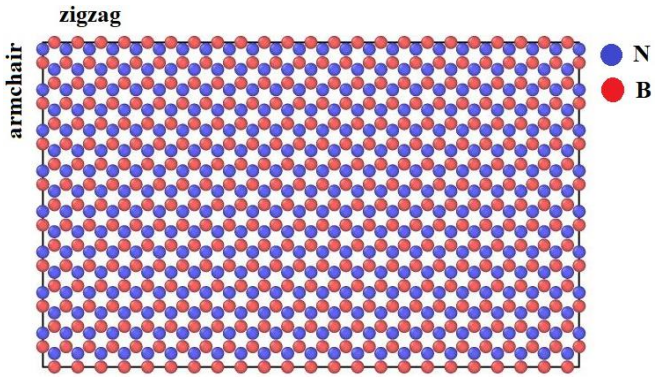

Figure 1. Zigzag and armchair orientations in a monolayer boron nitride sheet [8]

Molecular Dynamics (MD) simulation is a method based on the equations of motion, which, for a simple atomic system, are expressed as:

$$m_i\ddot{r}_i = f_i \quad (1)$$

This is essentially Newton's second law, where f_i is the force acting on each particle, m_i is its mass, and $\ddot{r}_i$ is its acceleration. To compute this, the forces acting on all atoms must be calculated, which are obtained from the potential energy of the system [6].

In the absence of external forces, the potential energy is represented as:

$$f_i = -\frac{\delta}{\delta r_i}u \quad (2)$$

Accordingly, the force on each atom is calculated via:

$$u = \sum_{i=1}^{n}\sum_{j>i}^{n} u(r_{ij}) \quad (3)$$

where:

$$f_i = -\sum_{i\neq j}^{n}\frac{\partial u(r_{ij})}{\partial r_{ij}} \quad (4)$$

is the relative position vector between atoms i and j.

Among various interatomic potentials proposed, one of the most accurate is the Tersoff potential, which is a subset of Lennard-Jones-type potentials. In this study, a three-dimensional Tersoff potential is used to evaluate atomic interactions in BN. This potential is formulated as:

$$E = \frac{1}{\delta r_{ij}}\sum_{i}^{n}\sum_{i\neq j}^{n} u_{ij} \quad (5)$$

The cutoff function $f_C(r)$ is defined piecewise:

$$u_{ij} = f_C(r_{ij})\,[f_R(r_{ij}) + b_{ij}\,f_A(r_{ij})] \quad (6)$$

$$f_C(r) = \begin{cases} 1 & r < R-D \\ \frac{1}{2} - \frac{1}{2}\sin\left(\frac{\pi}{2}\frac{r-R}{D}\right) & R-D < r < R+D \\ 0 & r > R+D \end{cases} \quad (7)$$

The repulsive and attractive components are expressed as:

$$f_R(r) = A\exp(-\lambda_1 r) \quad (8)$$

$$f_A r = -B\exp(-\lambda_2 r) \quad (9)$$

The bond order function is:

$$b_{ij} = (1+\beta^n\zeta_{ij}^n)^{-\frac{1}{2n}} \quad (10)$$

with the coordination function:

$$\zeta_{ij} = \sum_{k=i.j} f_C(r_{ik})\,g(\theta_{ijk})\,exp\,[\lambda_3^m(r_{ij}-r_{ik})^m \quad (11)$$

$$g(\theta) = \gamma_{ijk}\left(1+\frac{c^2}{d^2}-\frac{c^2}{[d^2+(cos\theta+cos\theta_0)^2]}\right) \quad (12)$$

Here, f_R represents the two-body interaction term, f_A includes three-body angular interactions, and i, j, and k refer to atomic indices with θ_{ijk} being the bond angle between i–j–k.

For gold atoms, the Embedded Atom Method (EAM) is employed. The potential parameters are adopted from references [25, 26]. The total potential energy in this method is defined as:

$$E_i = F_\alpha\left(\sum_{i\neq j}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{i\neq j}\phi_{\alpha\beta}(r_{ij}) \quad (١٣)$$

where:

- F_α is the embedding function representing the energy required to place an atom of type α into the electron cloud,
- $\rho\_\beta(r_{ij})$ is the electron density contribution from atom j of type β to atom i, and
- $\varphi\_\alpha\beta(r_{ij})$ is the pairwise potential between atoms i and j.

To describe the interaction between boron nitride and gold atoms, the Lennard-Jones potential (LJ) with cutoff is used (lj/cut), which is the standard 12-6 Lennard-Jones potential given by:

$$E = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]\ r < r_c \quad (14)$$

In this equation:

- ε is the depth of the potential well,
- σ is the distance at which the interatomic potential equals zero
- r is the interatomic distance
- r_c is the cutoff radius.

3. Modeling

Using the interatomic potentials described earlier, the interactions between boron nitride and gold atoms are computed. The simulations are conducted under periodic boundary conditions, in which particles at one boundary of the simulation box interact with those at the opposite boundary. This configuration allows atoms to exit one side of the simulation domain and re-enter from the other, effectively eliminating edge effects and ensuring a bulk-like environment.

In constructing the nanosheets, boron and nitrogen atoms are arranged in a hexagonal lattice to form a single-layer hexagonal boron nitride (H-BN) sheet. The models are designed in both square and rectangular geometries of various dimensions. To apply simple support boundary conditions, the outermost row of edge atoms on each side of the sheet is fixed. In molecular dynamics simulations, fixing a single row of atoms is sufficient to impose a pinned or simply supported boundary condition. Fixing more than one row may unintentionally represent a clamped (fixed) condition, which is not intended in this setup.

The time step used for sampling in the simulations is set to 1 femtosecond (fs). The NVE ensemble was initially employed to integrate Newton's equations of motion and update the positions and velocities of the atoms over time. This ensemble conserves total energy and provides a foundation for capturing the intrinsic dynamic response of the system.

To subsequently stabilize the temperature and pressure, the simulations are transitioned to NVT and NPT ensembles, respectively. These ensembles employ Nosé–Hoover thermostats and barostats, which modify the equations of motion using non-Hamiltonian formulations to generate statistically representative atomic trajectories from the canonical (NVT) or isothermal-isobaric (NPT) ensembles.

By applying the molecular dynamics framework and the governing interatomic force equations, it becomes possible to determine the positions of all atoms in the system at each time step, based solely on the forces acting between them. This enables tracking the displacements of atoms before and after excitation, which is critical for extracting vibrational characteristics such as natural frequencies and mode shapes.

These characteristics are obtained using the frequency decomposition method, a computational approach that decomposes the dynamic response of a structure into individual single-degree-of-freedom systems, each corresponding to a specific mode shape. In this method, the spectral density matrix is analyzed to extract modal parameters.

The eigenvalues and eigenvectors of the spectral density matrix are computed, and the peaks in the eigenvalue spectra indicate the natural

frequencies of the system. The corresponding eigenvectors, particularly those adjacent to the resonance peaks, represent the mode shapes. Although several vibrational modes contribute to the system's overall response, in the vicinity of a given natural frequency, a dominant mode typically emerges, which largely governs the observed response. Thus, at resonance, the system's displacement profile closely resembles that of its corresponding mode shape.

By decomposing the spectral power matrix into eigenvalues and eigenvectors at each frequency, one can determine the number of significant modes contributing to the response. The first non-zero eigenvalue generally corresponds to the first natural frequency, and the associated eigenvector provides the primary mode shape. This approach has proven effective in extracting modal properties from molecular dynamics simulations with high precision [27].

3.1 Mechanical Behavior Analysis

To evaluate the mechanical properties, a uniaxial tensile test is performed on a square-shaped boron nitride (BN) nanosheet with dimensions of 2.5 × 4.4 nanometers, at room temperature and under periodic boundary conditions.

At each simulation time step, a constant engineering strain rate is applied along the desired direction, causing the sheet to stretch accordingly. The stress component in the thickness direction is assumed to be zero, effectively reducing the problem to a two-dimensional plane-stress condition. During the simulation, both temperature and pressure are maintained constant using the NPT ensemble.

Figure 2 depicts the configuration of the nanosheet at different stages throughout the tensile test.

This setup allows for direct observation of atomic-level deformation behavior under mechanical loading. As strain increases, interatomic bonds stretch until the structure eventually yields or fractures, depending on the imposed strain and material properties. By analyzing the stress–strain response extracted from the simulation, key mechanical characteristics such as Young's modulus, yield strength, and ultimate tensile strength can be determined.

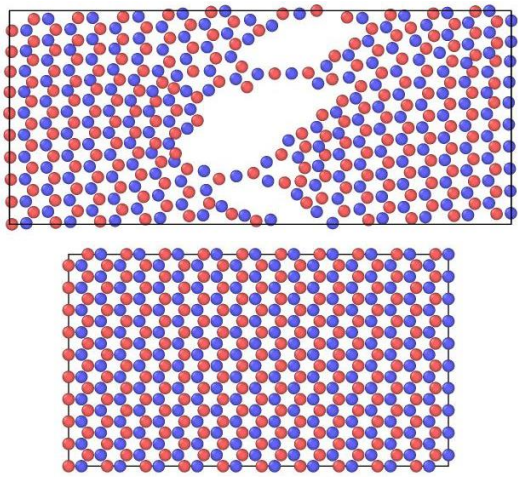

Figure 2. The condition of the plate during the tensile test

The slope of the initial linear portion of the stress–strain curve represents the Young's modulus of the boron nitride nanosheet. These results provide valuable insight into the material's elastic behavior and serve as a foundation for comparing the mechanical response of BN nanosheets to other two-dimensional materials such as graphene.

3.2 Vibrational Behavior Analysis

Single-layer boron nitride (BN) nanosheets with various sizes and rectangular geometries were modeled. The boron and nitrogen atoms were arranged in a hexagonal lattice structure as illustrated in Figure 3. In this configuration, blue atoms represent nitrogen, while red atoms correspond to boron.

To impose simple support boundary conditions, only the first row of atoms along the boundary was fixed. In molecular dynamics simulations, fixing a single row is sufficient to represent a simply supported (pinned) condition. Fixing multiple rows is generally considered an incorrect approach when simulating a pinned boundary and may instead resemble a clamped or fixed condition [28, 29].

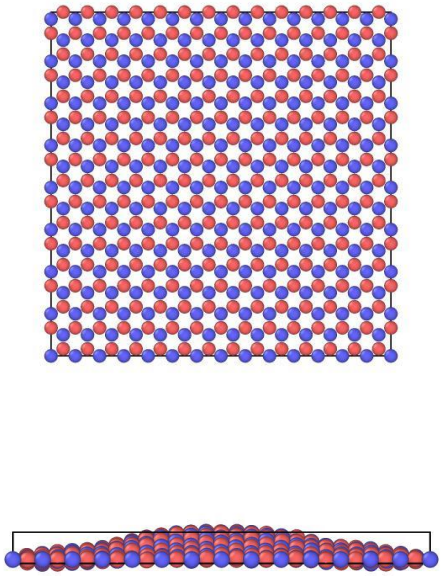

Figure 3. Atomic arrangement and plate condition during vibration

In all modeled sheets, the zigzag configuration was defined along the x-axis, while the armchair orientation was aligned with the perpendicular direction. To investigate the vibrational properties of the structure, an initial transient perturbation was applied to the center of the sheet for one femtosecond, after which the system was allowed to vibrate freely in its natural modes.

BN sheets were modeled with the following dimensions (in nanometers):

3.4 × 3.4, 2.5 × 2.5, 10 × 10, 6.79 × 5.26, and a series of asymmetric sizes including 3.4 × 5.0, 3.4 × 5.5, 3.4 × 6.0, 3.4 × 6.8, 5.0 × 3.4, 5.5 × 3.4, 6.0 × 3.4, and 6.8 × 3.4.

This broad range of geometries enables a comprehensive assessment of how changes in size and aspect ratio affect the vibrational characteristics of the BN sheets. Following the excitation phase, frequency decomposition analysis was used to extract the system's natural frequencies and associated mode shapes. These parameters offer fundamental insights into the dynamic response of the nanostructures and play a key role in applications such as nanoscale resonators and mass sensing platforms.

Beyond fundamental vibrational analysis, recent efforts have focused on improving the energy efficiency of such resonators. One notable approach involves the integration of boron-carbon-nitride (BCN) foams with graphene to mitigate energy dissipation and enhance the quality factor (Q-factor) of the system. These hybrid structures demonstrated improved vibrational stability and reduced damping, a direction that could be extended to BN-based sensors as well [30].

3.3 Mass Detection Capability Analysis

The capability of two-dimensional nanostructures for mass sensing applications remains a relatively underexplored area. In particular, the potential of hexagonal boron nitride (H-BN) nanosheets for mass detection has not been comprehensively studied. Therefore, this section focuses on evaluating the mass sensing performance of BN nanosheets in the presence of externally added gold nanoparticles.

To assess the frequency sensitivity of BN sheets to the presence of foreign particles, the sensitivity is calculated using the following

relation:

$$Sensitivity = \frac{\omega_1 - \omega_{Au}}{\omega_1} \quad (15)$$

Here ω_{Au} is the natural frequency of the sheet in the presence of the gold particle(s), and ω_1 is the frequency without any external mass.
The modeling procedure used to evaluate frequency sensitivity and mass detection capability is like the one previously employed for the pure BN sheets. The nanosheets are modeled in both square and rectangular geometries, with armchair and zigzag edge configurations, and are subject to simply supported boundary conditions. One or more gold atoms are placed above the surface of the nanosheets, as shown in Figure 4, and the interatomic interactions between gold and BN are described using the appropriate interatomic potentials.

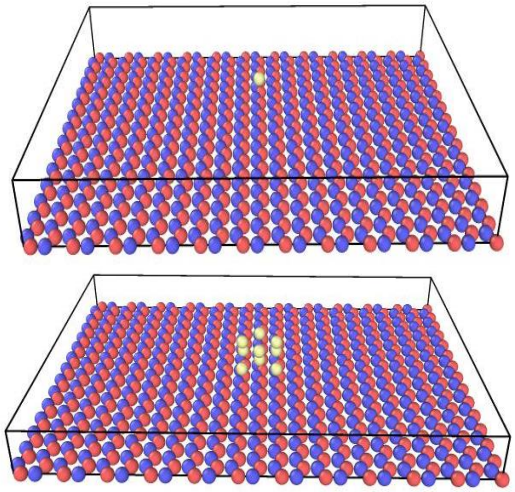

Figure 4. Plate condition in the presence of gold atoms.

As in the previous cases, a 1-femtosecond transient excitation is applied to the center of the sheet to initiate free vibration. Subsequently, the natural frequencies and mode shapes are extracted using the frequency decomposition method.
By comparing the vibrational response of the sheet with and without the presence of gold particles, the degree to which added mass influences the dynamic behavior can be quantified. While classical approaches have demonstrated the feasibility of using resonant frequency shifts for ultra-fine mass detection, more recent studies have introduced advanced architecture such as coupled graphene resonator arrays or optomechanical BN systems—that offer enhanced mass resolution and spectral selectivity. These configurations enable real-time detection of picogram-scale mass variations through modal interference and tunable frequency tracking [31, 32]. This analysis enables a precise evaluation of the sensitivity of the structure to added Nano masses, which is essential for determining its suitability as a nanoscale mass sensor.

4. Validation and Results

4-1. Verification of Mechanical Properties and Natural Frequency Extraction

To validate the mechanical behavior results, a rectangular boron nitride (BN) nanosheet was modeled under a uniaxial strain rate of 0.1 fs^{-1} using the same dimensions reported by Einalipour et al. [9]. The resulting stress–strain curve is shown in Figure 5.
This curve demonstrates the tensile response of the BN sheet, and as expected, the results are in good agreement with the referenced study, confirming the accuracy of the applied simulation method. The red curve represents the data from Einalipour et al. [9], while the blue curve corresponds to the present study. The slope of the linear region in the plot determines the Young's modulus of the material, which in this case is found to be 843 GPa.

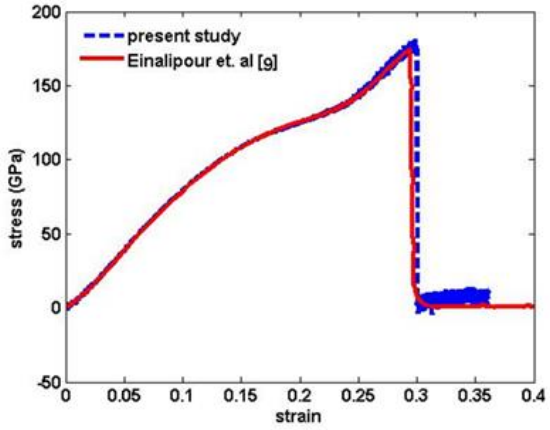

Figure 5. Stress–strain curve of the boron nitride nanosheet under a uniaxial strain rate of 0.1 fs^{-1}. The slope of the linear region indicates a Young's modulus of 843 GPa.

These simulation results are consistent with recent experimental measurements on freestanding few-layer graphene/BN heterostructures, where atomic force microscopy (AFM) and point-load indentation revealed Young's moduli in a comparable range. Finite element modeling further confirmed the mechanical integrity of such hybrid stacks, highlighting the strong interlayer coupling and anisotropic elasticity inherent in BN-containing composites [33].
For comparison, a graphene sheet with the same geometry was modeled under identical loading conditions. The corresponding stress–strain response is depicted in Figure 6.

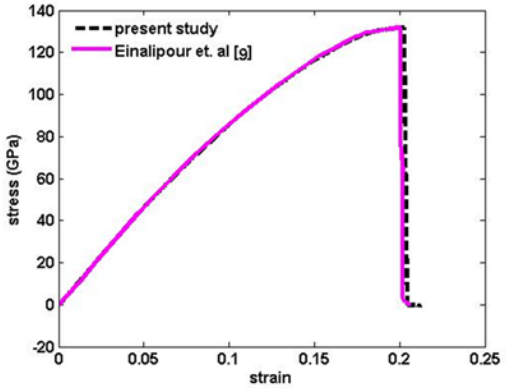

Figure 6. Stress–strain curve of graphene sheet

The slope of the linear region in this diagram indicates the Young's modulus. As shown in Table 1, the Young's modulus of BN is lower than that of graphene.

Table 1. Comparison of Mechanical Properties of BN and Graphene[34]

Material	E (TPa)	ν (Poisson's Ratio)	ρ (kg/m³)	h (nm)
Boron Nitride	0.843	0.27	2180	0.33
Graphene [34]	1.06	0.3	2300	0.34

The following equation relates the natural frequency to the elastic properties [34]:

$$\omega_{mn}^{C} = \sqrt{\frac{D(\alpha^2+\beta^2)^2}{M_{mn}\lambda_{mn}}} \quad (16)$$

Hence, under identical conditions, the natural frequencies of BN sheets are expected to be lower than those of graphene.

The natural frequency, mode indices, and other frequency parameters are obtained from the following equations:

$$\alpha = \frac{m\pi}{a} \quad , \quad \beta = \frac{n\pi}{a} \quad (17, 18)$$

$$\lambda_{mn} = 1 + \mu(\alpha^2 + \beta^2) \quad (19)$$

$$M_{mn} = m_0 + m_2 (\alpha^2 + \beta^2) \quad (20)$$

Here, m and n are the mode numbers, a and b represent the sheet dimensions, m_0 and m_2 represent the mass per unit surface and mass moment of inertia, μ is the non-local parameter and D is the flexural rigidity of the sheet, which is calculated as:

$$D = \frac{Eh^3}{12(1-\nu^2)} \quad (21)$$

To verify the accuracy of the obtained frequencies, a BN sheet with dimensions 5.26 × 6.79 nm was simulated in accordance with the study by Yi et al. [8]. The results are summarized in Table 2.

Table 2. Comparison of First Natural Frequency of BN Sheet (5.26 × 6.79 nm)

Material	a (nm)	b (nm)	Reference	ω (1,1) (THz)
BN	5.26	6.79	(MD) Yi et al. [8]	0.1755
BN	5.26	6.79	(FEM) Yi et al. [8]	0.1601
BN	5.26	6.79	Present Study (MD)	0.1679

As observed, the result from the present study closely matches the findings by Yi et al. [8].
A comparison of the first natural frequency of boron nitride and graphene nanosheets of equal dimensions is provided in Table 3.

Table 3. Comparison of First Natural Frequency of BN and Graphene

Material	b (nm)	a (nm)	Reference	ω (1,1) (THz)
Graphene	10.1200	10.0788	Mirakhory [34]	0.0603
BN	10.077	10.171	Present Study	0.027
Graphene	2.5300	2.5562	Mirakhory [34]	0.4834
BN	2.5375	2.5114	Present Study	0.331
Graphene	3.4	3.4	Mirakhory [34]	0.3149
BN	3.4	3.4	Present Study	0.2395

These findings confirm that boron nitride sheets exhibit lower natural frequencies than graphene sheets of identical geometry.

Next, Table 4 summarizes the first natural frequencies of BN nanosheets with various dimensions, illustrating the effect of size on vibrational response:

Table 4. First Natural Frequencies of BN Sheets without Gold Particles

Nominal Dimensions (nm) (Armchair × Zigzag)	Exact Dimensions (nm) (Armchair × Zigzag)	Frequency (THz)
3.4 × 3.4	3.5525 × 3.5160	0.2391
5 × 3.4	4.8575 × 3.5160	0.1933
5.5 × 3.4	5.2925 × 3.5160	0.1888
6 × 3.4	5.8725 × 3.5160	0.1799
6.8 × 3.4	6.5975 × 3.5160	0.1698
3.4 × 5	4.7718 × 3.4800	0.1922
3.4 × 5.5	3.4800 × 5.2740	0.1844
3.4 × 6	3.4800 × 5.7763	0.1788
3.4 × 6.8	3.4800 × 6.6554	0.1687

As expected, increasing the sheet dimensions leads to a reduction in the fundamental natural frequency.

Figure 7 compares the natural frequencies for zigzag and armchair configurations across different sheet sizes. For the square sheet, there is no difference, but for rectangular sheets, the armchair orientation exhibits higher frequencies than the zigzag counterpart.

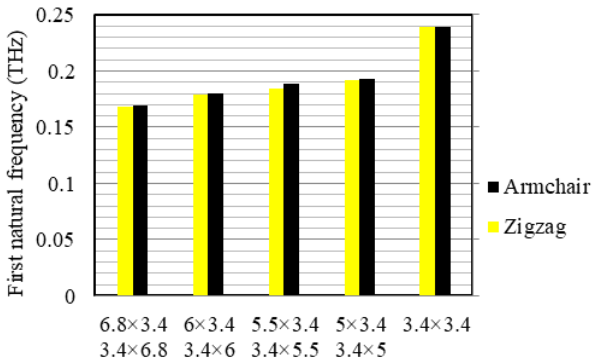

Figure 7. Comparison of natural frequencies for zigzag and armchair configurations

Also, the first vibrational mode shape of a 3.4 × 3.4 nm BN sheet without Gold Particles is presented in Figure 8.

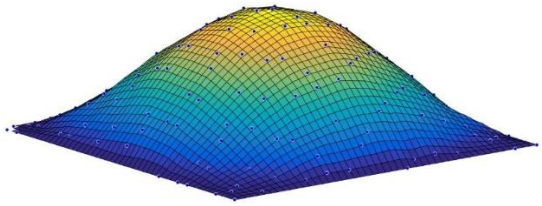

Figure 8. First mode shape of BN nanosheet (3.4 × 3.4 nm) without Gold Particles

4.2 Effect of Gold Nanoparticles on Natural Frequency

To assess the influence of added external mass on the vibrational behavior of boron nitride (BN) nanosheets, various numbers of gold atoms were deposited on the sheet surface and the first natural frequencies were extracted. The modeling was conducted on square and rectangular BN sheets with dimensions ranging from 3.4 to 6.8 nm in both armchair and zigzag orientations. The gold atoms were positioned above the sheet surface and the interactions were modeled using appropriate interatomic potentials.
The frequency extraction was performed using the same frequency decomposition method as in the unloaded state. Table 5 presents the natural frequencies of square BN sheets in the presence of various numbers of gold atoms.

Table 5. Natural Frequencies of BN Square Sheets with Gold Atoms (THz)

Number of Au Atoms	(no particle)	1	2	3	4	6	9
Frequency (THz)	0.2391	0.1967	0.1922	0.1877	0.1832	0.1788	0.1743

Also, the first natural frequency of a square BN sheet (3.4 × 3.4 nm) in the presence of increasing numbers of gold atoms is shown in Figure 9.

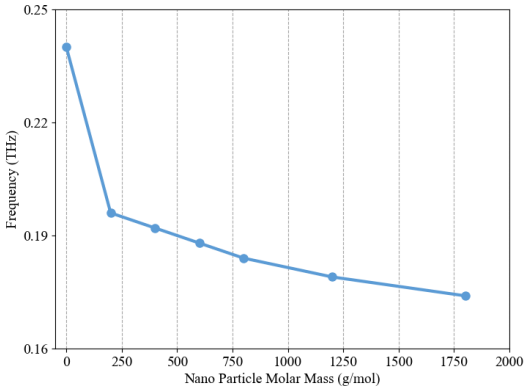

Figure 9. First natural frequency of a 3.4 × 3.4 nm square BN nanosheet versus molar mass of gold atoms

The results indicate that the frequency decreases with increasing particle number: from 0.24 THz in the absence of gold to 0.1967 THz with one gold atom and 0.1743 THz with nine atoms.
As defined in Equation (15), the frequency sensitivity quantifies the relative change in resonance frequency due to the added gold mass. The sensitivity for the same 3.4 × 3.4 nm sheet is shown in Figure 10.

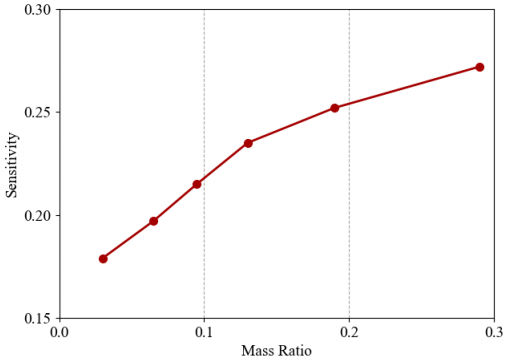

Figure 10. Frequency sensitivity of 3.4 × 3.4 nm BN nanosheet with gold atoms versus mass ratio

As can be seen in Figure 10, the sensitivity increases with the increasing number of gold atoms. Tables 6 and 7 present similar data for rectangular sheets in armchair and zigzag configurations.

Table 6. Natural Frequencies of Armchair BN Sheets (Armchair × Zigzag) with Au Atoms (THz)

Au Atoms	5×3.4	5.5×3.4	6×3.4	6.8×3.4
1	0.1654	0.1564	0.1518	0.1480
2	0.1609	0.1524	0.1476	0.1435
3	0.1520	0.1475	0.1436	0.1346
4	0.1473	0.1430	0.1387	0.1331
6	0.1428	0.1389	0.1342	0.1312
9	0.1386	0.1275	0.1250	0.1182

Table 7. Natural Frequencies of Zigzag BN Sheets (Armchair × Zigzag) with Au Atoms (THz)

Au Atoms	3.4×5	3.4×5.5	3.4×6	3.4×6.8
1	۰.۱۶۰۹	۰.۱۵۲۰	۰.۱۴۷۴	۰.۱۴۳۰
2	۰.۱۵۶۶	۰.۱۴۷۷	۰.۱۴۳۲	۰.۱۳۸۶
3	۰.۱۴۷۵	۰.۱۴۲۹	۰.۱۳۸۸	۰.۱۳۳۹
4	۰.۱۴۳۳	۰.۱۳۸۶	۰.۱۳۴۹	۰.۱۳۱۵
6	۰.۱۳۴۵	۰.۱۳۳۸	۰.۱۳۲۱	۰.۱۲۹۶
9	۰.۱۲۹۶	۰.۱۲۵۱	۰.۱۲۲۳	۰.۱۱۶۲

These results further confirm that as more gold atoms are deposited, the sheet's frequency drops significantly. Additionally, zigzag configurations consistently show slightly lower frequencies than armchair counterparts of the same nominal size. Figures 11 to 14 visualize the same trend graphically for various geometries:

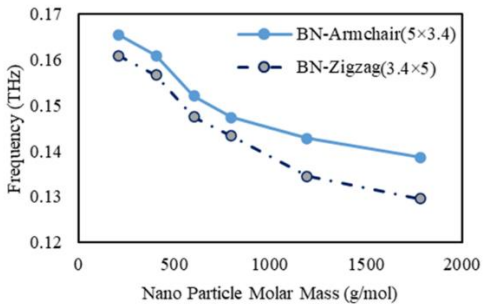

Figure 11. First natural frequency of 3.4×5 and 5×3.4 nm BN sheets with gold atoms

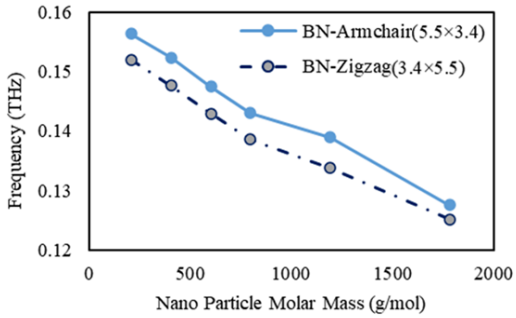

Figure 12. First natural frequency of 3.4×5.5 and 5.5×3.4 nm BN sheets

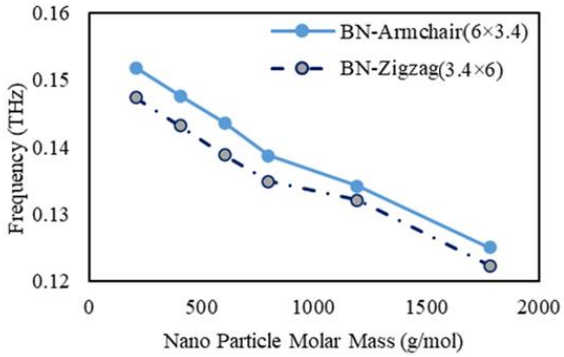

Figure 13. First natural frequency of 3.4×6 and 6×3.4 nm BN sheets

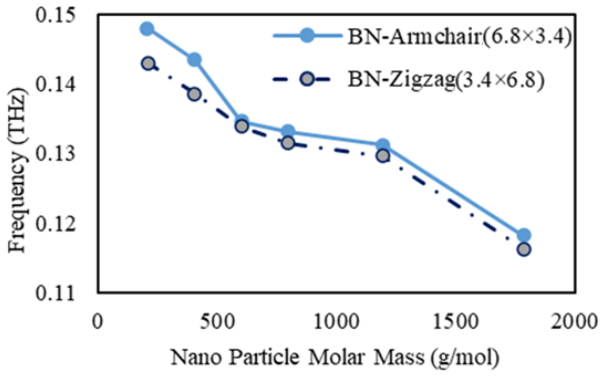

Figure 14. First natural frequency of 3.4×6.8 and 6.8×3.4 nm BN sheets

Across all dimensions, the same conclusion holds: the natural frequency decreases as external atomic mass increases.

4-3. Frequency Sensitivity Analysis to Added Mass

In this section, the sensitivity of boron nitride (BN) nanosheets to the presence of external atomic mass is analyzed across various sheet dimensions and orientations. Vibrational sensitivity is a crucial parameter in assessing the sheet's performance as a mass sensor.
The sensitivity values, calculated using Equation (15), are tabulated for a wide range of geometries in Table 8. As expected, increasing the number of gold atoms leads to greater shifts in the sheet's natural frequency, thereby enhancing the overall sensitivity.

Table 8. Frequency Sensitivity of BN Sheets to Gold Atom Adsorption

Dimensions (nm) (Armchair × Zigzag)	Number of Gold Atoms					
	1	2	3	4	6	9
5 × 3.4	0.144	0.167	0.213	0.237	0.261	0.282
5.5 × 3.4	0.167	0.192	0.218	0.242	0.264	0.324
6 × 3.4	0.156	0.179	0.201	0.229	0.254	0.305

6.8 × 3.4	0.128	0.154	0.207	0.216	0.227	0.303
3.4 × 5	0.162	0.185	0.232	0.254	0.300	0.320
3.4 × 5.5	0.175	0.199	0.225	0.248	0.274	0.321
3.4 × 6	0.152	0.178	0.206	0.220	0.231	0.311
3.4 × 6.8	0.152	0.178	0.206	0.220	0.231	0.311

These results reveal a clear trend: larger sheets and higher numbers of adsorbed atoms yield stronger sensitivity. Moreover, for sheets with identical nominal dimensions but different orientations, zigzag configurations consistently exhibit higher sensitivity than armchair ones.

This trend is also illustrated in Figures 15 to 18:

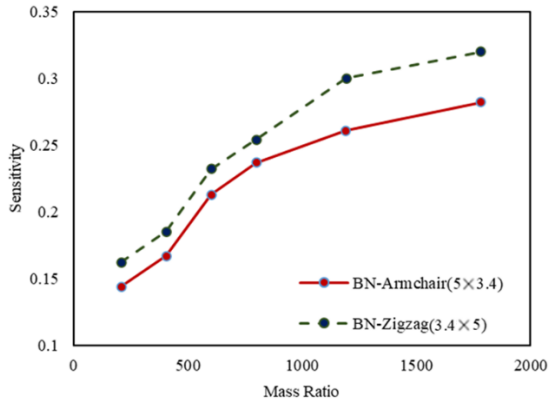

Figure 15. Frequency sensitivity of 3.4×5 and 5×3.4 nm BN sheets with varying numbers of gold atoms

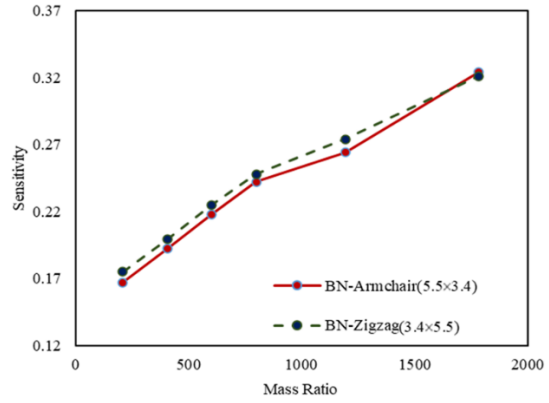

Figure 16.: Frequency sensitivity of 3.4×5.5 and 5.5×3.4 nm BN sheets with varying gold atoms

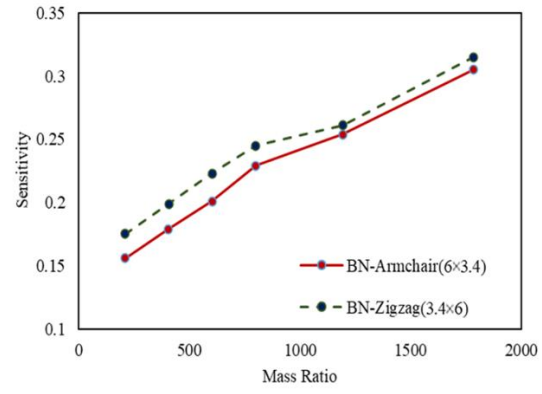

Figure 17. Frequency sensitivity of 3.4×6 and 6×3.4 nm BN sheets with varying gold atoms

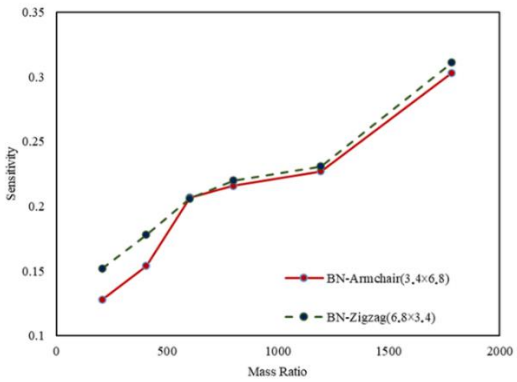

Figure 18. Frequency sensitivity of 3.4×6.8 and 6.8×3.4 nm BN sheets with varying gold atoms

The data confirms that:

- Sensitivity increases with the number of gold atoms.
- Zigzag-oriented sheets tend to be more sensitive than their armchair counterparts.
- For a fixed number of atoms, narrower sheets in the mass loading direction produce higher relative sensitivity due to more pronounced local inertia effects.

This strong sensitivity response highlights the high potential of boron nitride nanosheets for use in nanoscale mass sensors, especially in configurations optimized for maximum resonance shift.

5. Conclusion

In this study, the vibrational and mechanical properties of single-layer boron nitride (BN) nanosheets were investigated using molecular dynamics simulations. The frequency decomposition method was employed to extract the natural frequencies and mode shapes of the sheets. After validating the numerical results against existing experimental and analytical data, the following key conclusions were drawn:

- The first natural frequency of boron nitride nanosheets is lower than that of graphene sheets with identical geometry and boundary conditions. This is attributed to BN's lower Young's modulus and surface mass density.
- The natural frequency decreases with increasing sheet dimensions, a trend consistent with theoretical expectations and analytical models of vibrating plates.
- Mechanical behavior under uniaxial tension showed that the Young's modulus of the BN sheet is approximately 843 MPa, in agreement with previous studies.
- The presence of gold atoms on the sheet's surface significantly affects its dynamic response. As the number of adsorbed atoms increases, the sheet's natural frequency decreases due to the added inertial mass.
- The frequency sensitivity of the nanosheet increases proportionally with the number of gold atoms. This sensitivity is also influenced by the sheet's geometry and orientation.
- Among sheets with identical nominal sizes, those aligned in the zigzag direction exhibit higher sensitivity to added mass compared to their armchair counterparts.

Recent experimental studies have confirmed the optomechanical responsiveness of H-BN resonators under radiation pressure, highlighting their potential for integration in photonic mass sensors and frequency-tunable systems. Specifically, backaction effects such as optical spring softening and damping were observed in suspended BN structures, confirming their viability beyond purely mechanical applications [32].

These findings demonstrate that boron nitride nanosheets, due to their high sensitivity to nanoscale mass changes and consistent vibrational behavior, are promising candidates for use in nanoresonator-based mass detection devices. The results of this study can be applied toward

the development and optimization of extremely sensitive nanomechanical mass sensors based on two-dimensional materials.

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