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Nonlinear thermal vibration of a nanoplate attached to a cavity

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Abstract
Dynamic problems of a nanocircular plate-cavity system are investigated using molecular dynamics (MD) method. A nonlinear plate model considering gas action is developed. The results of the MD simulation show that the helium atoms adsorb on the wall of the cavity at low temperature, resulting in a negative deflection of the molybdenum disulfide (MoS$_2$) plate. As the temperature increases, the pressure in the cavity increases, leading to a gradual rise in the deflection of the plate. A nonlinear phenomenon of stiffness hardening is shown with increasing temperature. The nonlinear plate model can give a relatively good prediction compared with the results of MD simulations. The natural frequency of the plate is affected by temperature and the presence of gas in the cavity. The phenomenon of stiffness hardening and softening can be well simulated by the nonlinear plate model and MD method. The present study provides a reference for vibration experiments of two-dimensional nanostructures.

1. Introduction

Interest in electromechanical devices and systems of micrometre and nanometre scales has gradually increased due to their wide application in nanocomputers, mechanical signal processing, scanning probe microscopes, etc. The rapid development of these fields has led to the appearance of nanoelectromechanical systems (NEMS) [1–5]. More recently, NEMS based on two-dimensional crystals [6] such as graphene, MoS$_2$ and other materials have great potential for new types of drives and sensors due to their ultralow weight, high mechanical flexibility, low energy dissipation and high quality factor. The research methods for nanoscale two-dimensional materials mainly include experiment, MD simulation and continuum model, among which the conventional plate model is widely used due to its low computational cost and relatively simple formula. He et al. [7] established a Kirchhoff plate model to investigate the effect of the van der Waals interaction on the natural frequencies of multi-layered graphene sheets. Behfar and Naghdabadi [8] used the conventional continuum plate model to investigate nanoscale vibrational analysis of a multi-layered graphene sheet embedded in an elastic medium. Liew et al. [9] proposed a continuum-based plate model to study the vibration behaviour of multi-layered graphene sheets that are embedded in an elastic matrix. Lee et al. [10] measured the elastic properties and inherent fracture strength of free-standing monolayer graphene membranes using nanoindentation via an atomic force microscope. Duan and Wang [11] investigated the deformation of a circular single-layered graphene sheet under a central point load by molecular mechanics simulations and used von Karman plate theory to predict the graphene sheet behaviour under linear and nonlinear bending and stretching. Chen et al. [12] demonstrated the fabrication and electrical readout of monolayer graphene resonator, and investigated the response of a monolayer graphene nanomechanical resonator to mass and temperature changes. Li et al. [13] fabricated a field effect transistor and demonstrated the potential of thin black phosphorus crystals in nanoelectronic devices based on few-layer black phosphorus crystals with a thickness of only a few nanometers. Lee et al. [14] quantitatively demonstrated an ultrathin MoS$_2$ nanomechanical resonator with high quality factor vibration in the very high frequency band. Xiong and Gao [15] investigated the bending response of the single-layered MoS$_2$ using MD simulations. They showed that the bending behaviour of the single-layered MoS$_2$ is isotropic and can be predicted by the continuum mechanics theory. Sajadi et al. [16] fitted the resonance frequencies obtained from the Brownian
motion in MD simulations, to those obtained from a continuum mechanics model, with bending rigidity and pretension as the fit parameters. Liu and Wang [17] studied the nonlinear static and dynamic behaviour of a drum resonator based on double-layer MoS2 using MD simulation and a nonlinear circular sandwich plate model. However, a certain amount of gas is inevitably encapsulated in the cavity when the two-dimensional material is attached to the basal cavity in the experiment. The gas in the cavity has a remarkable influence on the vibration of two-dimensional materials [18, 19].

The free vibration of a plate with an enclosed cavity is of great interest to researchers. Such a model has a wide range of applications in vehicle and railway passenger cabins, aircraft fuselages and skin, acoustic instruments, and various aerospace structures. Frendi and Robinson [20] used a coupled model and an uncoupled model to study the effect of acoustic coupling on plate vibration under random and harmonic excitation. Li and Cheng [21] developed a coupled vibra-acoustic model for the study of flexible panels backed by a rectangular-like cavity introduced through a tilted wall. Tanaka et al [22] numerically solved and experimentally verified the eigenvalue problem of a coupled rectangular cavity. Lee [23] analysed the nonlinear resonant frequencies of a rectangular tube with one end open, the other end flexible and four rigid sides using harmonic balance and homotopy perturbation approaches. Lee [24] also studied the free vibration analysis of a nonlinear panel coupled with an extended cavity. The multilevel residual harmonic balance method was adopted to solve the nonlinear problem. Zhang et al [25] studied the coupling system of an acoustic cavity with rigid walls or impendence walls and a single or double thin laminated rectangular plate with various elastic boundary conditions based on an improved Fourier series method. Anvariye [26] investigated the nonlinear vibroacoustics of circular plates with air cavities under harmonic excitation. A plate equation based on von Karman theory and the pressure equation was obtained and solved.

In this paper, the influence of gas encapsulation in a nanometre resonator is investigated via MD simulation and a nonlinear plate model. The MD model and nonlinear plate model are illustrated in section 2. The results and discussion are presented in section 3. Finally, concluding remarks are given in section 4.

2. Models and methods

2.1. Molecular dynamics model

A monolayer MoS2 plate is attached to one side of a cylindrical cavity made of a carbon nanotube with graphene enclosed at the other side, as shown in figure 1. The cavity is filled with helium at a certain pressure. In this case, the carbon nanotube acts as the cavity. The red atoms of the MoS2 plate are fixed. The yellow part is in contact with the helium in the cavity and vibrates freely.

The parameters of the model in figure 1 are shown in table 1. In this section, an MD method is adopted to explore the thermal vibration of the system. The REBO potential [27] is chosen to describe the interatomic interaction of the MoS2 layer in the MD simulations. The interactions between helium and helium and helium and MoS2 are characterized by a 12-6 Lennard-Jones potential [28].

The mechanical effect of helium on the MoS2 can be considered as a uniform pressure. This pressure $p$ can be expressed by van der Waals (vdW) equation [29],

$$\left( p + \frac{a}{V_0} \right) (V_0 - b) = RT$$  \hspace{1cm} (1)

where $V_0$ is the volume of a vdW gas, and $a$ and $b$ are vdW corrections. For helium, the values of $a$ and $b$ are 0.00324 J m$^{-3}$mol$^{-2}$ and $2.34 \times 10^{-5}$ m$^{3}$mol$^{-1}$, respectively.

2.2. Nonlinear plate model

The unfixed part of the MoS2 plate in contact with the helium in the cavity is regarded as a circular von Karman plate model. The von Karman equation can be expressed as follows [30],

$$\nabla^2 \nabla^2 w + \frac{\rho}{D} w_{,tt} = \frac{q(r, \theta, t)}{D} + \frac{h}{D} \left[ w_{,rr} \left( \frac{1}{r} F_{,r} + \frac{2}{r^2} F_{,rr} \right) \right. $$

$$+ \left. F_{,r} \left( \frac{1}{r} w_{,r} + \frac{1}{r^2} w_{,rr} \right) - 2 \left( \frac{1}{r^2} w_{,rr} \right) \left( \frac{1}{r} F_{,r} \right) \right] ,$$

(2)

$$\nabla^2 \nabla^2 F = E \left[ \left( \frac{1}{r} w_{,r} - \frac{1}{r^2} w_{,rr} \right)^2 - w_{,rr} \left( \frac{1}{r} w_{,r} + \frac{1}{r^2} w_{,rr} \right) \right] ,$$

(3)

where $w$ is the transverse displacement and $F$ is the Airy stress function. The force and displacement are independent of the polar angle of the mode of the axisymmetric circular plate. By simplifying equations (2) and (3), we can get,
The boundary conditions of a clamped circular plate are,

\[
\begin{align*}
\frac{r}{D} = \frac{h}{D} (w_r^r)^r, \\
\frac{1}{r} \left[ \frac{r}{D} (w_r^r)^r \right] = \frac{E}{2} (w_{\gamma})^r.
\end{align*}
\]

(4)

(5)

The boundary conditions of a clamped circular plate are,

\[
\begin{align*}
w = 0, \\
w_r = 0 \text{ at } r = 1, \\
u_r = 0
\end{align*}
\]

(6)

where \(u_r\) is the radial displacement. Considering the stress caused by thermal expansion, the radial displacement is expressed as,

\[
u_r = \frac{1}{Eh} \left[ r N_{\gamma} + (1 - \nu) N_q \right] + \alpha T r,
\]

(7)

where \(\alpha\) is the coefficient of thermal expansion and \(T\) is the temperature. A circular plate of radius \(a\) and thickness \(h\) is subject to a uniform lateral pressure \(q_0\). The perturbation method is applied to obtain the approximate solutions of equations (4) and (5). The approximate fourth-order equations are calculated, and the
corresponding unknown coefficients are solved based on the boundary conditions. The relationship between the uniform distribution pressure \( q_0 \) and the central displacement \( w_0 \) is obtained as follows,

\[
\frac{q_0 a^4}{Eh^4} = \frac{1}{(1 - \nu^2)} \left[ \frac{2(173 - 73)(\nu + 1)w_0^3}{135h^3} + \frac{8[6 - 5(\nu + 1)]w_0^3}{9h} \right].
\] (8)

The pressure caused by helium in the cavity can be determined by using the wave equation as follows,

\[
\frac{\partial^2 q_t}{\partial r^2} + \frac{1}{r} \frac{\partial q_t}{\partial r} + \frac{\partial^2 q_t}{\partial z^2} - \frac{1}{c_s^2} \frac{\partial^2 q_t}{\partial t^2} = 0,
\] (9)

where \( z \) is the vertical displacement from the bottom of the cylindrical cavity and \( c_s \) is the sound speed. The boundary conditions of pressure \( q_t(r, z, t) \) are,

\[
\frac{\partial q_t}{\partial r} \bigg|_{r=a} = 0, \quad \frac{\partial q_t}{\partial z} \bigg|_{z=0} = 0, \quad \frac{\partial q_t}{\partial z} \bigg|_{z=\delta} = -\rho_{air} \frac{\partial^2 w(r, t)}{\partial t^2}.
\] (10)

Dimensionless parameters are introduced as follows,

\[
\xi = \frac{r}{a}, \quad U = \frac{au}{h^2}, \quad W = \frac{w}{h}, \quad \delta = \frac{z}{z_0}.
\] (11)

To investigate the nonlinear response of a rigid clamped circular plate under a sinusoidal uniform load \( q(t) \), the equation of motion for the circular plate can be expressed as,

\[
\frac{D}{\rho a^4} \nabla^2 \nabla^2 W + W_{rr} = \frac{q(\xi, t)}{\rho h} - \frac{q(\xi, \delta, t)}{\rho h} + \frac{c_s^2}{a^4} W_{\xi\xi} \left[ U_{\xi} + \frac{1}{2} W_{\xi}^2 + \frac{U_{\delta}}{\xi} \right] + \frac{c_s^2}{a^4} W_{\xi\xi} \left[ U_{\xi} + \frac{1}{2} W_{\xi}^2 + \frac{U_{\delta}}{\xi} \right],
\] (12)

\[
U_{\xi\xi} + \frac{1}{\xi} U_{\xi} - \frac{U}{\xi^2} + W_{\xi} W_{\xi\xi} + \frac{1}{2} W_{\xi}^2 = 0.
\] (13)

The boundary conditions are,

\[
U = 0, \quad W = 0, \quad W_{\xi} = 0 \text{ at } \xi = 1.
\] (14)

The separation forms of the transverse displacement and radial displacement are assumed as follows,

\[
W(\xi, t) = \hat{w}(t)(1 - \xi^2)^2, \quad (15a)
\]

\[
U(\xi, t) = \hat{w}(t)H(\xi), \quad (15b)
\]

where \( (1 - \xi^2)^2 \) is the assumed modal function satisfying the transverse boundary condition (14), and \( H(\xi) \) is an unknown function related to \( \xi \). Substituting the above equations into equation (13) and applying the in-plane boundary conditions, the expression for \( H(\xi) \) is obtained as,

\[
H(\xi) = \frac{5 - 3\nu}{6} \xi^5 - (3 - \nu) \xi^3 + \frac{10 - 2\nu}{3} \xi^5 - \frac{7 - \nu}{6} \xi^3.
\] (16)

Using the boundary conditions in equation (14) and combining the separation forms of the transverse and radial displacement in equations (15a) and (15b), the pressure exerted by the helium on the vibrating circular plate can be obtained as follows,

\[
q_{0}(\xi, \delta, t) = \rho_{air} \frac{h(1 - \xi^2)^2 u_{rr}}{\sqrt{k^2 + \lambda^2 \sin^2(\sqrt{k^2 + \lambda^2}z)}} \times J_0(k\alpha \xi) \cos(\sqrt{k^2 + \lambda^2}z\delta) + q_0',
\] (17)

where \( J_0 \) is a Bessel function of the first kind of order \( m \), \( q_0' \) is the static pressure caused by the helium, and \( k \) is the \( m \)th root of the following equation,

\[
J_0(k\alpha \xi) I_0(k\alpha) + I_0(k\alpha) J_0(k\alpha) = 0.
\] (18)

By substituting equations (15)–(17) into equation (12), the Galerkin method is applied to obtain the nonlinear ordinary differential equation about \( \hat{w}(t) \) as,
\[ \dot{\omega} + \omega^2 \dot{\psi} + \alpha^2 \dot{\psi}^3 = P \cos \omega t + P_0, \]  
(19)

where

\[ \omega_0^2 = \frac{320D}{3\rho a^4 \eta}, \]
(20a)

\[ \alpha^2 = -\frac{40(v + 1)D(9v - 23)}{21\rho a^4}, \]
(20b)

\[ P = \frac{5q}{3\rho a^4 \psi \eta}, \]
(20c)

\[ P_0 = \frac{5q_0}{3\rho \psi \eta}, \]
(20d)

\[ \eta = 1 + 10 \int_0^1 \frac{\xi(\xi - 1)^4(\xi + 1)^4 \rho_0 \rho(ka\xi)\cos(\sqrt{k^2 + \lambda^2} z)}{\sqrt{k^2 + \lambda^2} \rho_0 \sin(\sqrt{k^2 + \lambda^2} z)} d\xi. \]
(20e)

Setting \( \dot{\psi} = x + \tau \), equation (19) can be expressed as [31],

\[ x_{,tt} + 2\zeta x_{,t} + \theta^2 x + \alpha_2 x^2 + \alpha_3 x^3 = P \cos \omega t, \]
(21)

where

\[ \tau^3 + \frac{\omega^2}{\alpha^2} \tau - \frac{P_0}{\alpha^2} = 0, \]
(22a)

\[ \theta^2 = \omega_0^2 + 3\tau^2 \alpha^2, \]
(22b)

\[ \alpha_2 = 3\tau^2 \alpha^2, \]
(22c)

\[ \alpha_3 = \alpha^2. \]
(22d)

Equation (21) represents the forced vibration of a Duffing system [32, 33]. Supposing \( x = \varepsilon u, \zeta = \varepsilon^2 \mu \), and \( P = \varepsilon^0 k \), one obtains,

\[ u_{,tt} + \theta_0^2 u = -2\varepsilon^2 \mu u_{,t} - \varepsilon \alpha_2 u^2 - \varepsilon^2 \alpha_3 u^3 + \varepsilon^0 k \cos \theta t. \]
(23)

\[ \theta = \theta_0 + \varepsilon^2 \sigma. \]
(24)

The multiscale method is applied to solve equation (23). The approximate solution of the equation has the following form,

\[ u(t) = u_0(T_0, T_1, T_2) + \varepsilon u_1(T_0, T_1, T_2) + \varepsilon^2 u_2(T_0, T_1, T_2) + \ldots \]
(25)

The above equation is substituted into equation (23). Coefficients of the same power of \( \varepsilon \) on both sides are set to be equal. The operation of eliminating the secular term and separating the real and imaginary parts is carried out. The steady-state periodic motion equation is simplified and the amplitude-frequency relationship is finally obtained as follows,

\[ \left[ \mu^2 + \left( \frac{\varepsilon - \frac{9\alpha_3 \theta_0^2 - 10\alpha_2^2 a}{24 \theta_0^3}}{2 \theta_0^2} \right)^2 \right] a^2 = \left( \frac{k}{\theta_0} \right)^2. \]
(26)

3. Results and discussion

3.1. Static analysis

The variation in the thermal expansion coefficient in the armchair and zigzag directions of the single-layered MoS\(_2\) with increasing temperature is shown in figure 2. The two curves in the armchair and zigzag directions roughly coincide. This result illustrates that MoS\(_2\) can be regarded as isotropic in the thermal expansion.

To explore the correctness of extracting the transverse stress of a circular plate and converting it into an equivalent pressure, this result is compared with the different state equations of the gas, as shown in figure 3. The pressure from the ideal gas state equation, vdW equation and modified vdW equation are compared with the MD simulation pressure. The ideal gas equation of state is expressed as

\[ pV_0 = RT. \]
(27)

The vdW equation is shown in equation (1). The modified vdW equation [34] is expressed as

\[ p = \frac{RT}{V_0 - b} - \frac{a}{\sqrt{T}V_0(V_0 + b)}. \]
(28)
The pressure predicted by the ideal gas state equation is far less than the extracted result of the MD simulation. The pressure predicted by the vdW equation and the modified vdW equation is a little greater than the extracted result of the MD simulation.

The deflection of the MoS$_2$ circular plate with a radius of 6.78 nm is shown in figure 4. The cavity is filled with a certain amount of helium. The motion of the model at different temperatures is simulated by the MD method between 100 K and 1000 K. The nonlinear curves show typical geometric nonlinear phenomena, which suggests that the MoS$_2$ plate stiffens when subjected to helium pressure. The theoretical result of the nonlinear plate model considering thermal expansion increases slightly compared to the results not considering thermal expansion, but the overall difference is not significant. The theoretical value fits well with the simulated value of the MD simulation. To explore the static effect of helium motion on the MoS$_2$ plate, which is equal to the pressure created by the thermal motion of the helium exerted on the plate, the transverse stresses on the plate in the MD simulation at different temperatures are extracted. The model should be controlled at the corresponding temperature when pressure is applied to simulate the effect of temperature on the thermal vibration of the MoS$_2$ plate. The simulated result of applying pressure and controlling temperature is in good agreement with the original MD simulation result and theoretical result, indicating the correctness of the idea of applying equivalent pressure.

**Figure 2.** Pressure in the cavity obtained by using different theories and molecular dynamics simulation.

**Figure 3.** Thermal expansion coefficients of monolayer MoS$_2$ in the armchair and zigzag directions with increasing temperature.
3.2. Helium adsorption at low temperature

The vibration of the MoS$_2$ circular plate caused by helium in the cavity at temperatures from 5 K to 1000 K is simulated. The deflection of the centre point of the circular plate is shown in figure 5. When the temperature is under 15 K, the plate exhibits abnormal negative deflection. To explore the mechanism of this phenomenon, MD method is used to output .xyz files that contain all the coordinates of the atoms. Then the files are imported into molecular visualization program to display the motion process of molecules. The frame images in molecular visualization program are generated as shown in figure 6. At 5 K, helium atoms gather on the surface of the MoS$_2$ plate and the bottom of the graphene. At this time, the helium presents a state similar to a solid. The helium adsorbs on the surface of the MoS$_2$ due to the vdW force between MoS$_2$ and helium, and the vdW force between MoS$_2$ and helium attracts the plate downward. At 15 K, helium atoms begin to slide close to the MoS$_2$ plate and the graphene at the bottom, while a small number of helium atoms crawl vertically up and down along the cavity wall, showing a liquid-phase phenomenon. Zero deflection of the plate appears at this temperature. It is speculated that the offset of the attraction helium atoms to the plate leads to this phenomenon. As the temperature rises, the phase of helium in the cavity changes to the gaseous state with random thermal motion. At 1000 K, helium atoms with violent thermal motion in the cavity frequently impact the MoS$_2$ plate, resulting in a large bulge deflection.

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**Figure 4.** Central point deflection of the MoS$_2$ circular plate with increasing temperature.

**Figure 5.** Central point deflection of the MoS$_2$ circular plate.
3.3. Dynamic analysis

The model without helium in the cavity and the model filled with helium in the cavity are set up as shown in figure 7. The free thermal vibration of this system is simulated using the MD method. The time history of an atom in the centre of the MoS$_2$ plate is shown in figure 8. Using the fast Fourier transform (FFT), the frequency spectrum of the atom is presented in figure 9. The natural frequencies of the plate can be obtained from the peaks of the curve.

Then, the influence of temperature and whether helium is filled in the cavity on the first-order natural frequency of the MoS$_2$ is investigated. The first-order natural frequencies of the thermal vibration of the plate and that of the nonlinear plate model are summarized in table 2. It can be seen from table 2 that the first-order natural frequencies obtained by MD simulation and by the nonlinear plate model are close to each other at 15 K. The deflection of the MoS$_2$ plate is near 0 at 15 K, as shown in figure 5, so the static pressure exerted on the plate

Figure 6. Distribution of the helium atoms at different temperatures.
is also near 0. Whether helium in the cavity has little effect on the frequency of the plate. As the temperature rises to 200 K, the thermal vibration frequency of the plate without helium in the cavity decreases. This is because thermal expansion of the MoS$_2$ plate occurs as the temperature increases, which leads to normal stress in the plate and a decrease in the natural frequency. Meanwhile, the natural frequency of the plate with helium in the cavity increases due to the pressure caused by the thermal motion of the helium. Therefore, as the temperature rises to 200 K, the frequency of the plate with helium in the cavity increases substantially.

Figure 7. The model without helium in the cavity and the model filled with helium in the cavity.

Figure 8. Time history of a molybdenum atom of MoS$_2$. 
Amplitude-frequency curves can be obtained by the sweep frequency via MD simulation, as shown in figure 10. The sweep rate is 2.4 GHz ns$^{-1}$ starting from 0. The red curves are obtained from the nonlinear plate model at different temperatures with a density of helium in the cavity of 107.7 kg m$^{-3}$. The initial deflection of the plate due to static pressure increases with increasing temperature. The right inclination of the curve decreasing shows that the stiffness hardening phenomenon becomes weaker. In addition, the static pressure also leads to the asymmetry of the upper and lower deflections, as shown in figures 10(b) and (c).
The amplitude-frequency curves with different densities of gas at 100 K are shown in figure 11. As the density increases, the initial displacement due to static pressure increases, and the asymmetry in the equilibrium position of the deflection curves becomes more distinct. The hardening effect is weakened, and the softening effect is enhanced due to the increasing in density. The frequency sweep results in the figure show a stronger right inclination compared with the results of the nonlinear plate model. The rise in density of gas results in an increasing in natural frequency.

4. Conclusion

The MD model of a MoS$_2$ plate attached to a gas cavity and the dynamic nonlinear continuum model are developed. The results show that the pressure generated by helium can significantly change the deflection of a two-dimensional material. The solid phase and liquid phase of helium are observed at temperatures much higher than the melting points and boiling points. The nonlinear vibration behavior of the MoS$_2$ plate is investigated. The stiffness hardening phenomenon of the amplitude-frequency response of the MoS$_2$ plate

Table 2. First-order natural frequencies of the MoS$_2$ circular plates obtained using different methods.

|                | 15 K                   | 200 K                  |
|----------------|------------------------|------------------------|
|                | Thermal vibration      | Nonlinear plate model  | Thermal vibration      | Nonlinear plate model  |
|                | frequency GHz$^{-1}$   | frequency GHz$^{-1}$   | frequency GHz$^{-1}$   | frequency GHz$^{-1}$   |
| Without helium | 29.618                 | 31.143                 | 27.861                 | 31.143                 |
| Filled with helium | 29.294              | 31.143                 | 40.706                 | 36.806                 |

The amplitude-frequency curves with different densities of gas at 100 K are shown in figure 11. As the density increases, the initial displacement due to static pressure increases, and the asymmetry in the equilibrium position of the deflection curves becomes more distinct. The hardening effect is weakened, and the softening effect is enhanced due to the increasing in density. The frequency sweep results in the figure show a stronger right inclination compared with the results of the nonlinear plate model. The rise in density of gas results in an increasing in natural frequency.

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becomes weaker when the temperature increases. The hardening effect is weakened, and the softening effect is enhanced by an increasing in density of gas.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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