Vibrational analysis of fluid-filled carbon nanotubes using wave propagation approach

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ABSTRACT

This paper presents a method for vibrational analysis of fluid-filled double-walled carbon nanotubes using wave propagation approach. Simplified Flügge shell equations are proposed as the governing equations of vibration for the carbon nanotubes. The double-walled nanotubes are considered as two-shell model coupled together through the van der Waals interaction between two adjacent nanotubes. Based on the proposed theoretical approach, we investigate the influences of parameters, such as fluid properties and vibrational modes, on the vibrational characteristics of carbon nanotubes. In this study, we consider the double-walled nanotubes with an inner diameter of 2.2 nm and an outer diameter of 3.0 nm. The theoretical investigation may give a useful reference for potential application and design of nanoelectronics and nanodevices.

Key words:

62.30.+d Mechanical and elastic waves; vibrations

62.25.+g Mechanical properties of nanoscale materials

62.40.+I Anelasticity, internal friction, stress relaxation, and mechanical resonances

Ⅰ. INTRODUCTION

The discovery of carbon nanotubes (CNTs) has attracted much attention due to their remarkable mechanical and physical properties.[1-6] The CNTs may be used in a wide range of applications, such as material reinforcement, field emission and vacuum microelectronic devices, nano-sensors and nano-actuators. Owing mainly to perfect cylindrical channels and the remarkable mechanical properties, the CNTs hold substantial promise as artificial blood vessels[7], and nanopipes for conveying fluid or gas. The carbon nanotubes are from about 3 nm to 30 nm in the diameter, which are small enough to fit into blood vessels. Because medium properties of fluid-filled CNTs could affect the vibrational frequency, understanding the mechanical and physical properties of CNTs conveying fluids is essential for their potential designs and application.

Some studies on the vibration [8-11] and the wave propagation [12-14] have been reported in the literature. However, the experimental techniques to measure the properties of an individual CNT are quite difficult owing to their nanometer dimensions. Current simulation models for CNTs can essentially categorized as molecular dynamics (MD) method and continuum mechanics. Although the MD simulation is an effective method to predict the chemical and physical properties of nanostructures, it is very time-consuming and remains formidable especially for larger-scale systems. The simulation of larger systems must be currently left to continuum mechanics methods. At present, solid mechanics with elastic continuum model has been regarded as an effective method and widely used for analyzing the mechanical and physical properties of CNTs. [9-15]

In early studies on wave propagation and vibration of CNTs, the CNTs have been modeled as Bernoulli-Euler beam equation. [9,12,13] The Euler beam model ignored the influence of rotary and shear deformation on transverse wave propagation in CNTs. Recently, the vibration of multi-walled carbon nanotubes (MWNTs) and wave propagation of double-walled carbon nanotubes (DWNTs) have been studied based on Flügge shell equation.[10,11,14] These work show that the CNTs have the vibration and sound wave frequency over terahertz because of their nanoscale, which opens a new topic on wave characteristics. Wang and Varadan[15] have presented the elastic wave solution obtained from Euler-Bernoulli beam and Timoshenko beam models. They reported that the comparison between the two models could be inappropriate on the terahertz frequency range. This suggested that the Timoshenko beam model should be employed in analyzing the wave propagation for the high frequency range. Li et al.[16,17] have presented vibrational analysis of single- and double-walled CNTs using a

truss rod model. They predicted that single-walled nanotubes (SWNTs) could have fundamental frequency ranging from 10 GHz to 1.5 THz and the frequency depends on the diameter and length of CNTs.[17] At present, however, few studies on vibrational characteristics in CNTs, especially in filled-fluid CNTs, have been down. The investigation on dynamic characteristics of fluid-filled CNTs is quite significant for the designs of various nanosensor and nanopipe conveying fluid. Yoon et al. have studied the vibration in single-walled CNTs conveying fluid by a simple beam model.[18] The dynamic characteristics in fluid-filled CNTs still remain relatively unknown.

The main objective of this paper is to propose a theoretical approach as well as to investigate the vibrational characteristics in fluid-filled DWNTs. The constitutive behavior of CNTs is described by Flügge shell equation, and the motion equation of fluids in CNTs is given by Morse and Ingard.[19] Using wave propagation approach, we investigated and analyzed the influence of fluid properties on the vibrational behaviors in DWNTs filled with fluid. This investigation is very significant for potential application of nanopipe conveying fluid.

Ⅱ. DYNAMIC EQUATIONS OF FLUID-FILLED CNTs

A. Flügge equations

Approximate Flügge shell equations are proposed as the governing equations of vibration for CNTs. Figure 1 shows a cylindrical coordinate system of the continuum shell model of CNTs. The x coordinate is taken in the axial direction of the shell, where the θ and z coordinates are in the circumferential and radial directions, respectively. The displacements of the nanotube are defined by u, v and w in the directions of x, θ and z-axes, respectively. The CNT has a thickness of h, radius of R and length of L.

Based on Love's first approximation shell theory,[20] the equations of motion for nanotubes can be given by[14]

$$\begin{bmatrix} L_1 & L_2 & L_3 \\ L_2 & L_4 & L_5 \\ -L_3 & -L_5 & L_6 \end{bmatrix} \begin{Bmatrix} u \\ v \\ w \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ -pK \end{Bmatrix}, \tag{1}$$

where $L_j \ (j = 1, \cdots, 6)$ are the differential operators with respect to x and θ given by

$$
\begin{aligned}
L_1 &= \frac{\partial^2}{\partial x^2} + \frac{1-\sigma}{2R^2}\frac{\partial^2}{\partial \theta^2} - K\rho h\frac{\partial^2}{\partial t^2}, \qquad L_2 = \frac{1+\sigma}{2R}\frac{\partial^2}{\partial x \partial \theta}, \qquad L_3 = -\frac{\sigma}{R}\frac{\partial}{\partial x}, \\
L_4 &= \frac{1-\sigma}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{R^2}\frac{\partial^2}{\partial \theta^2} + \alpha\left[2(1-\sigma)\frac{\partial^2}{\partial x^2} + \frac{1}{R^2}\frac{\partial^2}{\partial \theta^2}\right] - K\rho h\frac{\partial^2}{\partial t^2}, \\
L_5 &= \frac{1}{R^2}\frac{\partial}{\partial \theta} - \alpha\left[(2-\sigma)\frac{\partial^3}{\partial x^2 \partial \theta} + \frac{1}{R^2}\frac{\partial^3}{\partial \theta^3}\right], \\
L_6 &= -\frac{1}{R^2} - \alpha\left(R^2\frac{\partial^4}{\partial x^4} + 2\frac{\partial^4}{\partial x^2 \partial \theta^2} + \frac{1}{R^2}\frac{\partial^4}{\partial \theta^4}\right) - K\rho h\frac{\partial^2}{\partial t^2},
\end{aligned}
\tag{2}
$$

where $K = \left(1-\nu^2\right)/Eh$, $\alpha = h^2/12R^2$. E and ν are the elastic modulus and Poisson's ratio of a graphene sheet folded into CNTs.

Eliminating u and v from Eq. (1), we have

$$
L_A w + L_B(pK) = 0, \tag{3}
$$

where

$$
\begin{aligned}
L_A &= L_5\left(L_2L_3 - L_1L_5\right) + L_3\left(L_2L_5 - L_3L_4\right) + L_6\left(L_2L_2 - L_1L_4\right), \\
L_B &= \left(L_2L_2 - L_1L_4\right).
\end{aligned}
\tag{4}
$$

B. Acoustic pressure field

For fluids with non-viscous and isotropic fluids, the motion equation of fluids in the cylindrical shell can be written by Morse and Ingard in the cylindrical coordinate system as[19]

$$
\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial p}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 p}{\partial \theta^2} + \frac{\partial^2 p}{\partial x^2} = \frac{1}{c_f^2}\frac{\partial^2 p}{\partial t^2} \tag{5}
$$

where p is the acoustic pressure and c_f is the sound speed of the fluid.

C. Vibrational frequency of double-walled nanotubes

The wave propagation approach is presented for analyzing the natural frequency of CNTs. In the cylindrical coordinate system as shown in Fig. 1, the displacement of simply supported DWNTs for the harmonic vibration can be expressed in the form of wave propagation:

$$
w_j = C_j \sin\frac{m\pi x}{L}\cos n\theta \exp(i\omega t) \qquad (j = 1,2) \tag{6}
$$

where $C_j\ (j=1,2)$ represents the amplitude of vibration in the inner and outer nanotubes. ω is the circular frequency of wave. The modal parameters m $(m>0)$ and n are the axial half-wave and the circumferential wave numbers, respectively, characterizing the vibrational

mode of CNTs.

The solution form of the acoustic pressure field of the cylindrical shell filled with fluid, which satisfies Eq. (5), can be expressed as

$$p_f = P_0 Z_n(k_r r)\sin\frac{m\pi x}{L}\cos n\theta \exp(i\omega t) \tag{7}$$

where Z_n denotes a Bessel function J_n of order n when $k_r^2 = \omega^2/c_f^2 - (m\pi/L)^2 > 0$, and the modified Bessel function I_n when $k_r^2 = (m\pi/L)^2 - \omega^2/c_f^2 > 0$. The parameter k_r presents the radial wave numbers.

Since the fluid remains in contact with the tube wall, the fluid displacement is equal to the radial displacement of the inner tube wall. This coupling condition is given by Fuller and Fahy[21] from the momentum equation. Thus, the fluid pressure amplitude to be written in terms of the radial displacement amplitude as

$$P_0 = \frac{\rho_f \omega^2 C_1}{k_r Z_n'(k_r r_1)} \tag{8}$$

where ρ_f is the fluid density. C_1 is the amplitude of vibration in the inner nanotube. Substituting Eq. (8) into Eq. (7), and using Eq. (6), we obtain

$$p_f = k_f(\omega, k_r) w_1, \qquad k_f(\omega, k_r) = \frac{\rho_f \omega^2 Z_n(k_r r)}{k_r Z_n'(k_r r)}. \tag{9}$$

DWNTs are regarded as nested SWNTs whose pressure between two adjacent nanotubes results from the vdW interaction. The vdW interaction energy potential, as a function of the interlayer spacing between the inner and outer nanotubes, can be estimated by the Lennard-Jones potential. Since the interlayer spacing of DWNTs is very close to equilibrium spacing, the initial vdW force remains zero for each of the tubes provided they deform coaxially. In case of small-amplitude vibration of CNTs, the interaction pressure between two adjacent nanotubes is assumed to be linear relative to the difference of their deflections in the radial direction. Therefore, the coupled equations of the pressure (p) in the Eq. (3) caused by the vdW interaction in DWNTs can be given by

$$\begin{aligned} p_1 &= p_f + c_{21}(w_2 - w_1) \\ p_2 &= c_{12}(w_1 - w_2) \end{aligned} \tag{10}$$

where w_1 and w_2 are the deflections in the inner and outer nanotubes, respectively.

In this simulation, the vdW interaction coefficient c_{ij} can be estimated as[22]

$$c_{ij} = \frac{\pi\varepsilon R_j \sigma^6}{a^4}\left[\frac{1001\sigma^6}{3} H_{ij}^{13} - \frac{1120}{9} H_{ij}^{7}\right], \tag{11}$$

where

$$H_{ij}^{m} = \left(R_i + R_j\right)^{-m} \int_0^{\pi/2} \frac{d\theta}{\left(1 - K_{ij}\cos^2\theta\right)^{m/2}}, \qquad (m = 7, 13), \tag{12}$$

and

$$K_{ij} = \frac{4R_i R_j}{\left(R_i + R_j\right)^2}. \tag{13}$$

where σ and ε are the vdW radius and the well depth of the Lennard-Jones potential, respectively.

Substituting Eq. (10) into Eq. (3), the coupled equations of the wave speed in DWNTs are written as

$$\begin{aligned} &L_A^1 w_1 + L_B^1\left[K k_f(\omega, k_r) w_1 + c_{21} K\left(w_2 - w_1\right)\right] = 0, \\ &L_A^2 w_2 + L_B^2\left[c_{12} K\left(w_1 - w_2\right)\right] = 0, \end{aligned} \tag{14}$$

By substituting Eqs. (7) and (9) into Eq. (14), the vibrational frequency in DWNTs can be determined by a nontrivial solution in Eq. (14) as

$$\begin{vmatrix} L_A^1(\omega, m, n) + K\left[k_f(\omega, k_r) - c_{21}\right] L_B^1(\omega, m, n) & c_{21} K L_B^1(\omega, m, n) \\ c_{12} K L_B^2(\omega, m, n) & L_A^2(\omega, m, n) - c_{12} K L_B^2(\omega, m, n) \end{vmatrix} = 0, \tag{15}$$

where L_A^j and L_B^j $(j = 1, 2)$ are the differential operators, which are given by Eqs. (2) and (4) for inner and outer tubes, respectively.

The amplitude ratio of the inner nanotube to the outer nanotube is given by

$$\frac{C_1}{C_2} = \frac{-c_{21} K L_B^1(\omega, m, n)}{L_A^1(\omega, m, n) + K\left[k(\omega, k_r) - c_{21}\right] L_B^1(\omega, m, n)}. \tag{16}$$

Ⅲ. NUMERICAL RESULTS AND DISCUSSION

Influences of fluid properties on the natural frequency in CNTs were investigated using the proposed method. In this simulation, the thickness of individual SWNT was assumed to be that of a graphite sheet with 0.34 nm. CNTs had an elastic modulus of 1 TPa, Poisson's ratio

of 0.27, and the density of 2.0 g/cm^3. The vdW parameters used in the Lennard-Jones potential are taken as $\varepsilon = 2.967\,\text{meV}$ and $\sigma = 0.34\,\text{nm}$ reported recently by Saito et al.[23] The inner and outer diameters of DWNTs are 2.2 nm and 3.0 nm, respectively.

Figure 2 shows the natural frequency of DWNTs as a function of nanotube aspect ratio. The following solution is obtained for low frequency vibrational modes of $m = n = 1$. In order to investigate the dependence of fluid parameters on the vibrational frequency, three types of filled fluids A, B and C are taken according to the fluid properties. The Fluids A and B have the same density, but not the same elastic modulus. The Fluids A and C have the different density but the same elastic modulus. As shown in Fig. 2, the vibrational frequencies in CNTs are largely affected by the fluid properties. The vibrational frequency shows logarithmically linear dependence on the aspect ratio of CNTs. Compared to the CNTs without fluid loading, the fluid-filled CNTs have higher vibrational frequency when the aspect ratio of CNTs is larger. However, the natural frequency exhibits a reversed trend in case of low aspect ratio of CNTs. The CNTs filled with high elastic modulus or low density fluids show larger vibrational frequency. The natural frequencies of CNTs with different vibrational modes are shown in Fig. 3 as a function of the elastic modulus. There is a logarithmically linear relation between the vibrational frequency and the elastic modulus.

For the CNTs filled with the Fluid A, the influences of vibrational mode on the frequency are shown in Fig. 4 as a function of nanotube aspect ratio. The vibrational frequency in CNTs decreases with an increase in the aspect ratio. But, the vibrational frequency increases increasing axial half-wave number. It can be found from Fig. 5 that the vibrational frequency of CNTs is in proportion to the axial half-wave number. However, the vibrational frequency of CNTs is hardly affected by the circumferential wave numbers (see Fig. 6). The value of vibrational frequency in CNTs with the aspect ratio 20 is around 32 GHz, which gives a high frequency response. Figure 7 shows the dependence of CNT diameter on the vibrational frequency. The vibrational frequency increases significantly with decreasing CNT diameter. It is seen that CNTs exhibit the vibrational frequency with near terahertz when CNTs have an extremely small diameter.

Figure 8 shows the vibration amplitude ratio of the inner tube to the outer tube. The amplitude ratios of the vibration are dependent on the circumferential wave numbers, but hardly affected by the axial half-wave number. The amplitude ratio of the inner to the outer nanotube is close to 1 when the CNTs have the low frequency vibrational mode of $m = n = 1$. This indicates that the vibrational models of CNTs are almost coaxial and that the deflection

of the inner to outer tubes has the same amplitude. For the circumferential wave number of $n \geq 2$, the vibrational displacement of the outer nanotube is larger than that of the inner nanotubes. The vibrational coupling amplitude rises with an increase in circumferential wave number.

Ⅳ. CONCLUSIONS

Vibrational analysis of fluid-filled double-walled carbon nanotubes is presented using wave propagation approach. Based on this theoretical approach, the influences of the fluid properties and the vibrational modes on the vibrational characteristics of carbon nanotubes are investigated in detail. The vibrational frequencies of the filled-fluid CNTs are largely affected by the fluid properties and the vibrational modes. The CNTs filled with high elastic modulus or low density fluids show high-frequency vibration. The natural vibrational frequency increases linearly with increasing axial half-wave number, but is insensitive to the circumferential wave numbers. The amplitude ratios of the vibration in the inner to the outer nanotube are dependent on the circumferential wave numbers, but hardly affected by the axial half-wave number.

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Figure captions

Figure 1 Geometry of nanotube and coordinate system

Figure 2 Vibrational frequency of DWNTs as a function of the aspect ratio. The properties of Fluid A: the elastic modulus of 1.0 GPa , the density of $1000\,\mathrm{kg/m^3}$; Fluid B: the elastic modulus of 0.1 GPa , density $1000\,\mathrm{kg/m^3}$; Fluid C: the elastic modulus of 1.0 GPa , density $500\,\mathrm{kg/m^3}$.

Figure 3 Relationship between the vibrational frequency and the elastic modulus (the fluid density: $1000\,\mathrm{kg/m^3}$; the aspect ratio: 20).

Figure 4 Relationship between the vibrational frequency and the aspect ratio. (Fluid A: the elastic modulus of 1.0 GPa , the density of $1000\,\mathrm{kg/m^3}$).

Figure 5 Variation of the vibrational frequency with the axial half-wave number (Fluid A: the elastic modulus of 1.0 GPa , the density of $1000\,\mathrm{kg/m^3}$; the aspect ratio of 20).

Figure 6 Variation of the vibrational frequency with the circumferential mode (Fluid A: the elastic modulus of 1.0 GPa , the density of $1000\,\mathrm{kg/m^3}$; the aspect ratio of 20).

Figure 7 Diameter dependence of the vibrational frequency for DWNTs (Fluid A: the elastic modulus of 1.0 GPa , the density of $1000\,\mathrm{kg/m^3}$; the aspect ratio of 20).

Figure 8. Amplitude ratio of the vibration in DWNTs of the inner tube to the outer tube (Fluid A: the elastic modulus of 1.0 GPa , the density of $1000\,\mathrm{kg/m^3}$; the aspect ratio of 20).

Figure 1 (T. Natsuki)

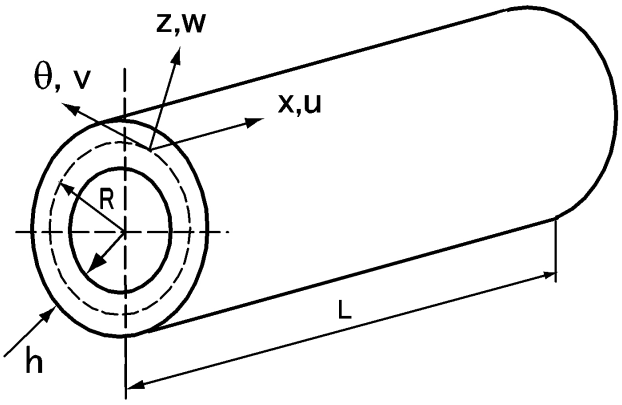
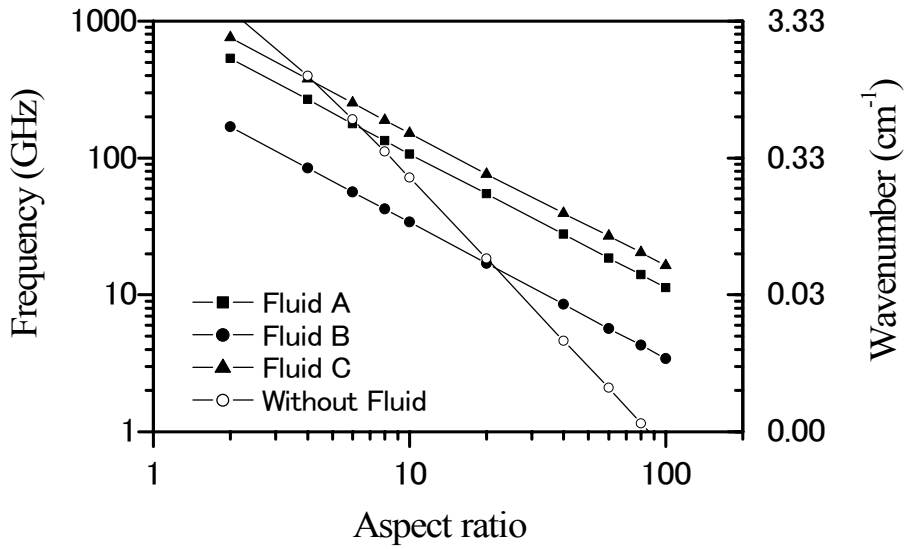


Fig.2 (T. Natsuki)



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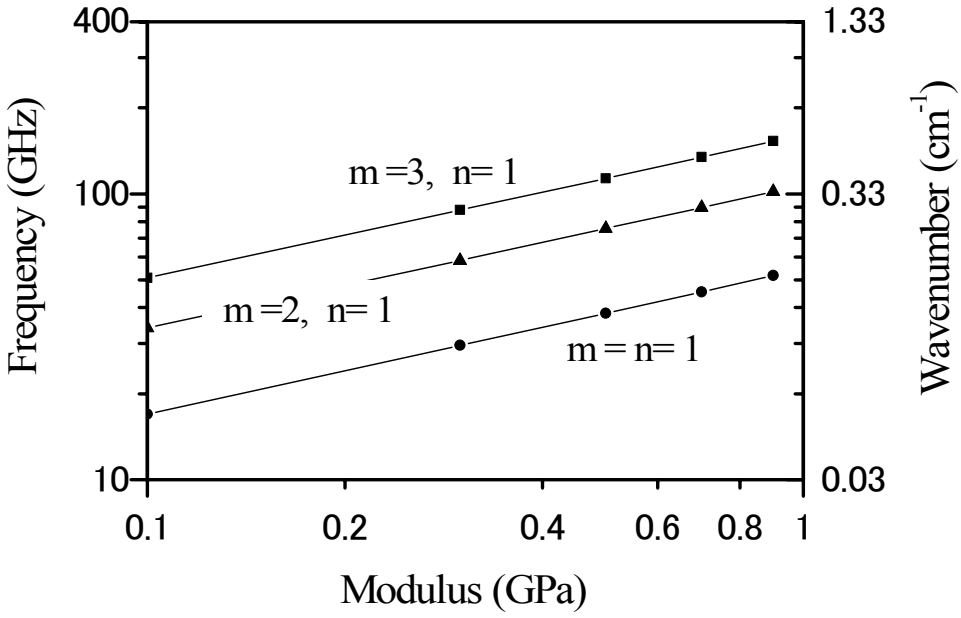

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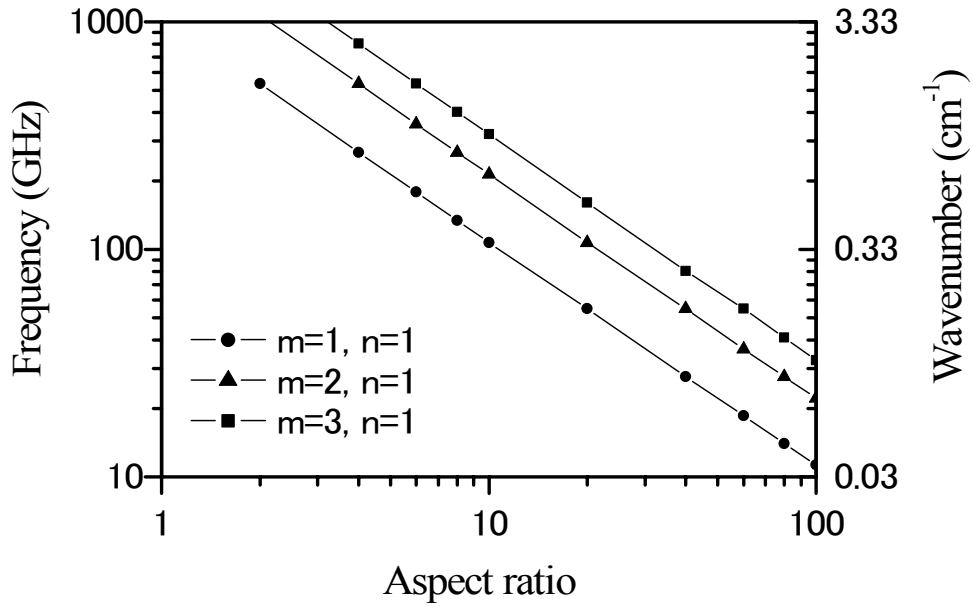

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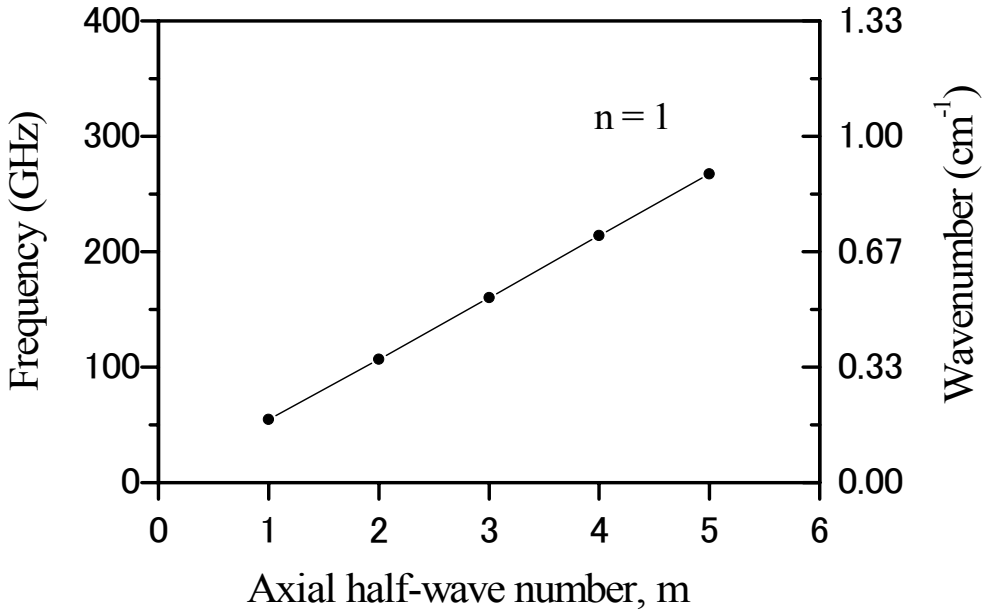

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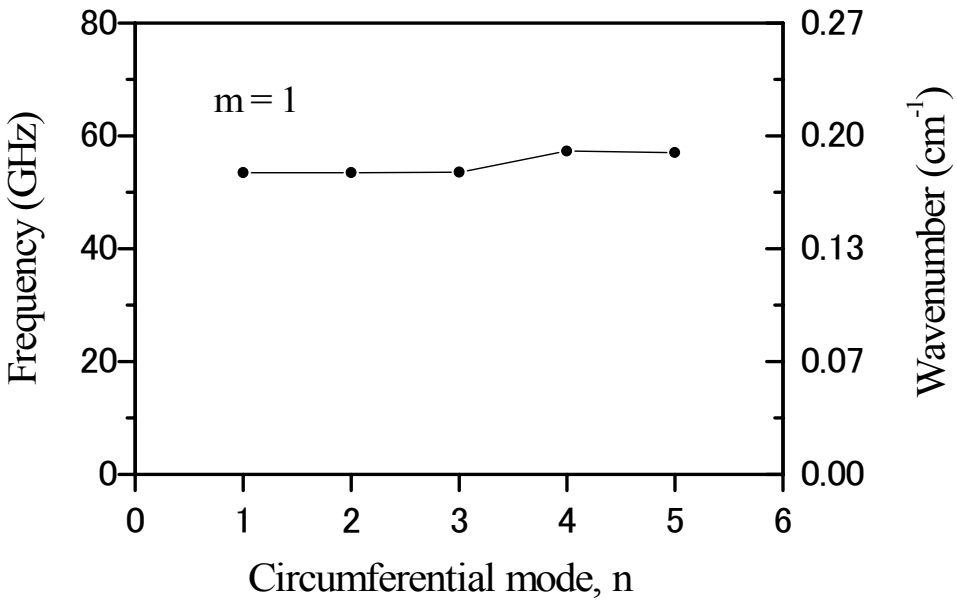

Fig.7 (T. Natsuki)

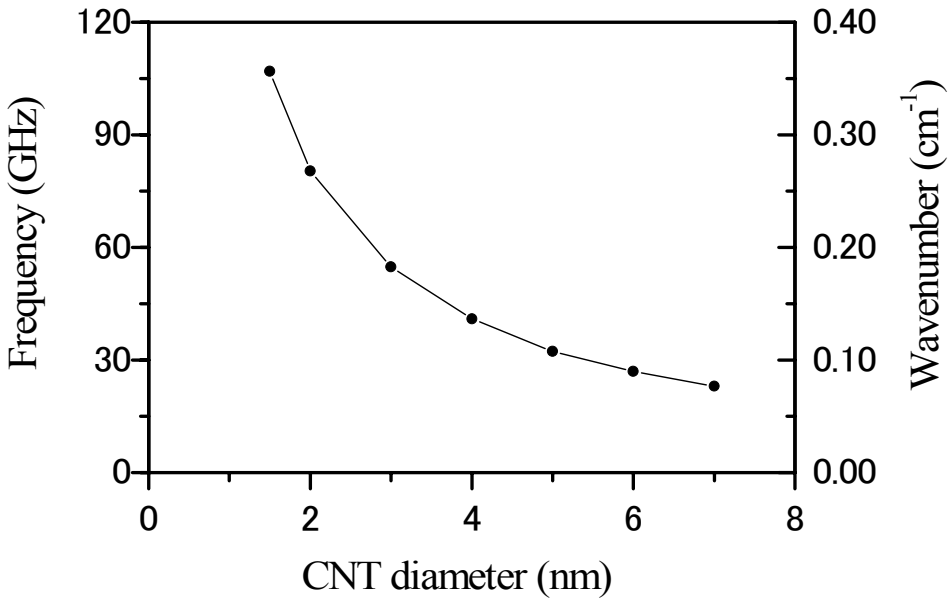

Fig.8 (T. Natsuki)