Investigation of wave propagation in architected uniform triangle mass center fractal nano-bio-filters based on microtubules

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ABSTRACT: Microtubules, polymer tubes stretched from the cell nucleus to the cell membrane, are the major parts of the cytoskeleton that provide the mechanical rigidity, organization, and shape retention for the cytoplasm of eukaryotic cells. These structures play a key role in some cellular processes such as cell division, intracellular transport, and the internal organization of cells. In all the above applications, the network structure of microtubules is the main reason for the importance of in-depth studies of their mechanical properties. In this paper, the propagation of elastic waves in periodic networks based on two-dimensional fractal microtubules of fixed mass-center triangles is analyzed. This study begins with the selection of a suitable beam model for a microtubule and examines the dynamic behavior of microtubules by creating periodic structures. To obtain dispersion curves, finite element models of microtubules and their networks are developed, and the bandgap equations are calculated based on Bloch's theory. The results show that depending on the topology of the selected unit cells as well as the considered periods, it is possible to design a frequency gap in specific ranges for the application of low and high-frequency bio-filters. This study helps researchers control or absorb some unwanted vibrations using periodic structures, and thanks to their better biocompatibility, these networks can be used in next-generation nanomechanical devices such as implantable biosensors.

1- Introduction

Nature has a unique complex of active bio-molecules developed during the centuries. Nowadays, our knowledge about nano-bio-structures is flourishing and with the development of new micro/nanofabrication techniques, the artificial synthesis of such bio-structures is becoming possible [1].

Microtubules are one of the very fascinating nano-bio-structures that are radially stretched from the cell nucleus to the cell membrane. They are the stiffest part of the cells tolerating the internal and external mechanical stresses. Hence, from the mechanical point of view, microtubules are the most important bio-polymer inside the cell. Koch et al. showed that it is possible to artificially synthesize microtubules and build small networks of them using optical tweezers [2]. The investigation of various mechanical behaviors of networked structures is an important research field these days [3, 4]. Hence, following the research by Koch et al. [2], in this work, we analyze wave propagation of architected uniform triangle mass center fractal nano-bio-filters based on microtubules using finite element method and Bloch's theorem [5]. The schematic representation of microtubules and their fractal structures studied in this work are shown in Fig. 1.

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2- Methodology

As shown in Fig. 2, microtubule elements have three degrees of freedom on each node, i. e. longitudinal translation (u), transverse translation (v), and bending (φ) about the z-axis.

According to Newton's second law, the governing equation of the in-plane motion of a microtubule is written as Eq. (1).

$$\left[M \right]_{6\times6} \begin{bmatrix} \ddot{u}_1 \\ \ddot{v}_1 \\ \ddot{\phi}_1 \\ \ddot{u}_2 \\ \ddot{v}_2 \\ \ddot{\phi}_2 \end{bmatrix} + \left[K \right]_{6\times6} \begin{bmatrix} u_1 \\ v_1 \\ \phi_1 \\ u_2 \\ v_2 \\ \phi_2 \end{bmatrix} = \begin{bmatrix} f_{1x} \\ f_{1y} \\ M_1 \\ f_{2x} \\ f_{2y} \\ M_2 \end{bmatrix} \quad (1)$$

where f_x, f_y, and M denote the axial force, transverse force and bending moment applied on each node. Also, $[M]_{6\times6}$ and $[K]_{6\times6}$ are the mass and stiffness matrices, respectively. The detailed formulations of these matrices [6] are presented in the full paper.
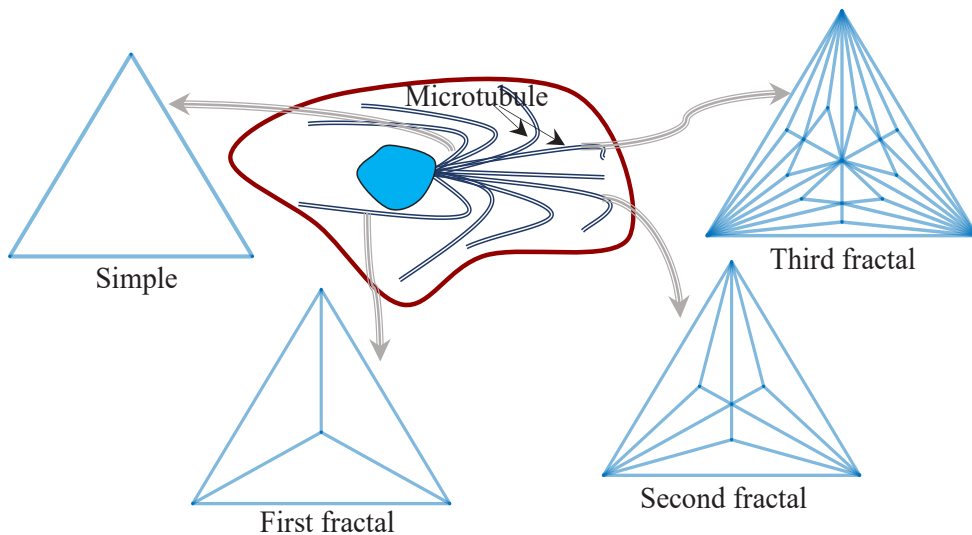
Fig. 1. Schematic representation of microtubules and their uniform triangle mass center fractal structures
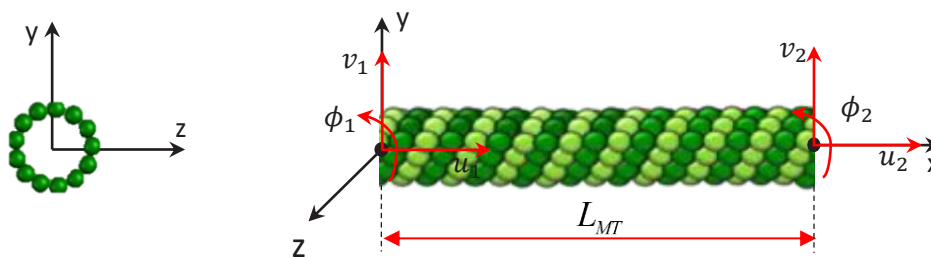

Fig. 2. Microtubule element and its degrees of freedom.

Via assembling the above elements into the unit cell of the networked structures in Fig. 1 and using the proper transformation matrices to transform the parameters from the local coordinate system to the global coordinate system, we can write the governing equation of the motion of the whole unit cell as Eq. (2).

$$[M]_{r \times r} \ddot{q}_r + [K]_{r \times r} q_r = f_r \qquad (2)$$

where r is the number of degrees of freedom of the unit cell and $\ddot{q}_r$, q_r , and f_r denote the acceleration, displacement, and force on each node, respectively. Eq. (2) is solved considering Bloch's theorem [5] and the dispersion curves of the periodic structures are obtained in the irreducible Brillouin zone [3].

3- Results ad Discussion

In this section, the results of the work are presented in the form of dispersion curves within the normalized frequency range $0 \leq \Omega \leq 5$. The frequencies are normalized by the fundamental frequency of a doubly clamped microtubule beam. The geometries and mechanical properties of the microtubules are presented in Table 1 [4].

Fig. 3 shows the dispersion curves of a periodic structure with the unit cell of the simple triangle made of microtubules. The dispersion curves in Fig. 3 have a local resonance bandgap blocking the waves in the shown frequency range.

Changing the structure of the simple triangle to the triangular first fractal without the change in the mass center of the unit cell leads to the dispersion curves of Fig. 4. As shown in this figure, adding more microtubules to the unit cell induces an additional bandgap at the expense of decreasing the width of the local resonance bandgap.

The dispersion curves of the second and third triangular fractals of microtubules are presented and analyzed in the main text of the full paper. However, the collective bandgap areas of the periodic structures studied in this work are compared in Fig. 5. According to this figure, the second fractal possesses the largest collective bandgap area.

4- Conclusions

This paper presented wave-propagation characteristics of architected uniform triangle mass center fractal nano-

Table 1. The geometries and mechanical properties of the microtubules [4].

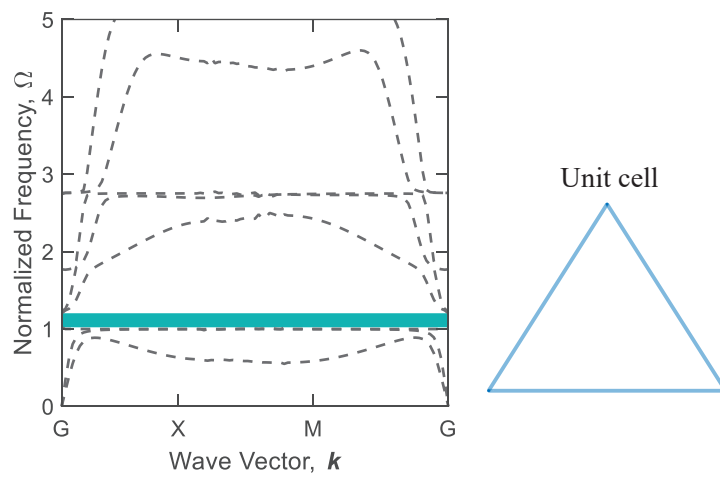| Geometries and mechanical properties	Numerical values
Length	1 µm
Inner diameter	16 nm
Outer diameter	25 nm
Elastic modulus	2 GPa
Poisson's ratio	0.3
Density	$1470 \frac{kg}{m^3}$

Fig. 3. Dispersion curves of a periodic structure with the unit cell of the simple triangle.
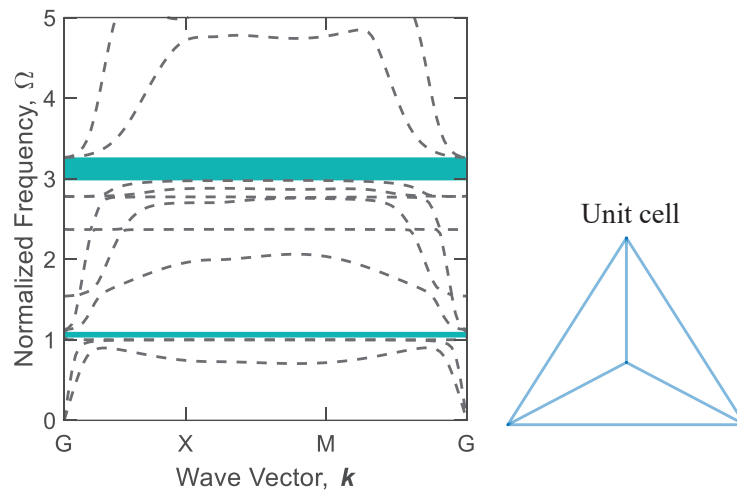

Fig. 4. Dispersion curves of a periodic structure with the unit cell of the first triangular fractal.

bio-filters based on microtubules. The zeroth, first, second, and third fractals were analyzed in the main manuscript and the results of the zeroth and first fractals were presented in this extended abstract. According to the results, the zeroth fractal has one bandgap but the first fractal has two. Also, the comparison of the collective bandgap areas revealed that the second fractal has the largest bandgap areas among all studied cases.
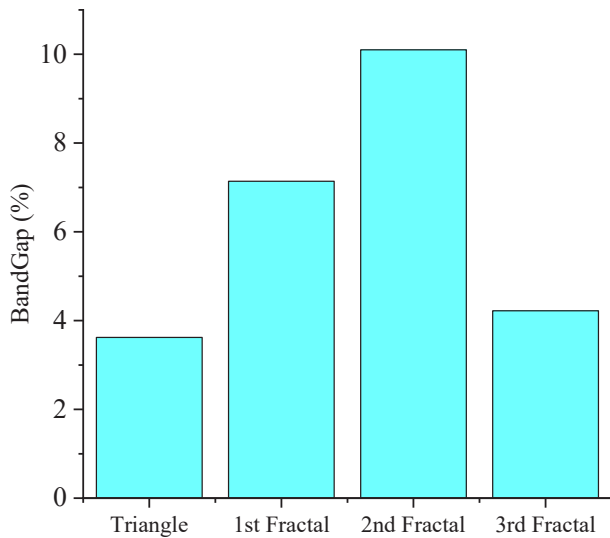
Fig. 5. Collective bandgap areas of the periodic structures studied in this work.

References

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