Numerical Study of Hollow-Walled Nanotubes Under Static Compression

ELZA M. M. FONSECA[1], CARLOS AURELIO ANDREUCCI[2]

[1]Department of Mechanical Engineering,
Polytechnic of Porto,
Rua Dr. António Bernardino de Almeida, 431, 4249-015 Porto,
PORTUGAL

[2]Department of Biomedical Engineering,
American International University of Koweit,
Saad Al Abdullah, Al Jahra, Koweit
KOWEIT

Abstract: In this work, different hollow-walled titanium Ti6Al4V nanotubes in chiral structures are modelled using the finite element method. Nine numerical models of chirality C (*n*, *m*) types were built. The structure of the titanium nanotube is named chiral and expressed by a vector C, depending on two base vectors, where *n* and *m* indicate the number of unit vectors in two directions, called the indices of the nanotube. The chiral designation is from the chirality as an essential geometric property of a mirror asymmetry used in several branches of science. In this work, several chirality measures have been computationally tested using the finite element method to quantify their characteristics and the physical behaviour.

Key-Words: - Finite Element Method, Hollow-Walled, Nanotube, Static Analysis.

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1 Introduction

The primary benefits of titanium dioxide (TiO_2) nanotube structures can be enumerated as follows: a 3-dimensional (3D) repetitive structure, an extensive surface area, and elevated mechanical stability. Moreover, the facilitated tissue attachment that characterises these structures has the potential to enhance bioactivity, a critical consideration in the biomedical field [1].

TiO_2 nanotubes possess a low elastic modulus of 36 to 43 GPa, a range that closely resembles that of natural bones [2]. It has been documented that TiO_2 nanotube arrays enhance cellular activity and significantly accelerate the proliferation of osteoblast cells [3].

The natural tissues of the human body are assembled from nanomodules; therefore, from a biomimetic perspective, nanostructures should exhibit enhanced biological activity. TiO_2 nanotubes demonstrate distinctive physical and chemical properties, attributable to their elastic modulus, substantial specific surface area, and regular hollow structure, which is analogous to that of bone tissue [4].

The application of oxidation technologies has been demonstrated to enhance the natural oxide formed on the surface of titanium. The oxide layer is typically composed of polymorphs of titanium oxide, including anatase, rutile, and brookite. Rutile has been identified as the most stable form of titanium oxide [5].

Contemporary plasma electrolytic technologies represent a progression from traditional anodising, utilising higher voltages to produce oxide ceramic coatings on Ti surfaces [6].

The morphology of materials with spatial complexity can significantly influence their physical properties, underscoring the indispensability of morphological characterisation in establishing structure-property relationships.

The process of biological surface modification is versatile, allowing for the deposition of a wide range of organic biological coating materials. Consequently, biological modification has evolved into a subject of extensive research in the field of implant surface modification.

Plasma Electrolytic Oxidation (PEO) and anodisation are cutting-edge techniques for surface treatment of titanium and its alloys. These materials hold significant interest in advanced engineering applications because of their high strength-to-weight ratio, corrosion resistance, biocompatibility, and other characteristics. During the processes of PEO and microarc oxidation (MAO), an anodic potential is applied between a metallic substrate and a counter electrode in aqueous electrolytes to form anodic oxide coatings on the surface of metals, including aluminium, magnesium, titanium, zirconium, and niobium [7].

The TiO_2 nanotube-coated surfaces exhibited hydrophobic properties in comparison to the plain CP-Ti surfaces. However, the wettability of the coating surfaces produced at high voltages exhibited enhanced properties in comparison to the surfaces produced at low voltages [8].

The protein adsorption capacity of the TiO_2 surface is indicative of its biological characteristics. Authors [9] evaluated a series of TiO_2 samples immersed in a solution containing proteins (fetal bovine serum). They found that the amount of protein adsorbed by the new type of titanate nanotube (TNT) coating samples was significantly increased compared to titanium surfaces without PEO, indicating that the TiO_2 nanotube structure facilitates protein adsorption.

The utilisation of porous implants is a well-established procedure that facilitates the ingrowth of cells and subsequent colonisation of the implant. The ideal porous implant is characterised by a 3D architecture that facilitates the rapid migration of incoming cells without inducing a substantial pro-inflammatory response from immune cells [10].

The controlled oxidation of surfaces on porous titanium structures exerts a direct effect on the cellular attachment and migration through the porous and nanotubes on the surface of those implants.

Different researchers have been studying the use of nanoparticles in consumer products, which are developed and manufactured [11]. Their development has been increased and successful in different areas, from textiles, electrical, and biosensors, among others, where so many companies worldwide work with nanoscale materials [12].

To obtain knowledge about the mechanical behaviour of nanotubes, different numerical models, using the finite element method, are presented in this study. Hollow-walled nanotubes are of particular interest as channel materials due to their unique structure and excellent characteristics.

2 Materials and Methods

In this work, different single-walled titanium [13] nanotubes in chiral structures are modelled. The nanotubes are vertical tubular structures with a uniform diameter. A total of nine mathematical models were constructed, each of the chirality C (*n*, *m*) type.

The structure of the titanium nanotube is named chiral and expressed by vector C [14], depending on two base vectors, where n and m indicate the number of unit vectors in two directions, called the indices of the nanotube.

The chiral designation is from the chirality as an essential geometric property of a mirror asymmetry used in several branches of science. Several chirality measures have been tested to quantify this property and to correlate them with physical and chemical properties [14].

Figure 1 shows all nine defined structures, with different lengths, obtained with the Nanotube Modeler, a program which generates x-y-z coordinates for Nanotubes [15].

This program is based on topological algebra as a continuous function of carbon rings [15]. The basis of the modeller structure is two nanotubes that can be connected, creating bonds between frontier atoms and adding new carbon atoms as required.

The nanotube structure is formed by rolling up into a cylinder, defined by the vector connecting two equivalent carbon positions that are matched together after the rolling, named the chiral vector C [14-15].

According to the chiral angle formed between the chiral vector C, the nanotubes are described in three types: zigzag type C (*n*, 0) with chiral angle equal to 0°; armchair type C (*n*, *n*) and angle equal to 30°, both types showing the higher of symmetry; and chiral C (*n*, *m*) without symmetry.

In this work, three-dimensional Zigzag chiral types, with different chiral index *n*=8, 10 and 12, different tube lengths (10, 20 and 30 A), with the same bond length equal to 1.241 A and the tube diameter equal to 1.47 A, were considered.

According to the geometries created, the atoms are represented by key points and their respective coordinates, and the lines are the connections between each one. The atomistic model generates the respective mesh to be used in the ANSYS® program, according to the previous use of a parametric program in APDL language (Ansys Parametric Design Language).

The main objective of the study is to examine the compressive effect of different samples in titanium nanotubes and their mechanical behaviour.

The numerical program ANSYS®, based on the finite element method, was used to identify the maximum compressive load which could be applied to the structure.

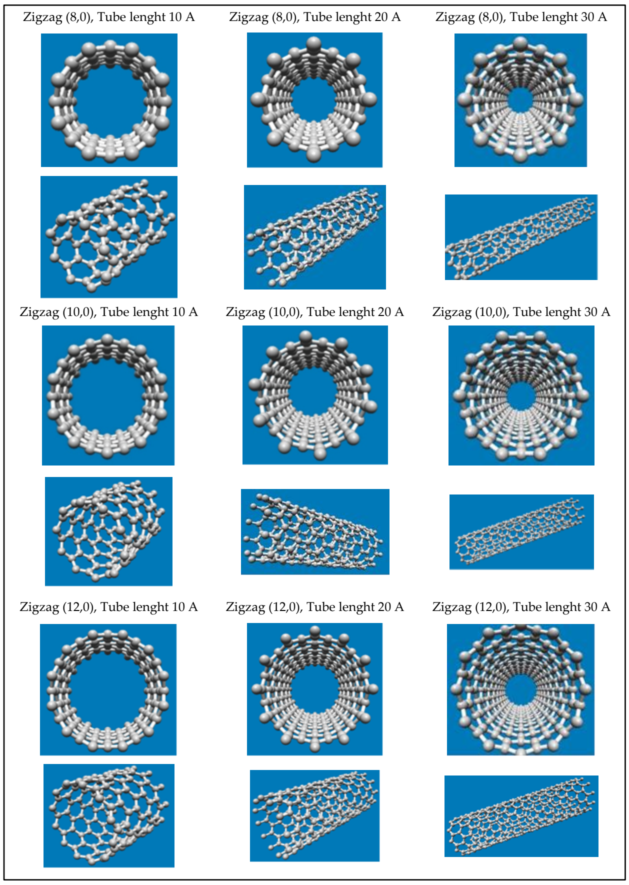

Fig. 1: Nanotube with different Zigzag chiral structure types.

The finite element used in the mesh was BEAM 188 with 2 nodes and 6 degrees of freedom per node. The boundary conditions for each nanotube are fixed on one side, and one incremental compressive load is applied on the other.

A structural and incremental analysis was performed. The maximum compressive load, along with its corresponding displacement and strains, were obtained.

The mechanical properties of the titanium Ti6Al4V nanotube are determined from other references [13] with the Young modulus equal to 43 GPa, Poisson ratio equal to 0.3 and yield stress of 384 MPa.

3 Numerical Results and Discussion

The numerical results using the finite element method allow us to verify the behaviour under a compressive force for a titanium nanotube of Zigzag type.

The compressive force was incremental and linearly applied until it reached a value in nanonewton (nN). Figures 2 to 4 show the results for chiral structures nanotubes Zigzag (8,0), (10,0) and (12,0), respectively, with the mesh, the axial displacement in Angstrom (A) and the calculated strain.

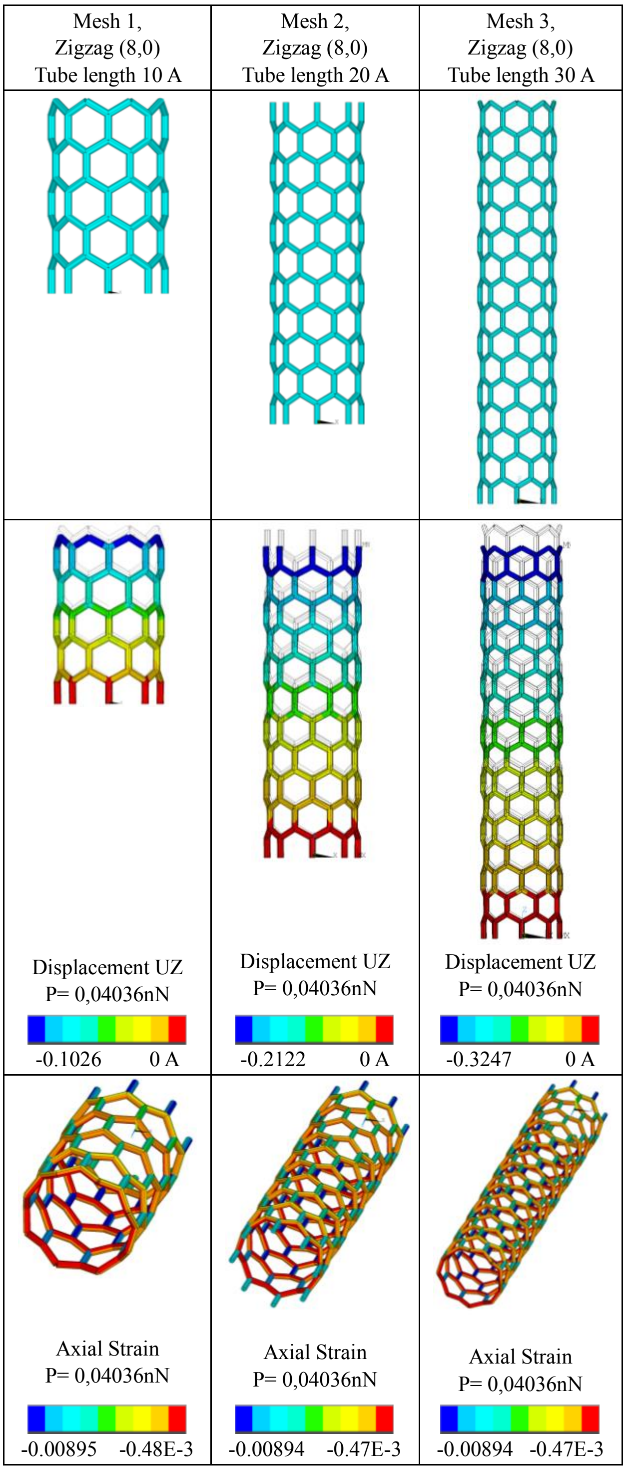

Fig. 2: Numerical results of the nanotube structures with different Zigzag (8,0) chiral types.

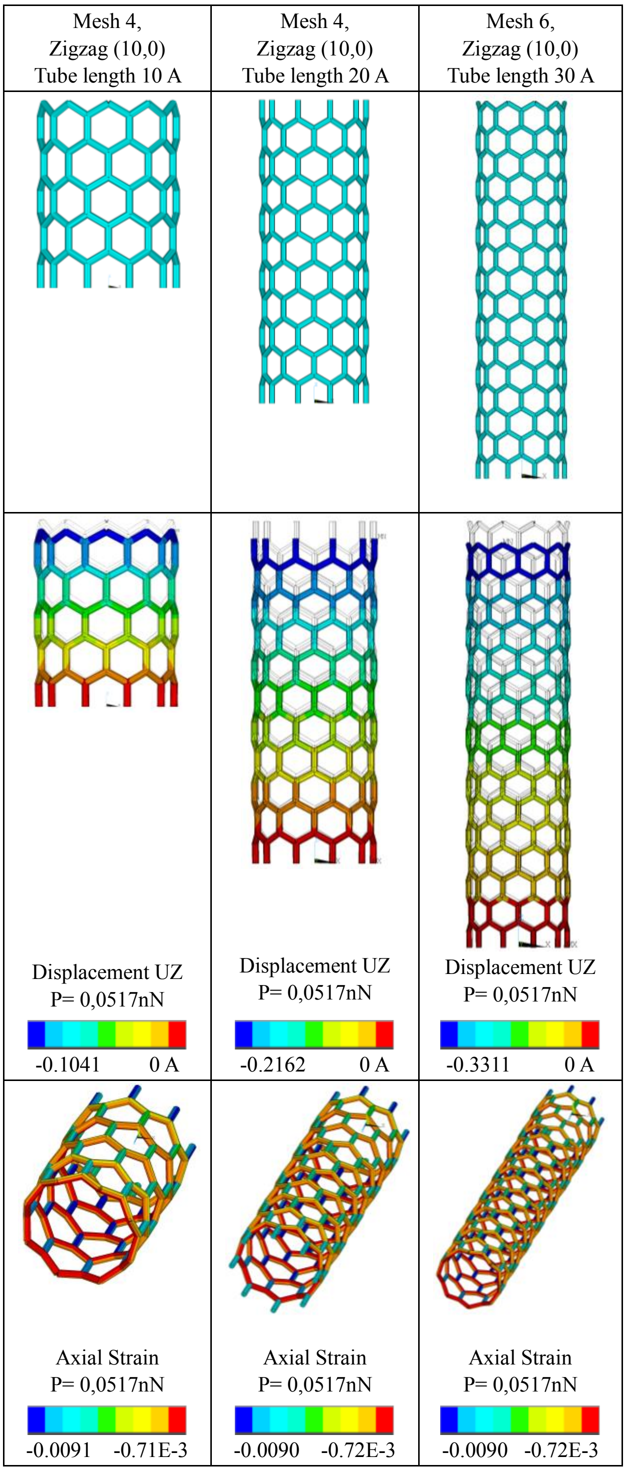

Fig. 3: Numerical results of the nanotube structures with different Zigzag (10,0) chiral types.

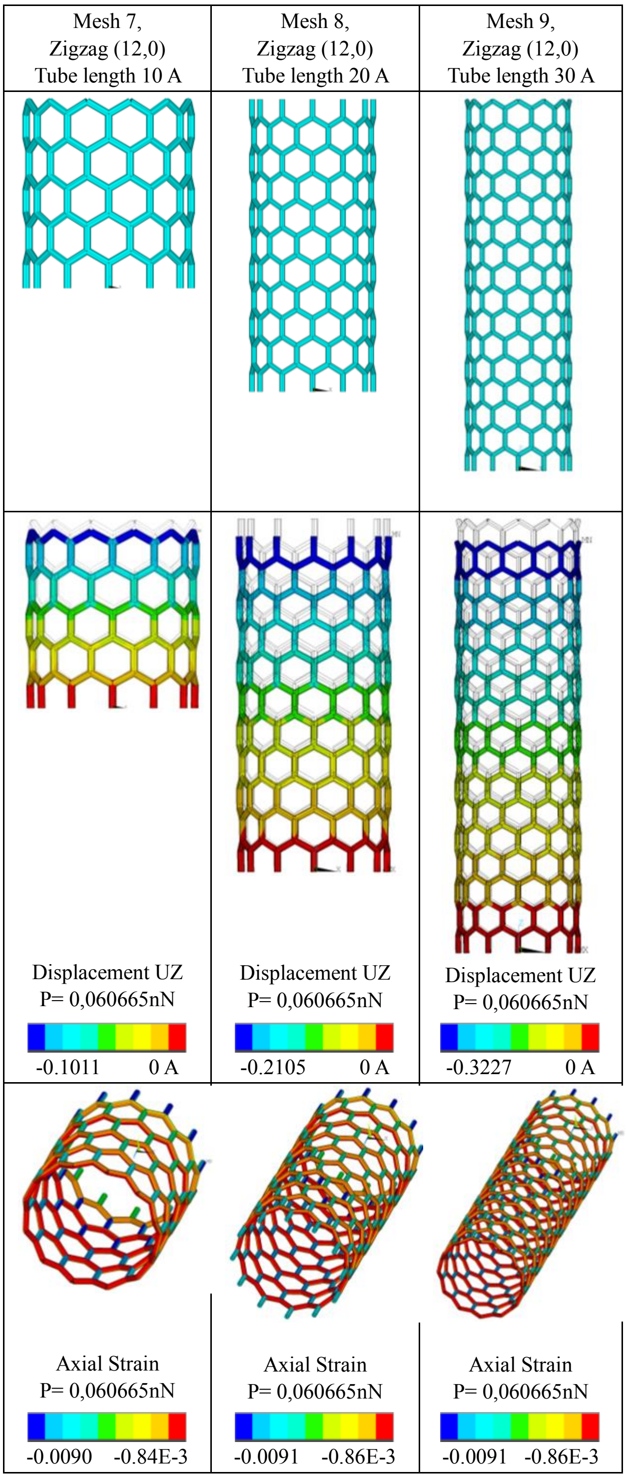

Fig. 4: Numerical results of the nanotube structures with different Zigzag (12,0) chiral types.

All the other chiral zigzag nanotubes referred to in Figure 1 were also analysed, and the results are presented in Table 1.

Table 1 shows the general conclusions of the mechanical behaviour of all Zigzag chiral types, related to the maximum compressive load and the obtained level of strain and axial displacement.

Table 1: Maximum compressive load and mechanical behaviour in all different Zigzag chiral types.

Maximum compressive load P= 0.04036nN	Zigzag (8,0) Tube length 10A	Zigzag (8,0) Tube length 20A	Zigzag (8,0) Tube length 30A
	Uz= 0.102592A	Uz= 0.212243A	Uz= 0.324738A
	Strain=- 0.008949	Strain=- 0.008938	Strain=- 0.008938
Maximum compressive load P= 0.0517nN	Zigzag (10,0) Tube length 10A	Zigzag (10,0) Tube length 20A	Zigzag (10,0) Tube length 30A
	Uz= 0.104069A	Uz= 0.216155A	Uz= 0.33111A
	Strain=- 0.009046	Strain=- 0.009037	Strain=- 0.009037
Maximum compressive load P= 0.060665nN	Zigzag (12,0) Tube length 10A	Zigzag (12,0) Tube length 20A	Zigzag (12,0) Tube length 30A
	Uz= 0.101136A	Uz= 0.210507A	Uz= 0.322663A
	Strain=- 0.009049	Strain=- 0.009049	Strain=- 0.009055

The numerical results allow us to draw the following main conclusions:

-For each Chirality with the same number of cells and the same maximum compression load, the displacement increases with the increase in the tube length, as well as the axial strain.

-The maximum compressive load increases with the number of Chirality cells, being independent of the tube length.

-From Chirality Zigzag (8.0) to (10.0), there was an increase in displacement and strain.

-From Chirality Zigzag (10.0) to (12.0), the displacement and strain are almost the same.

Table 1 quantitatively confirms expected mechanical behaviors: the maximum compressive load is proportional to the chiral index *n*, demonstrating that transversal stiffness increases with cell number. On the other hand, axial displacement and strain are dependent exclusively on tube length. However, the displacement and strain values are almost the same when transitioning from Chirality Zigzag (10,0) to Chirality Zigzag (12,0), despite an increase in maximum compressive load, suggesting a possible numerical artifact or material property limit that permits deeper discussion for future work using a different material behavior for a full nonlinear structural analysis. The used boundary conditions or the finite element convergence for higher chiral indices needs to be continued investigated.

The initial goal with this work was to understand the influence of cell arrangements and predict nanoscale mechanical response. In future work other finite element types will be chosen to accurately the discrete atomic interactions that define chiral mechanics and to obtain more conclusions.

4 Conclusion

The presented numerical method allows the prediction of the nanoscale mechanical response of nanotubes in compression and is useful to understand the influence of the cell arrangements obtained according to their behaviour.

Anodic oxidation technology is an important tool to prepare biomimetic TiO_2 nanotubes on the surface of Ti6Al4V. The nanotubes formed a series of vertical tubular structures with a uniform diameter. This results in improved roughness and biomimetic properties of titanium, such as those of trabecular bone, as well as enhanced corrosion resistance.

In particular, the TiO_2 nanotube structure shows a propensity for protein adsorption, thus demonstrating favourable biocompatibility, bioactivity and potential for clinical application.

The computational method used thus allows the prediction of the nanoscale mechanical response of the nanotubes, being useful to understand the influence of the cellular arrangements to be obtained by the anodization technology, as future work in the continuation of development. Different chiral structure types can be studied using other configurations.

Considering the current knowledge on the growth mechanism of hollow-walled nanotubes, we would say that current approaches are not yet fully undeveloped.

There is still a long way to go to achieve the selective production of hollow-walled nanotubes by bulk chirality.

Major efforts to develop advanced equipment, in situ characterisation and computational models are essential to address these fundamental challenges.

References:

[1] Nabavi, H.F.; Aliofkhazraei, M. "Morphology, composition, and electrochemical properties of bioactive-TiO2/HA on CP-Ti and Ti6Al4V substrates fabricated by alkali treatment of hybrid plasma electrolytic oxidation process (estimation of porosity from EIS results)," *Surf. Coat. Technol*. vol.375, pp.266–291, 2019.

[2] Macák JM, Tsuchiya H, Schmuki P. "High-aspect-ratio TiO2 nanotubes by anodization

of titanium," *Angew Chem Int Ed Engl*. vol.44(14), pp.2100-2102, 2005. doi:10.1002/anie.200462459.

[3] Lu, H.F.; Li, F.; Liu, G.; Chen, Z.G.; Wang, D.W.; Fang, H.T.; Lu, G.Q.; Jiang, Z.H.; Cheng, H.M. "Amorphous TiO2 nanotube arrays for low-temperature oxygen sensors," *Nanotechnology*, vol.19(40), 405504, 2008.

[4] Zheng, H.; Xu, L.; Jiao, Y.; Xia, Y.; Wu, X.; Lu, K.; Zhang, P.; Zhao, Q.; Zhang, L.; Ni, X. "Fabrication and surface characterization of titanium dioxide nanotubes on titanium implants," *Front. Mater*. vol.10, 1325997, 2023. doi:10.3389/fmats.2023.1325997.

[5] Diebold, U. "The surface science of titanium dioxide," *Surf. Sci. Rep*. vol.48(5-8), pp.53–229, 2003.

[6] Pesode, P.; Barve, S. "Surface modification of titanium and titanium alloy by plasma electrolytic oxidation process for biomedical applications: A review," *Mater. Today: Proc*. vol.46, pp.594–602, 2021.

[7] Geetha, M.; Singh, A.K.; Asokamani, R.; Gogia, A.K. "Ti based biomaterials, the ultimate choice for orthopedic implants—a review," *Prog. Mater. Sci.* vol.54(3), pp.397–425, 2009. doi:10.1016/j.apsadv.2021.100121.

[8] Zheng, H.; Xu, L.; Jiao, Y.; Xia, Y.; Wu, X.; Lu, K.; Zhang, P.; Zhao, Q.; Zhang, L.; Ni, X. "Fabrication and surface characterization of titanium dioxide nanotubes on titanium implants," *Front. Mater*. vol.10, 1325997, 2023. doi:10.3389/fmats.2023.1325997.

[9] Yang, K.; Shi, J.; Wang, L.; Chen, Y.; Liang, C.; Yang, L.; Wang, L.-N. "Bacterial anti-adhesion surface design: Surface patterning, roughness and wettability: A review," J. *Mater. Sci. Technol*. vol.99, pp.82–100, 2022. doi:10.1016/j.jmst.2021.05.028.

[10] Chaves, R.R.; Fanton, L.; Figueiredo, R.S.; Caram, R.; Cremasco, A. "Influence of anodically grown TiO2 nanotubes on shear strength and fatigue behavior of pure titanium,". *Surf. Coat. Technol*. vol.494, 131358, 2024. doi:10.1016/j.surfcoat.2024.131358.

[11] Maryam Subalya1; Rajeeva Voleti; D. Alexander Wait. "The Effects of Different Solid Content Carbon Nanotubes and Silver Quantum Dots on Potential Toxicity to Plants through Direct Effects on Carbon and Light Reactions of Photosynthesis,''. *WSEAS TRANSACTIONS on ELECTRONICS*, vol. 13, pp.11-18. 2022. doi:10.37394/232017.2022.13.2

[12] Mark J. Schulz; Sung Yong Kim; Ashley Kubley; David Mast; Vesselin Shanov. "Nanotube Sheet and Yarn Manufacturing and Commercialization,''. *WSEAS TRANSACTIONS on BUSINESS and ECONOMICS*, vol.18, pp.1149-1163, 2021. doi:10.37394/23207.2021.18.108.

[13] Quan, U.; Drescher, P.; Zhang, F.; Burkel, E.; Seitz, H. "Cellular Ti6Al4V with Carbon Nanotube-Like Structures Fabricated by Selective Electron Beam Melting," *Rapid Prototyping J*., vol. 20(6), pp.541–550, 2014. doi:10.1108/RPJ-05-2013-0050

[14] Cha, M.; Ma, J.; Kim, J.-Y.; Emre, E.S.T.; Kotov, N.A. "Graph-Theoretical Chirality Measure and Chirality–Property Relations for Chemical Structures with Multiscale Mirror Asymmetries," *Chirality*, vol.36(6), e23678, 2024. doi:10.1002/chir.23678.

[15] Melchor, S.; Dobado, J.A. "CoNTub: An Algorithm for Connecting Two Arbitrary Carbon Nanotubes," J. Chem. *Inf. Comput. Sci*., vol.44(5), pp.1639–1646, 2004. doi:10.1021/ci049857w.

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The authors have no conflicts of interest to declare that are relevant to the content of this article.