



Finite Element Analysis of the Effect of Carbon Nanotube Content on the Compressive Properties of Zirconia Nanocomposites

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ABSTRACT

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This work continues the assessment of the application of carbon nanotubes (CNTs) mixed with zirconia (ZrO_2). The study examined the compressive, bending, and bond strengths of samples containing and lacking carbon nanotubes. Zirconia carbon nanotubes (ZrO_2) in the concentrations of 0.00 %, 0.01 %, 0.02 %, 0.03 %, 0.04 %, and 0.05 % were the subjects of six mixtures whose resistance was measured. The results were analyzed using the finite element method with the ANSYS 15.0 program. ANSYS 15.0 software is used to analyze compressive and bending loads as well as the conventional zirconia model. Showcase the advantages of moderately utilizing carbon nanotubes. Zirconia's mechanical properties can be improved more effectively by mineral/chemical mixtures or fibers without the issues related to carbon nanotube dispersion. Provide evidence of the advantages of moderately utilizing carbon nanotubes. Without the issues related to carbon nanotube dispersion or the health hazards of handling Nanomaterials, zirconia's mechanical properties can be improved more effectively by mineral/chemical mixtures or fibers. The maximum and ideal load for the load was found to be 163.5 MPa, which was approved in all tests after the six models were finished with their designs in the ANSYS program. This was based on the von mises stress value and the maximum shear stress value less than the yield strength of the basic material used. After making numerous attempts, this load was selected by increasing the load by a specific percentage until it reached the ideal load, at which point the original model was able to support the load without experiencing any problems. The results of the ANSYS program were compared and examined, and they showed that the models' resistance to deformations, displacements, stresses, and various strains greatly increased when carbon nanotubes were added. By adding more carbon nanotubes, those models will be more resilient to the strains and deformations caused by compressive loads. The deformation rate decreased by 60%, which was a very noticeable decrease, especially in the sixth model where the carbon percentage was 5%.

1. INTRODUCTION

Owing to their exceptional potential and distinct characteristics, ceramic matrix composites offer a new generation of technically advanced applications with exceptional efficiency. Thanks to their strength, light weight, and exceptional resistance to wear, ceramic matrix composites are a great class of materials for use in great tribological applications, aerospace engineering (think hot structures), and automotive applications (think oxygen sensors and brake systems) [1-5].

Furthermore, ceramic materials have a strong reputation for being chemically inert, resistant to corrosion, strong, and thermally stable, which makes them ideal for applications that involve exposure to high temperatures or harsh environmental conditions. Low density ceramic materials with high wear and break resistance are needed in related industries like metallurgy and chemical to use them in cutting-edge applications [6-8]. Well-known biomaterials are ceramics

based on the simultaneous presence of diopside ($CaMg(SiO_3)_2$) and wollastonite ($CaSiO_3$). The majority of the experiences are related to glass-ceramics from the regulated crystallization of glasses with B_2O_3 , Na_2O , CaF_2 , and P_2O_5 additives that belong to the $CaO-MgO-SiO_2$ system [9-11]. However, recent studies have shown the high bioactivity and biocompatibility of ceramics based only on the two silicate phases (in particular, based on eutectic point of the pseudo binary $CaSiO_2-CaMg(SiO_3)_2$ system [12]. The additives may cause the formation of additional phases, such as fluorapatite [11]. One of the most extensively studied and technologically resilient ceramic materials utilized in numerous applications are ZrO_2 -based nanocomposites. Highly ionic conductivity, low density, chemical inertness, good wear resistance, high mechanical strength, and stability at elevated temperatures are just a few of the significant properties of ZrO_2 that have made it widely applicable in a variety of difficult structural, tribological, and multifunctional applications [13, 14]. Common uses are made to withstand challenging conditions and to meet the growing

global demand for clean energy. This can be achieved directly through the use of electrochemical power generation, as in the case of solid oxide fuel cell (SOFC) devices, or indirectly through the use of engines' thermal barrier layer, which guarantees that customers will be able to purchase inexpensive electricity because of the motor's high efficiency [15]. Further significant uses are in the domain of dental implants and load-bearing prostheses [16], where mechanical characteristics are crucial [17]. The first significant advancement in the synthesis and characterization of various structures containing zirconia nanotubes (ZNTs) was reported in 1997 [18]. Single-walled Zirconia nanotubes (SWZNT) have been synthesized and characterized using a variety of techniques, including hydrothermal treatments [19], the sol-gel method [20], anodization [21], bottom-up synthesis by impregnation [22], template-assisted depositions [23], and others. Numerous experimental studies [18, 24-26]. Determined a number of ZNT's physical, thermal, optical, electrical, and other properties. The scientific communities have been very interested in carbon nanotubes (CNTs) since their discovery [27], as evidenced by [28, 29]. These days, it is possible to produce large amounts of carbon nanotubes through the pyrolysis of hydrocarbons [30] or arc discharge [31]. Efficient growth of carbon nanotubes in terms of length, diameter, and straightness is crucial for prospective uses as well as in-depth property characterization. The direct pyrolysis of hydrocarbon gas to create insulated carbon nanotubes could be one new

technological advancement. Using atomic force microscopy or transmission electron microscopy, numerous studies on physical properties, including flexural stiffness [32] and Young's modulus [33], have been conducted to date. Single-walled zirconia nanotube (SWZNT) properties have already been the subject of numerous simulations; however, these studies were limited to their physical and chemical aspects, including surface adsorption and diffusion, phonon dispersion, and atomic structures [34-42]. The ANSAS program will be used to run finite element method simulations on the mechanical properties (compressive loads, bending loads) of SWZNTs. For this study, ratios (Zirconia (ZrO_2) with carbon nanotubes in the concentrations of 0.00%, 0.01%, 0.02%, 0.03%, 0.04%, and 0.05%) will be used to create SWZNT structural models, which will then be subjected to various mechanical simulation forces. Lastly, an analysis and discussion of the deformations, stresses, and strains seen in SWZNT will be conducted.

2. MATERIALS USED

A total of twelve mathematical models were constructed, six for bending tests and six for compression tests. The first model was composed entirely of zirconia, while the other five models, as indicated in Table 1, included varying amounts of Nano carbon mixed with zirconia.

Table 1. Ratios of zirconia and carbon added to it in various models [43-47]

Model	Materials Friction Weight	Density, ρ , (g/mm ³)	Weight, g	Volume, mm ³	Volume Fractions	Modulus of Elasticity, E , (GPa)	Passion's Ratio	Tensile Strength MPa	Yield Strength MPa
Model - 1	Zirconia, (ZrO_2)	0.005832	3.5192	603.429	1.00	200	0.32	330	230
Model - 2	Zirconia & Carbon Nanotubes	Zirconia; (99%)	0.005832	2.6135	448.131	0.74	200	330	230
		Carbon Nanotubes; (1%)	0.00017	0.0264	155.288	0.26	1200	150000	102000
Model - 3	Zirconia & Carbon Nanotubes	Zirconia; (98%)	0.005832	2.0700	354.931	0.59	200	330	230
		Carbon Nanotubes; (2%)	0.00017	0.0422	248.494	0.41	1200	150000	102000
Model - 4	Zirconia & Carbon Nanotubes	Zirconia; (97%)	0.005832	1.7101	293.229	0.49	200	330	230
		Carbon Nanotubes; (3%)	0.00017	0.0529	311.171	0.51	1200	150000	102000
Model - 5	Zirconia & Carbon Nanotubes	Zirconia; (96%)	0.005832	1.4484	248.362	0.41	200	330	230
		Carbon Nanotubes; (4%)	0.00017	0.0604	355.012	0.59	1200	150000	102000
Model - 6	Zirconia & Carbon Nanotubes	Zirconia; (95%)	0.005832	1.3167	225.772	0.36	200	330	230
		Carbon Nanotubes; (5%)	0.00017	0.0693	407.647	0.64	1200	150000	102000

Table 2. The mechanical characteristics of composite materials produced by the software Mathcad 15

Models	Materials	K	E, GPa	G, GPa	μ
Model - 1	Zirconia, (ZrO_2)	-----	200	76	0.32
Model - 2	Zirconia & Carbon Nanotubes 74% - 26%	0.375	265	99.98	0.325
Model - 3	Zirconia & Carbon Nanotubes 59% - 41%	0.431	330.2	124.3	0.328
Model - 4	Zirconia & Carbon Nanotubes 0.49% - 0.51%	0.469	384.9	144.7	0.330
Model - 5	Zirconia & Carbon Nanotubes 41% - 59%	0.499	435.1	163.4	0.332
Model - 6	Zirconia & Carbon Nanotubes 26% - 74%	0.518	524	195.3	0.342

Table 3. Results of compression deformations, stresses and strain

Model	Maximum Comp. Deformations (mm)				Maximum Stresses Compressive (MPa)												Maximum Strains Compressive (μe)							
	Ux	Uy	Uz	Usum	σ _x	σ _y	σ _z	τ _{xy}	τ _{yz}	τ _{xz}	σ ₁	σ ₂	σ ₃	σ _{int}	σ _{von}	ε _x	ε _y	ε _z	ε _{xy}	ε _{yz}	ε _{xz}	ε _{int}	ε _{von}	
M - 1	0.0011	0.0011	0.0096	0.0967	142.61	143.19	304.31	15.00	80.78	92.29	99.76	143.20	347.15	247.40	230.02	0.00041	0.00040	0.00106	0.00203	0.00110	0.00122	0.00163	0.00115	
M - 2	0.0008	0.0008	0.0073	0.0073	147.28	147.86	307.14	15.58	85.03	94.02	102.80	147.87	351.60	248.80	230.84	0.00032	0.00031	0.00079	0.00016	0.00085	0.00094	0.00124	0.00087	
M - 3	0.0006	0.0006	0.0058	0.0059	150.14	150.73	308.86	15.71	85.92	95.06	104.67	150.74	354.32	249.65	231.33	0.00025	0.00024	0.00063	0.00012	0.00069	0.00076	0.00101	0.00070	
M - 4	0.0005	0.0005	0.0050	0.0050	152.07	152.67	310.02	15.80	86.51	95.60	105.93	152.68	356.15	250.21	231.66	0.00022	0.00022	0.00054	0.00010	0.00059	0.00066	0.00086	0.00060	
M - 5	0.0005	0.0005	0.0044	0.0044	154.03	154.63	311.18	15.88	87.11	96.45	107.21	154.64	357.99	250.78	231.99	0.00020	0.00019	0.00048	0.00009	0.00053	0.00059	0.00077	0.00053	
M - 6	0.0004	0.0004	0.0037	0.0037	164.18	164.79	317.14	16.30	90.11	99.97	113.83	164.81	367.47	253.64	233.63	0.00017	0.00016	0.00039	0.00008	0.00046	0.00051	0.00065	0.00044	

Table 2 shows the findings of the mechanical characteristics of the composite materials as determined by the Mathcad-15 program. Table 3 lists the models, codes, particular disciplines, element kinds, and load types applied by the ANSYS 15.0 program.

Fiber Composites with Random Orientation and Discontinuity Typically, in situations where short, discontinuous fibers with random orientation are employed, an expression known as the "rule-of-mixtures" for the elastic modulus can be employed, which is comparable to equations:

$$E_C = K \cdot E_f \cdot V_f + E_m \cdot V_m \tag{1}$$

$$\mu_c = \mu_f + \mu_m \tag{2}$$

$$G_c = \frac{E_c}{2(1 + \mu_c)} \tag{3}$$

where, E_C =Randomly Oriented Composite Modulus of Elasticity; K =Fibre Efficiency Parameter; E_f =Elastic Modulus of the Fibre; E_m =Elastic Modulus of the Matrix; V_f =Volume Fraction of the Fibre; V_m =Volume Fraction of the Matrix.

The fiber efficiency parameter (K) is dependent on the of (V_f & E_f/E_m ratio). Its magnitude will, of course, be less than unity; typically, it will be between 0.1 and 0.6. The fibers are uniformly and randomly distributed within a specific plane, which accounts for the value of ($K=0.375$) [48-50].

3. SIMULATING AND MODELING

3.1 Zirconia nanotube structures

For each of the six models, pressure screening specimens are created and prepared using composite materials in compliance with ASTM E9 standards. ANSYS software was utilized to conduct compression tests utilizing the finite element technique. For the purpose of compression testing, specimens measuring 8 mm in diameter and 12 mm in height were ready, as seen in Figure 1.

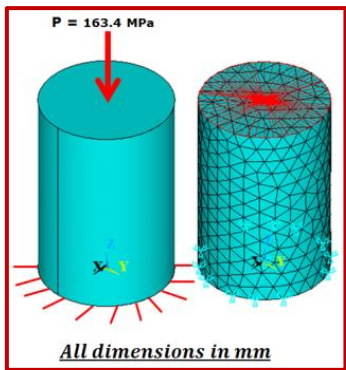


Figure 1. Schematic illustration of a compression test sample's dimensions [43]

4. RESULTS AND DISCUSSION

Table 3 and Figures 2-14 present the most significant findings from this investigation, which came from applying a compressive load of (163.4 MPa) to the models, (To find the load at which the first model collapses, the load was achieved

through numerous attempts to load the model). By adding more of these materials to each model, the amounts of nanomaterial's in the various models were varied.

Table 3 and Figures 2-4, deformation, sum displacement, and displacement in direction - Z results, which were acquired by loading the six models, show a decline in its value, when comparing the five models to the first model in the following proportions: 24.6, 39.5, 48.1, 54.1, and 61.9%, respectively, with increasing ratios the Carbon Nanotubes in the models. Figure 5, which shows the normal stress in direction - Z results obtained by loading the six models, shows an increase in its value when comparing the five models to the first model in the following proportions: 0.93, 1.48, 1.87, 2.26, and 4.22%, respectively, as the ratio of carbon nanotubes in the models increases. Shear stress in direction-XZ results obtained by loading the six models are displayed in Figure 6, which demonstrate an increase in its value with increasing ratios of carbon nanotubes in the models. This increase is seen when comparing the five models to the first model in the following proportions: 1.87, 2.99, 3.75, 4.51, and 8.14%, respectively. Figure 7 present the shear stress in direction-ZY results obtained by loading the six models, showing an increase in its value with increasing ratios of carbon nanotubes in the models. The following proportions show this increase: 1.77, 2.84, 3.43, 4.27, and 7.86%, respectively, when comparing the five models to the first model. Figure 8 shows the intensity stress results of loading the six models, showing a marginal increase in its value as the models' carbon nanotube ratios rise. The percentages that demonstrate this increase between the first model and the five models are: 0.57, 0.91, 1.14, 1.77, and 2.52%, respectively.

The von Mises stress results obtained from loading the six models are shown in Figure 9, which indicates a very slight increase in their value as the models' proportions of carbon nanotubes increase. When comparing the five models to the first model, the following percentages demonstrate this increase: 0.36, 0.57, 0.72, 0.86, and 2.52%, respectively.

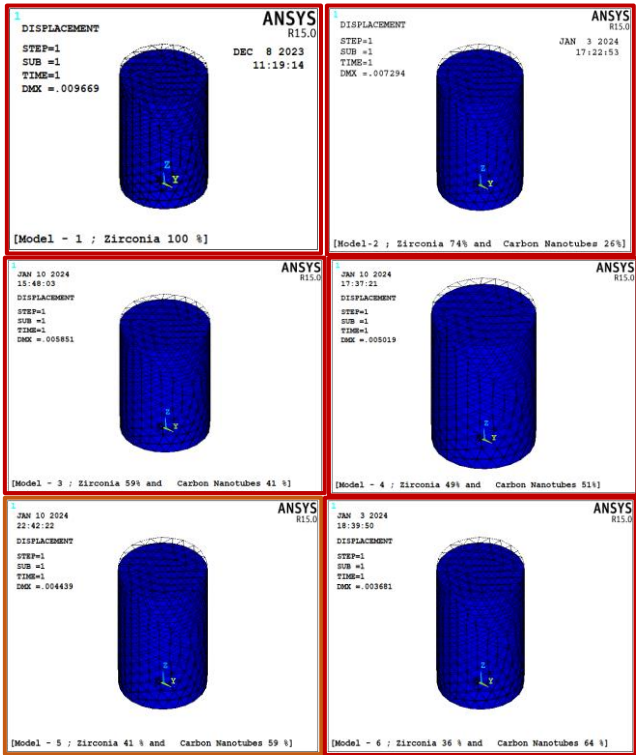


Figure 2. The results of the deformation for each model

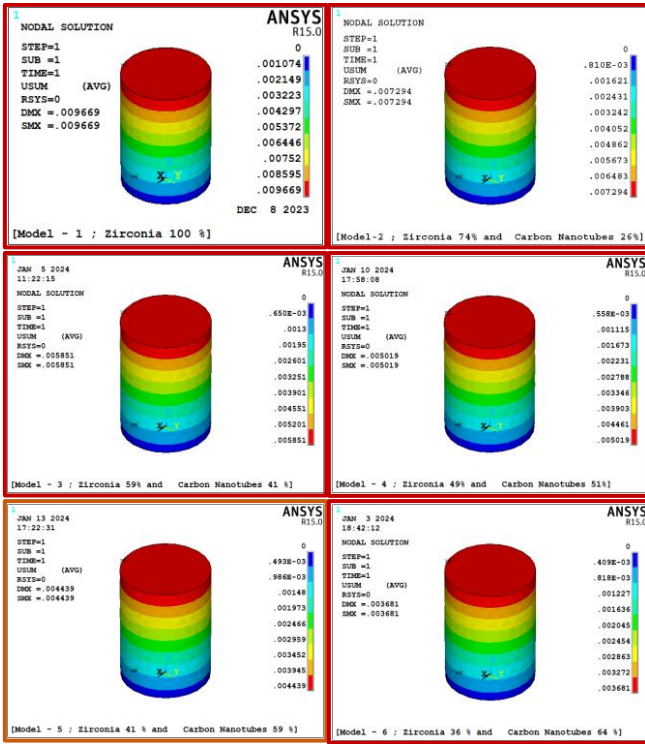


Figure 3. The results of the sum displacement (U_{sum}) for each model

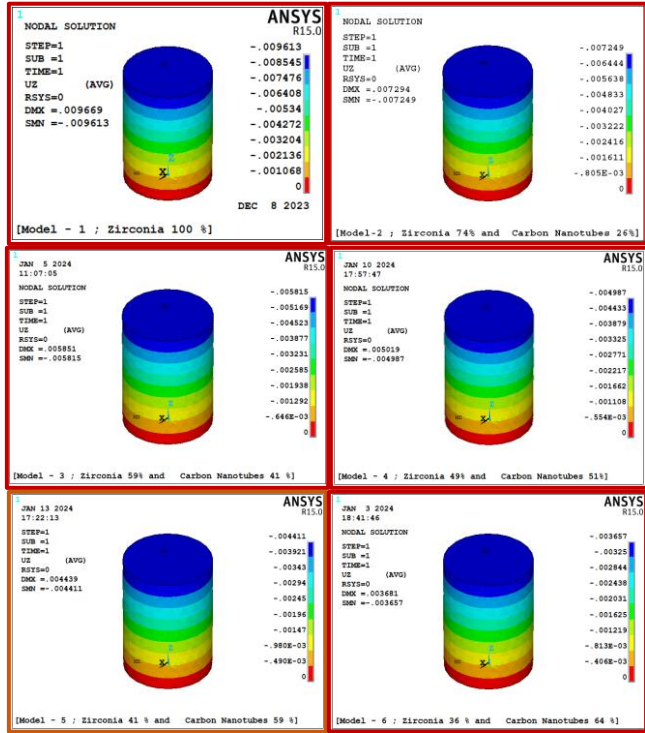


Figure 4. The results of the sum displacement (U_z) for each model

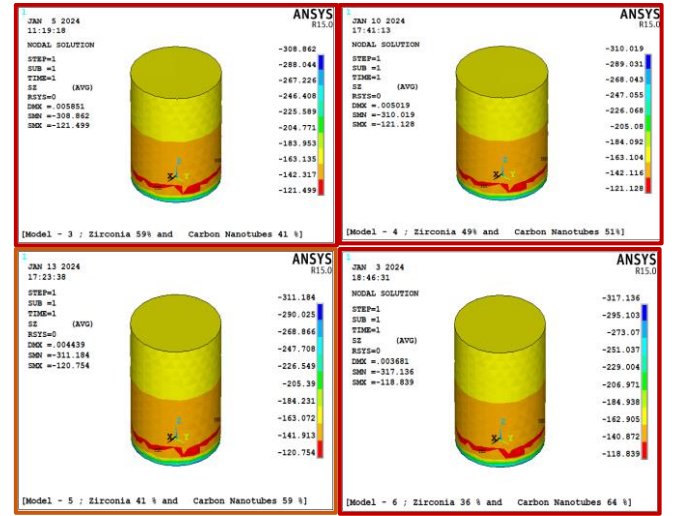
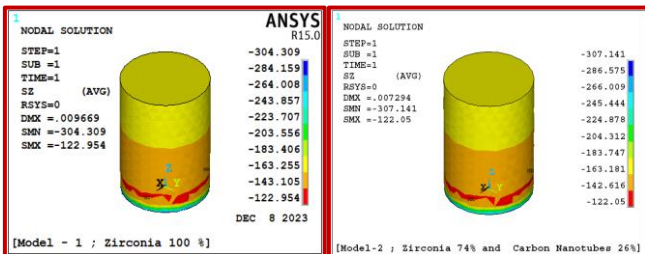


Figure 5. The results of the normal stress (σ_z) for each model

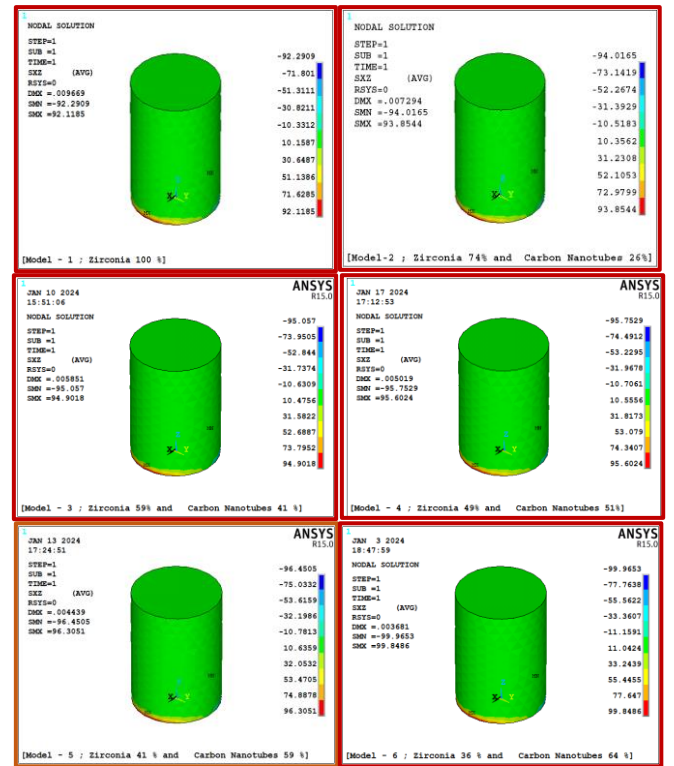
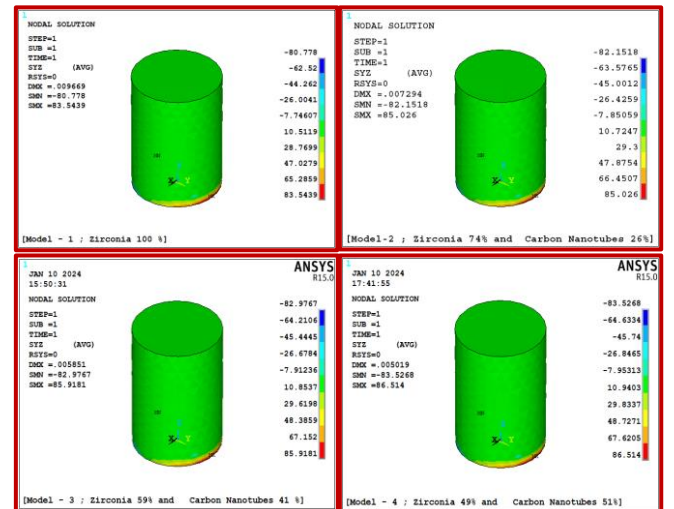


Figure 6. The results of the shear stress (τ_{xz}) for each model



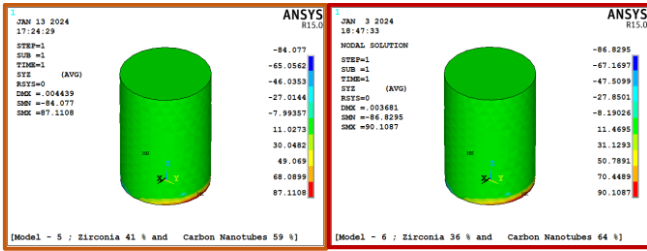


Figure 7. The results of the shear stress (τ_{yz}) for each model

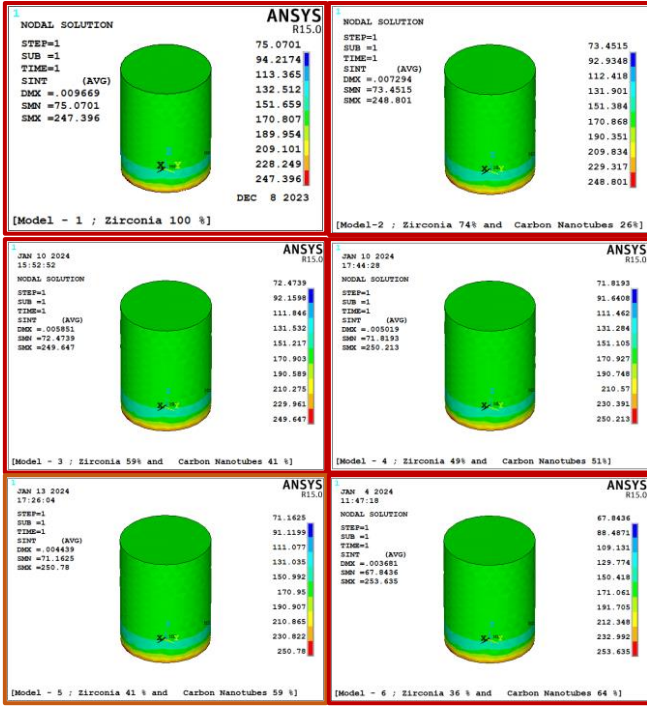


Figure 8. The results of the intensity stress (σ_{int}) for each model

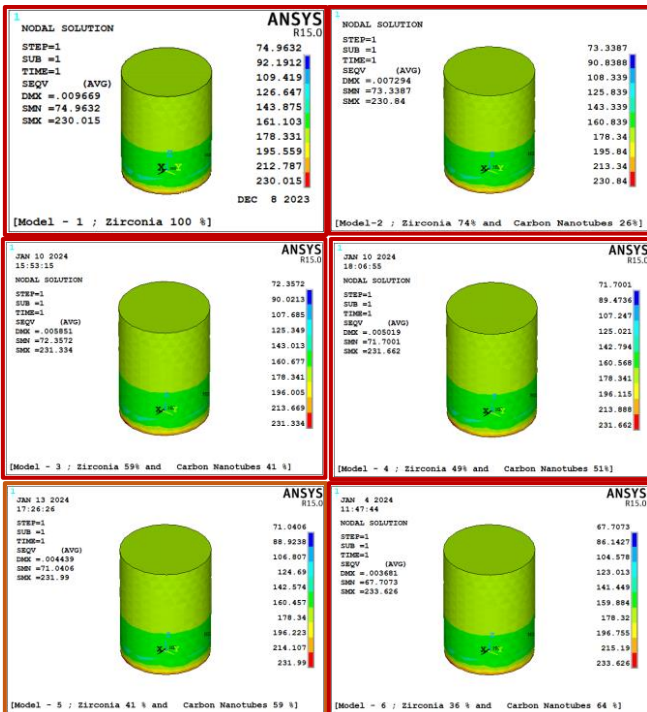


Figure 9. The results of the von mises stress (σ_{von}) for each model

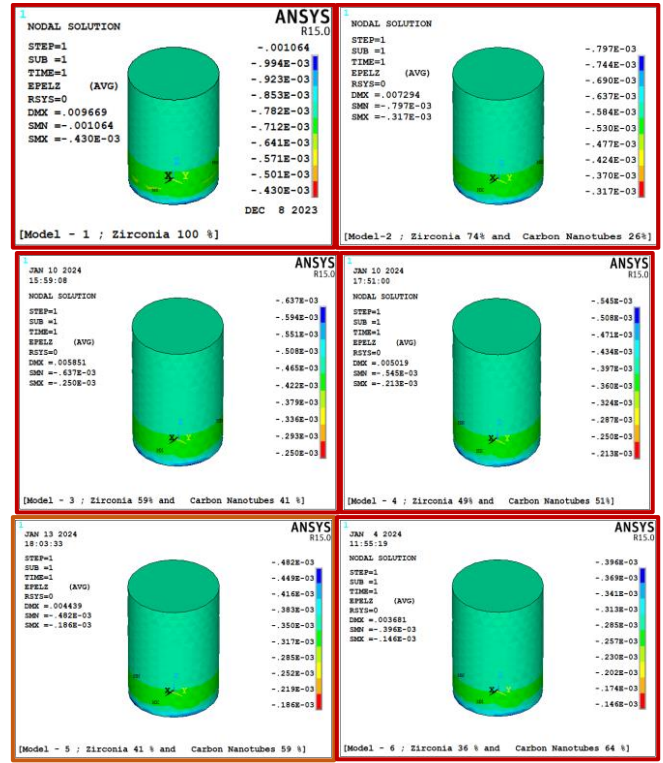


Figure 10. The results of the normal strain (ϵ_z) for each model

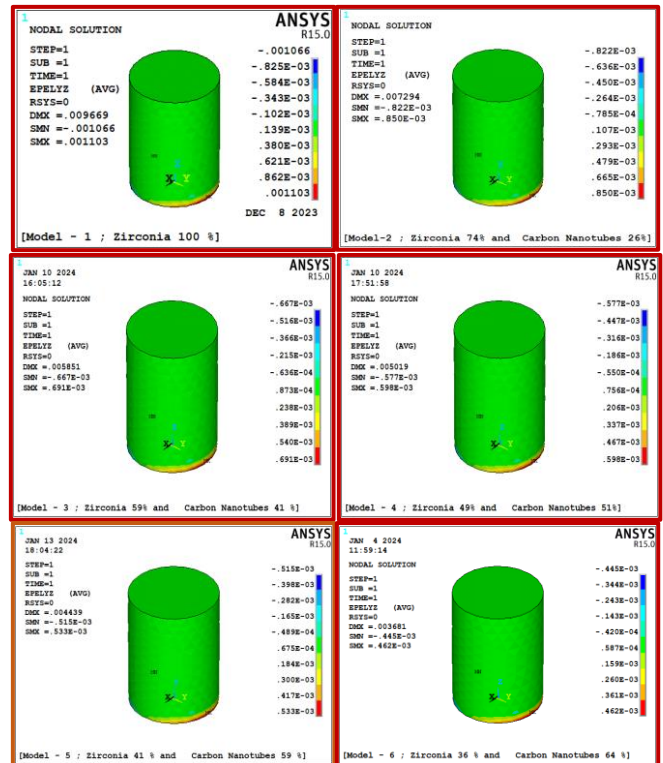


Figure 11. The results of the shear strain (ϵ_{yz}) for each model

Carbon nanotubes cause the crystalline structure of the material they are added to become rougher, which explains why stress results change very slightly when the content of carbon nanotubes is increased ($\sim 5\%$ in most cases).

The results of loading the six models in Figure 10 show that there is a noticeable increase in strain in the direction of Z as the proportion of carbon nanotubes in the models increases. The following percentages demonstrate this increase when

comparing the five models to the first model: 25.47, 40.57, 49.06, 54.72, and 63.21%, respectively. Figure 11 shows the strain results in the direction of YZ that were obtained from loading the six models. It shows that the strain increases significantly as the proportion of carbon nanotubes in the models increases. The following percentages demonstrate this increase when comparing the five models to the first model: 22.73, 37.27, 46.36, 51.82, and 58.18%, respectively. Figure 12 shows the strain results in the XZ direction that were obtained after loading the six models. It demonstrates that when the amount of carbon nanotubes in the models rises, the strain increases noticeably. When comparing the five models to the first model, the following percentages show this increase: 22.95, 37.70, 45.90, 51.64, and 58.20%, respectively.

Figure 13 shows the intensity strain results that were obtained after the six models were loaded. It shows that there is a discernible increase in intensity strain with an increase in the number of carbon nanotubes in the models. The following percentages demonstrate this increase when comparing the five models to the first model: 23.93, 38.04, 47.24, 52.76, and 60.12%, in that order. Figure 14 shows the von Mises strain results that were obtained after loading the six models. It shows that the von Mises strain increases significantly with an increase in the number of carbon nanotubes in the models. The following percentages demonstrate this increase when comparing the five models to the first model: 24.35, 39.14, 47.83, 53.91, and 61.74%, respectively.

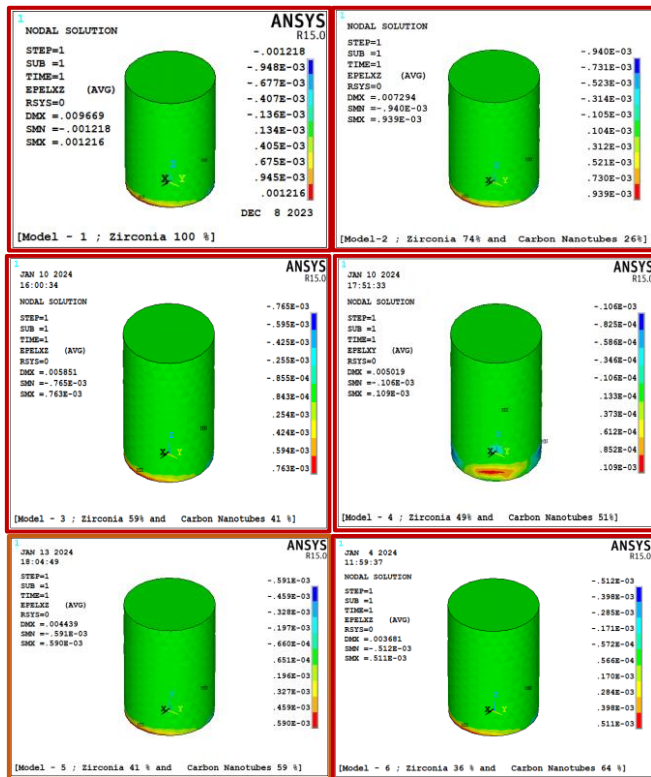


Figure 12. The results of the shear strain (ϵ_{xz}) for each model

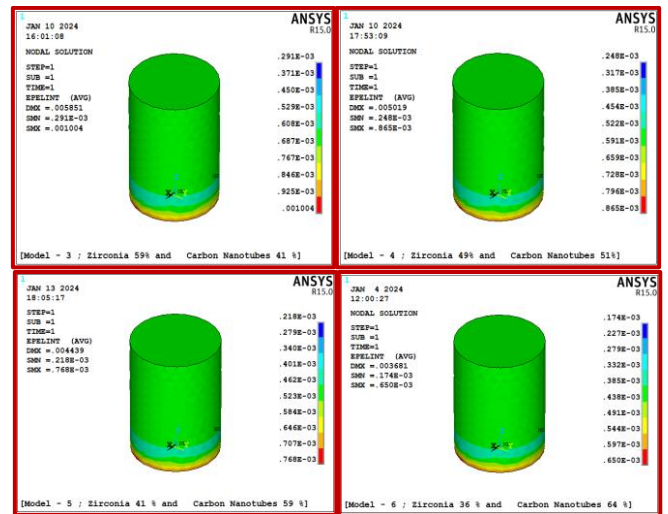
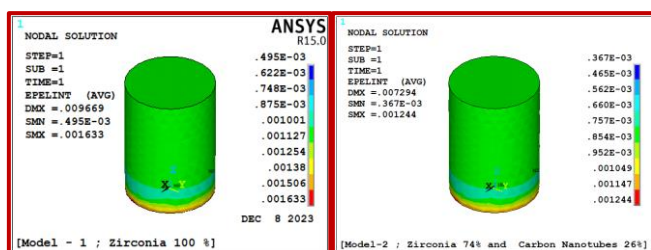


Figure 13. The results of the intensity strain (ϵ_{int}) for each model

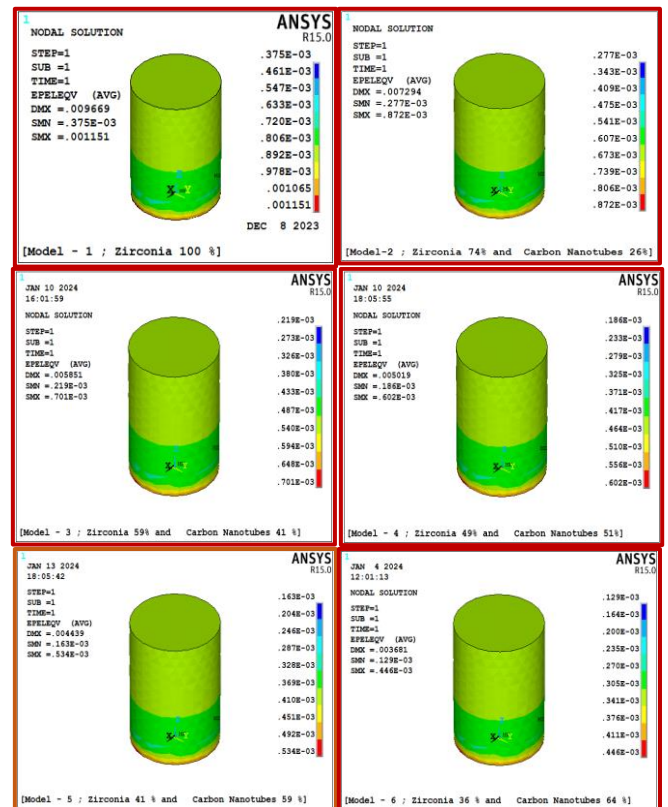


Figure 14. The results of the von mises strain (ϵ_{von}) for each model

The material to which the carbon nanotubes are added has a rougher crystal structure, which accounts for the very small change in the stresses results when compared to the high strains results.

5. CONCLUSIONS

The following was concluded from this theoretical study of composite materials composed of materials of different proportions by creating six models made of different materials, testing each model's compressive resistance, and comparing the results to one another in order to obtain materials with high

compressive resistance:

1. The results obtained show a significant decrease in deformation and deflection in the models, when the percentage of carbon nanotubes is increased at very high rates, which may reach 61.9% in the sixth model.

The primary cause of deformation sensing in carbon nanotube-polymer composites is the conductive carbon nanotube network's compressive strength inside the polymer matrices. Consequently, its deformation decreases due to the change in the mechanical deformation of the carbon nanotube network upon loading when its proportion in the material increases to a certain amount.

2. It is observed that applying a load of 163.5 MPa is the maximum optimal load for the models to bear this load without any failure occurring in them when using von Mises theory to compare the results obtained for the six models with the yield compressive strength of these materials.

3. It is also observed that the applied load is suitable for these models to function without failure when comparing the results with the theory of maximum shear stress.

6. FUTURE STUDIES

The researchers propose to create a number of mathematical models for different engineering materials, including aluminum alloys, composite materials, and magnesium alloys used in the medical field. They advise looking into how different loads in daily life affect engineering materials. withstand loads from impacts, twists, tensile and compression, torsion and fatigue, heat, and other sources. Using state-of-the-art engineering software, like the ANSYS program, carefully examine them to determine the deformations, stresses, and strains they experience during loading.

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NOMENCLATURE

δ Deformed and unreformed

U_x	Component of the displacement (x-direction)
U_y	Component of the displacement (y-direction)
U_z	Component of the displacement (z-direction)
σ_x	Normal stress
τ_{xy}	Shear stress
τ_{xz}	Shear stress
$\sigma_{int.}$	Stress intensity
σ_{von}	Von mises stress
ϵ_x	Normal strain (x-direction)
ϵ_{xy}	Shear strain (xy-direction)
ϵ_{xz}	Shear strain (xz-direction)
ϵ_{first}	First principal elastic strain
ϵ_{third}	Third principal elastic strain
$\epsilon_{intensity}$	Elastic strain intensity
ϵ_{von}	Von mises elastic strain

Greek symbols

E	Modulus of elasticity
ρ	Density
G	Modulus of rigidity
μ	Poisson's ratio

Subscripts

SNC	Surface Nano Crystallization
Si	Silicone
Mn	Manganese
C	Carbon
Ni	Nickel
Ti	Titanium
Cr	Chrome
Fe	Iron