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Studying buckling of composite rods made of hybrid carbon fiber/carbon nanotube-reinforced polyimide using multi-scale FEM

M. Ahmadi[a], R. Ansari[a], and H. Rouhi[b,*]

a. *Department of Mechanical Engineering, University of Guilan, Rasht, P.O. Box 3756, Iran.*
b. *Department of Engineering Science, Faculty of Technology and Engineering, East of Guilan, University of Guilan, P.C. 44891-63157, Rudsar-Vajargah, Iran.*

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Abstract. In this paper, the buckling behavior of rods made of carbon fiber/carbon nanotube-reinforced polyimide (CF/CNT-RP) under the action of axial load is investigated based on a multi-scale finite element method. A dual-step procedure is first adopted to couple the micro- and nano-scale effects in order to obtain the equivalent elastic properties of CF/CNT-RP for various volume fractions of CF and CNT. The interphase effect between CNTs and the polymer matrix is taken into consideration. Further, the dispersion of CF/CNT into the polymer matrix is assumed to be random. Then, rods with square and circular cross-sections are considered whose stability characteristics are analyzed. The finite element modeling is performed using two models including a 3D brick model and a 2D beam model. Selected numerical results are given to study the effects of volume fraction of CNT/CF, interphase, and geometrical properties on the axial buckling response of the multiscale composite rods.

1. Introduction

Hybrid composite materials have been the focus of several research works in recent years [1–7]. This attention is mainly given to a wide range of possibilities available to modify the properties of such materials on different length scales. In particular, polymer matrix composites reinforced with Carbon Nanotubes (CNTs) and Carbon Fibers (CFs) have attracted much attention from the research community due to their excellent mechanical and electrical properties together with multifunctionality. For example, CNT/CF/epoxy composites indicated $\sim 30\%$ enhancement of the interlaminar shear strength in comparison with that of CF/epoxy composites without CNTs and demonstrated considerably improved out-of-plane electrical conductivity [1]. Alipour Skandani and Al-Haik [5] revealed that the surface grown CNTs could enhance the CF-reinforced composite resistance to viscoplastic deformation. Pal and Kumar [6] showed that, even at low CF content, dispersing CNTs in the CF-polymer composite significantly improved the effective electrical conductivity and electrical percolation threshold of the resulting composite. The properties and performance of CNT-reinforced composites are dependent on different parameters. Synthesizing strategy, morphology of CNTs, type of matrix (e.g., metal, polymer, etc.),

*. *Corresponding author. Tel. /Fax: +98 13 42688447*
E-mail addresses: masoud_ahmadi_pr@yahoo.com (M. Ahmadi); r_ansari@guilan.ac.ir (R. Ansari); h_rouhi@guilan.ac.ir (H. Rouhi)

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dispersion of CNTs, and interfacial reactions between CNTs and matrix can be mentioned as some examples. The reader is referred to [8] for more details.

Up to now, many micromechanical models have been developed to estimate the mechanical properties of CNT-reinforced composites [9–15]. Moreover, there are some research works in which the mechanical behaviors (e.g., vibration, buckling, and bending) of structural elements made of nanocomposites have been studied [16–32].

Since the lattice structure of CNTs is not incorporated into the micromechanical models, the direct application of continuum micromechanical models may lead to inaccurate results in the analysis of CNT-reinforced composites [33]. Furthermore, CNT/polymer matrix interphase region is one of the most important factors in the analysis of reinforced polymers with CNTs [34]. The interphase is formed by non-bonded van der Waals interaction between the CNT and the surrounding matrix. Therefore, multi-scale modeling approaches to the coupled micro- and nano-scale effects have been proposed in a number of studies [35–43].

Moreover, there are some size-dependent generalized continuum theories to capture small-scale effects. The nonlocal, strain gradient, and couple stress theories are well-known non-classical elasticity theories capable of considering size influences on micro and nano scales. On the basis of nonlocal elasticity theory, the stress tensor at a reference point in a body depends on the strain tensor not only at that point but also at all other points of the body. The nonlocal parameter of this theory can be determined based on experimental data or results of atomistic approaches like molecular dynamics simulations. The nonlocal theory has been applied to various problems such as buckling of microtubules and boron-nitride nanotubes embedded in an elastic medium [44,45] and bending/buckling/free vibration analyses of nanobeams [46,47]. The reader is also referred to [48–52] as some examples for the applications of strain gradient and couple stress theories.

As cited earlier, there are some papers on the finite element multi-scale modeling of structural elements made of nanocomposites. However, to the authors' knowledge, the buckling behavior of rods made of CNT/CF-reinforced polyimide considering coupled effects of micro and nano scales based on a finite element approach has not been investigated yet. Therefore, in the present paper, the multi-scale buckling analysis of composite rods made of CNT/CF-reinforced polyimide is presented by employing the Finite Element Method (FEM). To this end, the elastic properties of CNT/CF-RP including Young's modulus and Poisson's ratio are first determined using a dual-step procedure. In the first step, CNTs with three values of volume fraction (1%, 3%, and 5%) are randomly dispersed into the polymer matrix (polyimide). In the selected Representative Volume Element (RVE), the interphase region between CNTs and the polymer matrix is taken into account. Then, a random distribution of CFs into the CNT-reinforced polymer is modeled according to six cases of hybrid CNT/CF reinforcement. The elastic properties of the composite are calculated with and without considering the interphase influence. After that, the axial buckling of rods made of CNT/CF-RP with circular and square cross-sections is analyzed. The analysis is performed via two models: a 3D brick model and a 2D beam model. The effects of some important factors including interphase, volume fraction of CNT/CF, and size on the critical buckling loads are investigated. Moreover, a comparison is made between the predictions of brick and beam models.

2. Dual-step multi-scale finite element modeling

In order to estimate the elastic constants of polyimide reinforced by CFs and CNTs, a dual-step procedure is adopted herein [38]. In the first step, CNTs are dispersed into the polymer matrix (polyimide) with three volume fractions including 1%, 3%, and 5%. The RVE model of this step is observed in Figure 1. The dispersion of CNTs is considered to be random from the viewpoint of orientation and coordinates. In addition, they are dispersed almost homogenously without aggregation. The RVE consists of three phases: CNTs, polymer matrix, and interphase. The interphase is formed due to the non-bonded van der Waals interaction between the CNT and the surrounding matrix. It is modeled as a layer developed around the CNT. Shen

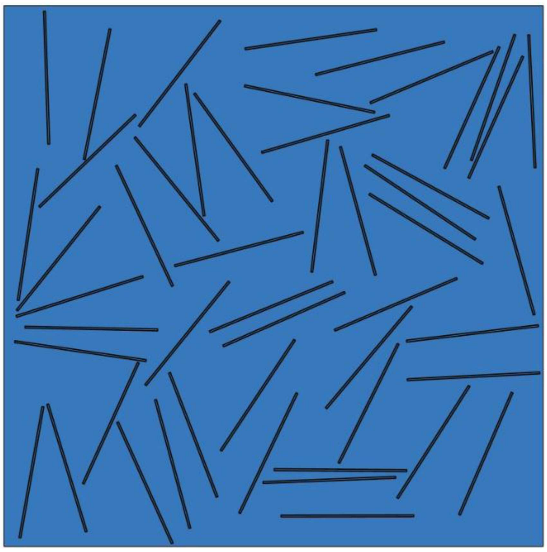


Figure 1. Representative Volume Element (RVE) model of composite with random Carbon Nanotube (CNT) distribution.

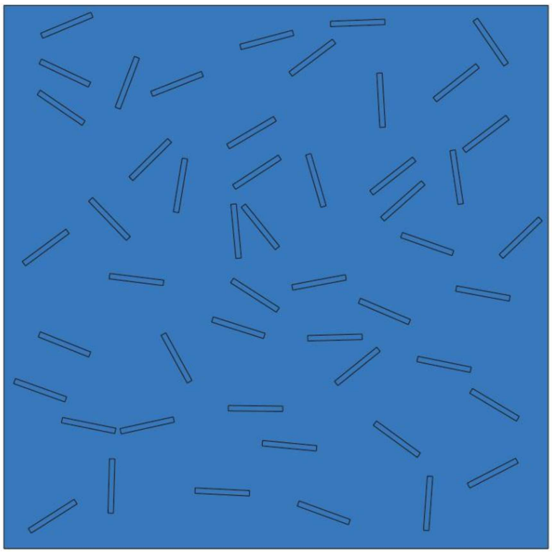


Figure 2. Representative Volume Element (RVE) model of composite with random Carbon Fiber (CF) distribution.

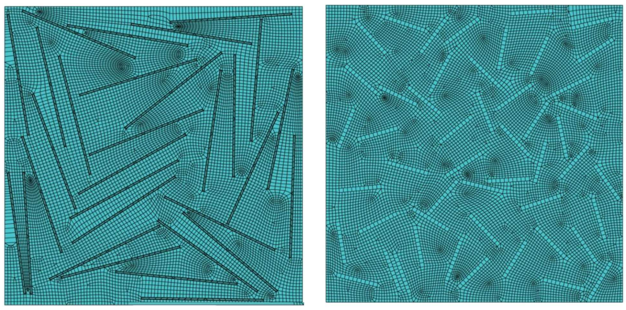
and Li [53,54] showed that CNTs were transversely isotropic materials. Consequently, CNTs are modeled as transversely isotropic materials in the present finite element modeling. Further, the polymer matrix and interphase are considered as isotropic.

In the next step, CFs are distributed in the CNT-Reinforced Polyimide (CNT-RP), considered to be homogenous materials with the properties that were evaluated in the first step. Six cases as follows are studied for the hybrid reinforcement:

- 0.95% CNT + 5% CF + Polyimide,
- 2.85% CNT + 5% CF + Polyimide,
- 4.75% CNT + 5% CF + Polyimide,
- 0.9% CNT + 10% CF + Polyimide,
- 2.7% CNT + 10% CF + Polyimide,
- 4.5% CNT + 10% CF + Polyimide.

The RVE model of nanocomposite with the random dispersion of CFs is indicated in Figure 2. Similar to CNTs, CFs are assumed to be transversely isotropic. The Python programming language is utilized to create randomly distributed/oriented CNTs/CFs inside the RVE. It should be noted that the positions of CNTs/CFs are determined such that no overlapping occurs between them.

Figure 3 shows examples of meshed RVEs. Figure 4 represents the loading and boundary conditions of RVE to obtain Young's modulus. It is assumed that the effective properties of the nanocomposite are similar to those of RVE. By measuring the fixed boundary reaction force and calculating stress value (σ), the equivalent elastic modulus (E) of nanocomposite RVE is obtained based on Hooke's law as follows:



(a) (b)

Figure 3. Examples of meshed Representative Volume Elements (RVEs) for (a) CNT-reinforced polyimide, and (b) Carbon fiber-reinforced polyimide.

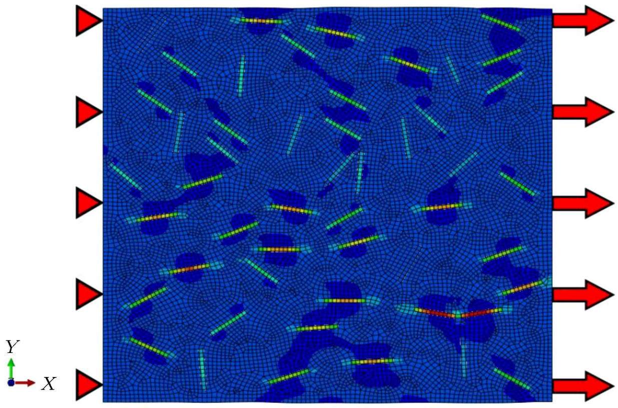


Figure 4. Stress distribution contour (tensile test for obtaining elastic modulus of nanocomposite).

$$E = \frac{\sigma}{\varepsilon}, \tag{1}$$

where ε is the RVE strain in the load direction. Poisson's ratio is also defined as the ratio of transverse strain to axial strain. It should be noted that the results are obtained for each reinforcement type using the average values of three analyses with various random microstructures in order to reduce the effect of chance on the results because of random dispersion. Besides, the present calculations reveal that there is a negligible difference between the results of 2D and 3D RVEs. Hence, 2D RVEs are used instead of 3D ones due to the high computational cost of 3D models.

After calculating Young's modulus and Poisson's ratio of CNT/CF-RP for various reinforcement types with and without the interphase influence, the buckling analysis of rods with circular and square cross-sections is performed. The finite element modeling is performed using two models: a 3D brick model and a 2D beam model, as shown in Figure 5. On a micro scale, an 8-node biquadratic plane stress quadrilateral element is used. Moreover, on a macro scale, a 3-node quadratic beam in space is used for the 2D beam model, and a 20-node quadratic brick is used for the 3D brick model.

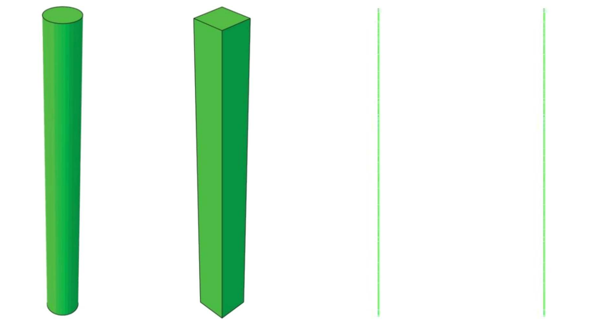


Figure 5. (a) 3D brick and (b) 2D beam models for the buckling analysis of rods.

3. Results and discussion

First, in order to validate the proposed multi-scale FEM, the present results of Young's modulus of polypropylene reinforced with randomly oriented CNTs are compared with the experimental results given in [55]. Table 1 shows the normalized Young's modulus of CNT-reinforced polypropylene for different volume fractions of CNT. It is seen that the present results are in good agreement with those reported in [55].

The material properties of composite constituents are given in Table 2. In this table, longitudinal Young's modulus (E_L), transverse Young's modulus (E_T), longitudinal Poisson's ratio (ν_L), transverse Poisson's ratio (ν_T), longitudinal shear modulus (G_L) and mass density (ρ) of CNTs, interphase, CFs, and the polymer matrix are presented. The aspect ratio and diameter of CFs are selected as 10 and 10 μm, respectively. Moreover, the aspect ratio and diameter of CNTs are taken as 100 and 0.78 nm, respectively. Moreover, the thickness of interphase is considered to be 0.3333 nm.

Table 1. Dimensionless Young's modulus of CNT-reinforced polypropylene.

CNT[a] volume fraction (%)	Present FEM[b]	Experiment [55]	Difference percentage
1.6	1.161	1.19	2.4
3.2	1.319	1.29	2.2
4.8	1.526	1.39	9.8

[a]CNT: Carbon nanotube; [b]FEM: Finite Element Method.

Table 3. Mesh convergence study in the case of 2.85% CNT −5% CF-RP[a].

No. of elements	E (GPa)	Error (%)
3933	7.0723	0.54
6963	7.0568	0.32
13808	7.0456	0.16
22834	7.0407	0.09
29953	7.0378	0.05
43499	7.0365	0.03
52276	7.0357	0.02
68465	7.0346	0.00
83270	7.0343	0.00
129724	7.0343	0.00

[a]CNT: Carbon Nanotube; CF: Carbon Fiber; RP: Reinforced Polyimide.

To study the mesh convergence, as an example, Young's modulus of 2.85% CNT −5% CF-RP (without interphase) is computed with various mesh sizes, as shown in Table 3. This table reveals a converged trend with a mesh size that is getting smaller. It is worth mentioning that the fining mesh is performed to reach a change smaller than 0.005% in the solution.

The values of equivalent Young's modulus, Poisson's ratio, and mass density of CNT/CF-reinforced polyimide for different volume fractions of CNT/CF are tabulated in Table 4. The results of this table are generated with and without considering interphase in order to show such an effect. The elastic properties of pristine material (polyimide) are also given so as to study the effect of reinforcement. According to the results, given the interphase effect, Young's modulus is computed to be larger than that obtained without considering the interphase effect. For example, there is a 4.5% increase in the value of Young's modulus for (4.75% CNT + 5% CF + polyimide) when the interphase is considered.

As expected, reinforcing polyimide with CNT/CF results in increasing the elastic modulus. For instance, when 5% CNT is added to the polymer matrix, an 88% increase in the elastic modulus of the resulting composite material is observed. Further, the increase reaches 133% in the case of (4.5% CNT + 10% CF + polyimide). It is also observed that the effect of reinforcement on Poisson's ratio is insignificant.

Table 2. Material properties of Carbon Nanotube (CNT), interphase, Carbon Fiber (CF), and polyimide.

Material	E_L (GPa)	E_T (GPa)	ν_L	ν_T	G_L (GPa)	ρ (kg/m^3)
CNT [34]	1382.5	645	0.272	0.2	1120	1300
Interphase [34]	19.29	19.29	0.34	0.34	7.2	1305
CF [56]	294	18.5	0.27	0.3	25	1760
Polyimide [57]	4.2	4.2	0.4	0.4	1.5	1310

Table 4. Equivalent Young's modulus, Poisson's ratio, and mass density of polyimide reinforced with CNT/CF.

Material	E (GPa)	ν	ρ (kg/m^3)
Polyimide	4.200	0.400	1310.00
1% CNT-RP (without interphase)	4.786	0.399	1309.90
1% CNT-RP (with interphase)	4.830	0.399	1309.86
3% CNT-RP (without interphase)	6.223	0.398	1309.70
3% CNT-RP (with interphase)	6.411	0.397	1309.57
5% CNT-RP (without interphase)	7.554	0.396	1309.50
5% CNT-RP (with interphase)	7.898	0.395	1309.29
0.95% CNT − 5% CF-RP (without interphase)	5.434	0.397	1332.41
0.95% CNT − 5% CF-RP (with interphase)	5.483	0.397	1332.36
2.85% CNT − 5% CF-RP (without interphase)	7.034	0.396	1332.22
2.85% CNT − 5% CF-RP (with interphase)	7.242	0.395	1332.09
4.75% CNT − 5% CF-RP (without interphase)	8.505	0.394	1332.03
4.75% CNT − 5% CF-RP (with interphase)	8.884	0.393	1331.82
0.9% CNT − 10% CF-RP (without interphase)	6.036	0.395	1354.91
0.9% CNT − 10% CF-RP (with interphase)	6.090	0.395	1354.87
2.7% CNT − 10% CF-RP (without interphase)	7.787	0.394	1354.73
2.7% CNT − 10% CF-RP (with interphase)	8.015	0.393	1354.61
4.5% CNT − 10% CF-RP (without interphase)	9.388	0.392	1354.55
4.5% CNT − 10% CF-RP (with interphase)	9.798	0.391	1354.36

Note: CNT: Carbon Nanotube; CF: Carbon Fiber; RP: Reinforced Polyimide.

Now, the buckling results of composite rods made of CNT/CF-RP are given and discussed. It is considered that the rods are under an axial point load applied to the center of cross-sections (circular and square). Furthermore, the boundary condition of rods is assumed to be clamped-free.

In Table 5, the results of multi-scale FEM are compared with those obtained through Euler's formula. The critical load based on Euler's formula is given by:

$$F_{cr}=\frac{\pi^2 EI}{(KL)^2}, \tag{2}$$

where E, I, L, and K denote elastic modulus, second moment of inertia of the cross-section, length, and effective length factor of the rod, respectively. The comparison is done for rods with both circular and square cross-sections using 3D brick and 2D beam models. In addition, various values of diameter are considered. It is observed that the finite element results agree well with the ones obtained based on Euler's formula.

Tables 6 and 7 show the critical buckling loads of rods made of different materials with circular and square cross-sections, respectively. The results of these tables are obtained by both brick and beam models. The effects of interphase, material, and geometrical properties on the buckling behavior of rods can be investigated herein. It is seen that with the hybrid CNT/CF reinforcement at hand, the resistance of rods to applied axial load improves significantly. For example, for a cylindrical rod with a radius of 20 mm, the critical buckling load increases by 123% when the material changes from polyimide to (4.5% CNT + 10% CF + Polyimide).

Besides, the interphase effect on the calculated critical buckling loads is observed in Tables 6 and 7.

Table 5. Comparison between the results of the present multi-scale Finite Element Method (FEM) and those of Euler's formula for the buckling of rods with circular and square cross-sections.

Rods with circular cross section				Rods with square cross section			
d	3D brick	2D beam	Euler's critical load	d	3D brick	2D beam	Euler's critical load
2 mm	13.057	13.013	13.023	2 mm	1.3842	1.3814	1.3817
5 mm	509.53	506.24	508.70	4 mm	22.176	22.084	22.108
10 mm	7804.8	7984.2	8139.148	10 mm	862.14	857.78	863.59

Table 6. Critical buckling load (N) of rods with a circular cross-section.

Material	r (mm)	3D brick		2D beam	
		Without interphase	With interphase	Without interphase	With interphase
Polyimide	1	0.81499		0.81376	
	2	13.057		13.013	
	5	509.53		506.24	
	10	7804.8		7984.2	
	20	102384		120846	
1% CNT-RP	1	0.92870	0.93723	0.92730	0.93582
	2	14.879	15.015	14.828	14.964
	5	580.62	585.96	576.87	582.18
	10	8893.7	8975.5	9098.2	9181.8
	20	116669	117742	137706	138972
3% CNT-RP	1	1.2075	1.2440	1.2057	1.2421
	2	19.346	19.930	19.280	19.863
	5	754.95	777.76	750.08	772.74
	10	11564	11913	11830	12187
	20	151699	156282	179053	184462
5% CNT-RP	1	1.4658	1.5326	1.4636	1.5303
	2	23.484	24.553	23.404	24.470
	5	916.43	958.16	910.51	951.97
	10	14037	14677	14360	15014
	20	184145	192531	217349	227247
0.95% CNT – 5% CF-RP	1	1.0544	1.0639	1.0528	1.0623
	2	16.893	17.045	16.836	16.988
	5	659.23	665.18	654.98	660.89
	10	10098	10189	10330	10423
	20	132466	133660	156351	157761
2.85% CNT – 5% CF-RP	1	1.3649	1.4053	1.3628	1.4031
	2	21.867	22.514	21.793	22.437
	5	853.34	878.57	847.83	872.90
	10	13071	13458	13372	13767
	20	171469	176540	202388	208372
4.75% CNT – 5% CF-RP	1	1.6503	1.7239	1.6479	1.7213
	2	26.440	27.618	26.350	27.525
	5	1031.8	1077.8	1025.1	1070.8
	10	15805	16509	16168	16888
	20	207328	216567	244712	255617
0.9% CNT – 10% CF-RP	1	1.1713	1.1817	1.1695	1.1799
	2	18.765	18.932	18.701	18.868
	5	732.27	738.82	727.54	734.05
	10	11217	11317	11474	11577
	20	147141	148457	173672	175226
2.7% CNT – 10%CF-RP	1	1.5110	1.5553	1.5087	1.5529
	2	24.208	24.917	24.126	24.832
	5	944.69	972.35	938.59	966.08
	10	14470	14894	14803	15237
	20	189825	195383	224053	230614
4.5% CNT – 10% CF-RP	1	1.8217	1.9012	1.8189	1.8984
	2	29.185	30.460	29.086	30.356
	5	1138.9	1188.7	1131.6	1181.0
	10	17445	18207	17847	18626
	20	228853	238848	270119	281915

Table 7. Critical buckling load (N) of rods with a square cross-section.

Material	d (mm)	3D brick		2D beam	
		Without interphase	With interphase	Without interphase	With interphase
Polyimide	2	1.3842		1.3814	
	4	22.176		22.084	
	10	862.14		857.78	
	20	12851		13453	
	40	183615		199463	
1% CNT-RP	2	1.5773	1.5918	1.5741	1.5886
	4	25.270	25.502	25.165	25.397
	10	982.43	991.46	977.46	986.45
	20	14644	14778	15330	15471
	40	209234	211157	227293	229382
3% CNT-RP	2	2.0509	2.1129	2.0467	2.1086
	4	32.857	33.850	32.721	33.710
	10	1277.4	1316.0	1270.9	1309.3
	20	19041	19616	19933	20535
	40	272056	280275	295538	304466
5% CNT-RP	2	2.4896	2.6029	2.4845	2.5976
	4	39.885	41.701	39.720	41.528
	10	1550.6	1621.2	1542.8	1613.0
	20	23113	24166	24196	25298
	40	330245	345284	358748	375085
0.95% CNT – 5% CF-RP	2	1.7909	1.8070	1.7872	1.8033
	4	28.691	28.950	28.572	28.830
	10	1115.4	1125.5	1109.8	1119.8
	20	16627	16776	17406	17563
	40	237563	239705	258067	260394
2.85% CNT – 5% CF-RP	2	2.3182	2.3867	2.3135	2.3819
	4	37.139	38.237	36.985	38.079
	10	1443.9	1486.6	1436.6	1479.1
	20	21522	22159	22531	23197
	40	307511	316605	334053	343931
4.75% CNT – 5% CF-RP	2	2.8030	2.9279	2.7973	2.9219
	4	44.906	46.907	44.720	46.713
	10	1745.8	1823.6	1737.0	1814.4
	20	26023	27183	27242	28456
	40	371820	388390	403912	421912
0.9% CNT – 10% CF-RP	2	1.9893	2.0071	1.9852	2.0030
	4	31.870	32.155	31.738	32.022
	10	1239.0	1250.1	1232.8	1243.8
	20	18469	18634	19334	19507
	40	263881	266242	286657	289221
2.7% CNT – 10%CF-RP	2	2.5664	2.6415	2.5611	2.6361
	4	41.115	42.319	40.945	42.144
	10	1598.4	1645.3	1590.4	1636.9
	20	23826	24524	24942	25673
	40	340431	350399	369814	380642
4.5% CNT – 10% CF-RP	2	3.0940	3.2291	3.0877	3.2225
	4	49.568	51.733	49.363	51.519
	10	1927.1	2011.2	1917.3	2001.1
	20	28725	29979	30071	31384
	40	410423	428348	445847	465318

For example, for the square rod made of (4.75% CNT + 5% CF + Polyimide) with a diameter of 40 mm, the critical buckling load, considering the interphase, is calculated as 4% larger than that obtained without taking the interphase into consideration.

In addition, the comparison between the results generated based on the 3D brick model and 2D beam model indicates that the discrepancy between the predictions of two models can be neglected in the case of small values of radius/diameter. However, the difference increases as the radius/diameter gets larger.

4. Conclusion

A dual-step multi-scale FE procedure was employed in this work in order to investigate the buckling behavior of rods made of polyimide reinforced with the combination of CNT and CF. To this end, the elastic modulus and Poisson's ratio of CNT/CF-RP for various reinforcement types were first calculated. It was shown that the elastic modulus considerably increased when polyimide was reinforced by the combination of CNT and CF. Moreover, the effect of interphase on the results was examined. It was indicated that the elastic modulus obtained with considering the interphase effect was larger than that obtained without the interphase effect. It was also concluded that the effect of reinforcement on Poisson's ratio was insignificant. After determining the elastic properties of CNT/CF-RP, the critical buckling loads of hybrid polymer composite rods with circular and square cross-sections were calculated. The results revealed that the buckling behavior of rods was significantly affected by the type of reinforcement. It was observed that there was a notable improvement in the resistance of rods to buckling when their material was a hybrid CNT/CF-polyimide composite instead of neat polyimide. A comparison was also made between the results of 3D brick and 2D beam models.

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Biographies

Masoud Ahmadi received his BSc and MSc degrees in Mechanical Engineering in 2013 and 2016, respectively, from the Razi University and University of Guilan, Iran. His research interests include finite element analysis, structural analysis, and biomechanics.

Reza Ansari received his PhD degree in 2008 from the University of Guilan, Iran, where he is currently a faculty member at the Department of Mechanical Engineering. He was also a visiting fellow at Wollongong University, Australia from 2006-2007. He has authored numerous refereed journal papers and book chapters. His research interests include computational nano- and micro-mechanics, advanced numerical techniques, nonlinear analyses, and prediction of the mechanical behavior of smart composite/FGM shell-type structures.

Hessam Rouhi received his PhD degrees in Mechanical Engineering in 2016 from the University of Guilan, Iran. He is currently a faculty member at the Department of Engineering Science, Faculty of Technology and Engineering, East of Guilan, University of Guilan, Iran. His research interests include computational micro- and nano-mechanics and the mechanical behavior of structures including buckling and vibration.