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A theoretical investigation on mechanical behavior of PEEK/MWCNT/bioactive glass composites for dental and bone implant applications

Mehdi Khanmohammadi ^a, Reyhaneh Nasr Azadani ^{b*}

^a Kroto Research Institute, School of Chemical, Materials and Biological Engineering, University of Sheffield, Sheffield S3 7HQ, UK.

^b Department of Bioengineering, McGill University, Montreal, QC, H3A 0E9, Canada.

ABSTRACT

Due to having an elastic modulus similar to that of bone, polyetheretherketone (PEEK) is a good choice for personalized bone and dental implants; however, its non-bioactive nature hinders its usage. The present study establishes innovative predictive models that optimize the flexural strength and elastic modulus of PEEK composites with multi-walled carbon nanotubes (MWCNT) and bioactive glass (BG). Eight different composite types containing 0 to 5 wt% of MWCNTs and 0 to 10 wt% of BG were made and then assessed. To quantify model uncertainty, response surface methodology (RSM) combined with bootstrap resampling (2000 iterations) was applied. The full quadratic model predicts flexural strength accurately ($R^2 = 0.9851$) and indicates that the ideal composition is 3 wt% MWCNT and 5 wt% BG with a flexural strength of 209.47 MPa, which is a 60.9% increase compared to pure PEEK. Negative quadratic and interaction coefficients confirmed the influence of agglomeration processes of fillers and stress concentration at higher levels of material concentration. In terms of elastic modulus, the reduced linear model ($R^2 = 0.6460$) confirmed an important effect of the reinforcement material, i.e., MWCNT, on the enhancement of elastic modulus, while no particular effect of BG was confirmed.

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1. Introduction

Implementation of patient-specific implants (PSI) necessitates the use of materials whose mechanical attributes are nearly equivalent to those of natural bones in order to avoid inducing stress shielding. Compared to titanium (Ti), polyetheretherketone (PEEK) has several desirable properties that have made it the choice for PSI, chiefly the fact that it has almost similar mechanical strength and elastic modulus (E-modulus) as those of bones [1-4]. Although body PEEK is characterized by good mechanical properties, it can be tailored to improve its load-bearing state; e.g., the incorporation of carbon fibers can enhance the E-modulus of the material to match that of cortical bones [4,5].

Carbon nanotubes (CNTs) are highly effective in providing a radical enhancement of the flexural strength of PEEK in composite materials owing to their exceptional mechanical properties. CNTs, which are believed to be one of the strongest materials available, possess greater possible flexural strengths than metals and ceramics at 14.2 ± 8 GPa, 11–52 GPa in tensile strengths, and 32–

1470 GPa in E-modulus [6,7]. The enhancement of flexural strength and mechanical properties of the composite highly depends on the uniform distribution of CNTs in the polymer matrix and good interfacial adhesion so that effective stress transfer from CNT to polymer can be performed [8-10]. Poor properties of dispersion and adhesion of CNT to the polymer matrix can lead to increased local stresses and lowered energy to fracture, thus reducing flexural and mechanical properties of the composite [11-13].

When trying to add other bioactive materials like bioactive glasses (BGs) to enhance osseointegration [14-16], the mechanical properties of the produced ternary composites (PEEK-MWCNT-BG composites) need to be preserved. Earlier research works reported that preparation techniques for such composites include methods like adsorption coprecipitation and injection molding with different BGs and MWCNTs concentrations [12,17]. The mechanical performance of these composites includes flexural and compressive strength, which can be influenced by interfacial

* Corresponding author: Reyhaneh Nasr Azadani, Email: Reyhaneh.nasrazadani@mail.mcgill.ca

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effects and dispersion level of fillers in addition to their energy to failure.

Khallaf and colleagues [18] conducted a study where they evaluated both mechanical and biological characteristics of PEEK composites that have been augmented with the incorporation of multi-walled carbon nanotubes (MWCNTs) and nano-bioactive glass (BG) for custom-made implants. The conducted three-point bending tests pointed out that adding fillers led to an increase in the flexural strength of the substance. The ternary composite that includes 3% of MWCNTs and 5% of BGs has demonstrated the highest flexural strength of 209.47 MPa, which is 60.9% higher in comparison with the pure PEEK (130.16 MPa). It needs to be emphasized that any of the obtained composites were stronger in comparison to the cortical bone (50-150 MPa) and cancellous bone (10-20 MPa), and thus they can be used for load-bearing tasks. Although the main aim of the research was to evaluate the flexural strength and elastic modulus of PEEK composites, the study is also in line with the existing literature where the addition of nano-BGs improves the compression strength of PEEK matrices and thus points out the great prospect of ternary composites in structural bone and dental implant applications.

The promising mechanical enhancements provided by the MWCNTs and BGs are encumbered by the complicated and non-linear behavior of MWCNTs and BGs in relation to the PEEK matrix, making it hard to predict mechanical properties based on experiment-oriented knowledge. In order to overcome this problem, the current study employs advanced statistical modeling and empirical data to create an efficient predictive system. Thus, the Response Surface Methodology (RSM) has been coupled with the Bootstrap resampling method in order to evaluate the influence of MWCNT and BG content on the bending rigidity and elastic modulus of the composite. Working on the predictive modelling based on experimental data presented in [18], this approach allows the quick identification of the optimal proportions of fillers that account for excellent mechanical properties as well as enables the determination of statistical uncertainty associated with such predictions. Thus, the presented data-driven modeling approach can provide an efficient mathematical instrument to control the mechanical properties of PEEK-based ternary composites.

2. Materials and methods

2.1. Statistical modeling and uncertainty analysis

In order to quantitatively assess both the individual and interactive impacts of MWCNT and bioactive glass (BG) concentrations on the mechanical behavior of PEEK composites, a methodology known as response surface methodology (RSM) was implemented. RSM is an amalgamation of statistical and mathematical methods that is commonly applied in materials science for solving problems where the sought-after result depends on various factors while aiming to achieve the best possible outcome [19, 20].

2.1.1. Quadratic regression model for flexural strength

Based on the experimental design with two independent variables, MWCNT content (x_1 , wt%) and BG content (x_2 , wt%), a full second-order polynomial model was fitted to the flexural strength (FS) data. The general form of the model is expressed as Eq. (1).

$$Y_{FS} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \epsilon \quad (1)$$

where Y_{FS} is the predicted flexural strength (MPa), β_0 is the intercept (constant term), β_1 and β_2 are the linear coefficients, β_{11}

and β_{22} are the quadratic coefficients representing the curvature of the response surface, β_{12} is the interaction coefficient capturing the synergistic or antagonistic effects between the two fillers, and ϵ is the residual error term. The coefficients were estimated using the ordinary least squares (OLS) method, and the model adequacy was evaluated by the coefficient of determination (R^2) and adjusted R^2 .

2.1.2. Reduced linear model for E-modulus

For the elastic modulus (E-modulus), initial analysis and rational reasoning suggested that including BG has an insignificant effect on PEEK stiffness, which is in agreement with experimental findings discussed in the results section. In order to prevent statistical overfitting, especially in view of a small number of samples ($N=8$) and small variance of E-modulus values (3.5–4.2 GPa), a simpler linear model considering only the main effects was used (Eq. (2)):

$$Y_E = \alpha_0 + \alpha_1 x_1 + \alpha_2 x_2 + \epsilon \quad (2)$$

where Y_E is the predicted E-modulus (GPa), and α_0 , α_1 , and α_2 are the intercept and linear coefficients, respectively. This parsimonious approach follows the principle of model simplicity and prevents the inflation of variance that typically arises when higher-order terms are fitted to datasets with low signal-to-noise ratios [21].

2.1.3. Bootstrap resampling for uncertainty quantification

Given the limited number of experimental data points, conventional parametric assumptions for confidence intervals may not be fully reliable. Therefore, a non-parametric bootstrap resampling technique was employed to quantify the uncertainty of the estimated regression coefficients and model predictions [22, 23].

In this procedure, $B = 2000$ bootstrap samples were generated by random sampling with replacement from the original dataset of size $N = 8$. For each resampled dataset, the regression model was refitted, and the distribution of the resulting coefficients was used to construct the 95% confidence intervals (CI) based on the 2.5th and 97.5th percentiles of the bootstrap distribution. The bootstrap mean of each coefficient was reported alongside its 95% CI, providing a robust measure of the statistical reliability of the model terms.

A coefficient whose 95% CI does not include zero is considered statistically significant at the $\alpha = 0.05$ level, indicating a meaningful contribution to the response. Conversely, when the CI includes zero, the corresponding term is deemed statistically non-significant, which may reflect either a genuine lack of effect or the limited statistical power arising from the small sample size. All statistical computations and graphical representations were performed using Python 3.12 with the libraries NumPy, scikit-learn, statsmodels, and Matplotlib.

2.2. Systems under study and mechanical testing

2.2.1. Systems under study

In order to assess the impact of the different reinforcing fillers, eight composite systems were created and characterized according to the wt% of MWCNTs and BG nanoparticles mixed in the PEEK matrix. The studied systems included the control pure PEEK (P), binary PEEK-MWCNT composites (PC3 with 3 wt% MWCNTs and PC5 with 5 wt% MWCNTs) mixtures of PEEK and BG at 5 wt% (PG5) and at 10 wt% (PG10), and hybrid PEEK-MWCNT-BG composites (PC3G5 at 3 wt% MWCNTs and 5 wt% BGs;

PC3G10 at 3 wt% MWCNTs and 10 wt% BGs; PC5G5 with 5 wt% MWCNTs and 5 wt% BGs).

2.2.2. Mechanical testing

The mechanical characteristics of the samples that were developed were assessed through flexural and compressive examination. To determine flexural strength and elastic modulus, a three-point bending test was conducted using a universal testing device (Instron 3365, MA, USA) according to relevant standards. The bar-type samples measuring $15 \times 2.5 \times 1.5$ mm were placed in one row on two round supports with a span of 10 mm. The use of a wedge-shaped indenter with a rounded edge at the central point of the samples had a constant crosshead speed of 1 mm/min till breaking. The mechanical properties were evaluated using relevant software (Instron Bluehill 3).

Furthermore, as the measurement of compressive strength is necessary for evaluating the load-carrying capacity of composites under axial loading conditions in connection with dental and orthopedic implant applications, the compressive strength was measured according to standard methods for rigid materials (e.g., ASTM D695). The performed test worked by applying the compressive load along the axis of the specimens until the full breakdown of the specimen materials at a certain speed. This study provides another aspect of mechanical evaluation that allowed checking whether the developed materials have enough structural integrity under bending and compressive stresses.

3. Results and discussion

To quantitatively evaluate the individual and interactive effects of MWCNT and bioactive glass (BG) contents on the mechanical responses of the PEEK composites, predictive regression models were developed and validated using non-parametric bootstrap resampling (2000 iterations).

The flexural strength (FS) data was fitted with a comprehensive quadratic response surface model. The model proved to be effective since it adequately fits the experimental data and provides a coefficient of determination $R^2=0.9851$. The predictive equation of the model, based on the average bootstrap coefficients, is given by the equation $Y_{FS} = 140.180 + 15.636 x_1 + 10.170 x_2 - 1.333x_1^2 - 0.583x_1x_2 - 0.583 x_1 x_2 - 0.717 x_2^2$

Bootstrap analysis produced robust confidence intervals (CI=95%) for every determined coefficient. The linear coefficients were 15.636 (95% CI: [-1.179, 38.580]) for MWCNT and 10.170 (95% CI: [-6.411, 25.430]) for BG, respectively. The very severe observation is that all bootstrap estimates for the quadratic coefficients, which are MWCN2 and BG2, along with the interaction coefficients, MWCN×BG, have negative values as follows: -1.333, -0.717, and -0.583, respectively.

It should be emphasized that the computed 95% confidence interval for the mentioned higher-order terms includes value 0 (e.g., [-4.896, 5.165] for $MWCNT^2$ and [-2.256, 2.721] for BG^2), which is somewhat anticipated because the sample size here ($N = 8$) is fairly small in comparison to the count of model parameters (6), which leads to the increase of variance in resampled datasets. Nevertheless, the negative tendency of the mean values of coefficients comes to prove the above-mentioned phenomenon of filler agglomeration and stress concentration on introducing larger amounts of the loading. Using a simplified linear model accounting only for the main factors, the E-modulus was calculated. This approach was deemed appropriate due to the small variations measured in stiffness (3.5 to 4.2 GPa), as well as the fact that BG addition is unlikely to modify the stiffness of

PEEK significantly. The resulting model's R^2 was equal to 0.6460. The formula is the following: $E = 3.645 + 0.094x_1 - 0.014x_2$.

A bootstrap test was conducted (2000 iterations) to define 95% confidence intervals of the coefficients. The linear coefficient of MWCNT is equal to 0.094 with 95% CI [0.001, 0.160]. The fact that the interval does not encompass zero verifies the existence of a significant positive effect of MWCNT on the composite's stiffness.

In contrast, the coefficient for BG yielded a result of -0.014 with a confidence interval of 95%: [-0.065, 0.036]. The presence of zero in this interval indicates that the impact of BG on E-modulus is statistically insignificant. The calculated result is in complete harmony with the laboratory results because the E-modulus values of the binary PEEK-BG groups were the same as that of pure PEEK (for example, 3.6 GPa for PG5 and PG10). This means that in this specific matrix, BG acts mainly as a bioactive filler and not as a stiffener.

In order to obtain a quantitative value for the total impact of MWCNT and BG incorporation into the flexural strength of PEEK composites, a full quadratic response surface model was obtained from the experimental results [18]. The obtained three-dimensional surface plot (Fig. 1) shows the predicted flexural strength as a continuous function of both filler contents, with experimental data represented by red spheres for comparison.

The model exhibited an excellent fit to the experimental data, yielding a coefficient of determination of $R^2=0.985$. As clearly visible in the surface plot, the flexural strength increases progressively from pure PEEK (130.16 MPa at 0 wt% MWCNT and 0 wt% BG) toward a well-defined maximum in the region of 3 wt% MWCNT and 5 wt% BG. This peak corresponds to the PC3G5 group, which recorded the highest experimental flexural strength of 209.47 MPa, representing a 60.9% improvement over pure PEEK.

Beyond this optimal composition, the response surface exhibits a noticeable downward curvature, particularly along the BG axis. At 10 wt% BG (e.g., the PC3G10 and PG10 groups), the predicted and experimental flexural strengths decline to 167.73 MPa and 158.88 MPa, respectively. This negative curvature is mathematically captured by the negative quadratic coefficients of the model (-1.333-1.333 for $MWCNT^2$ and -0.717-0.717 for BG^2) and is physically attributed to the agglomeration of fillers at higher loadings. As confirmed by the SEM micrographs (Fig. 1), increased BG concentration leads to the formation of agglomerates that act as stress concentration sites, restrict polymer chain mobility, and ultimately reduce the load-bearing capacity of the composite. The negative interaction coefficient (-0.583 for $MWCNT \times BG$) further indicates that the simultaneous presence of high concentrations of both fillers hinders their homogeneous dispersion, thereby diminishing the expected synergistic reinforcement.

In order to facilitate better visualization of the optimal composition area, the three-dimensional response surface was projected onto a two-dimensional contour map (Fig. 2). Here color gradient denotes predicted flexural strength values, while the overlaid black contour lines connect the points of the same strength (iso-strength lines). The eight experimental results are also projected onto the response surface as red points so that the experimental results can be compared with the predicted results.

The contour map has clearly defined an elliptical area with maximum flexural strength (>205 MPa) lying approximately at the area of composition (3 wt% MWCNT and 5 wt% BG).

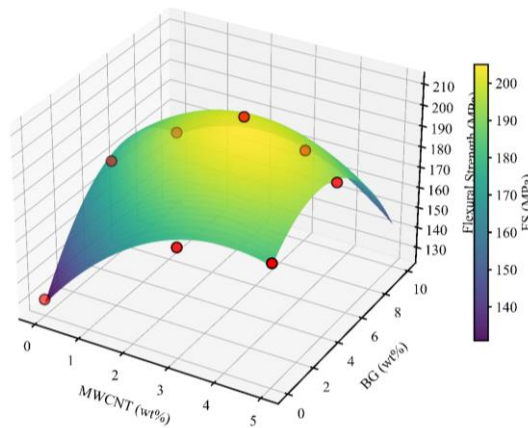


Fig. 1. Three-dimensional response surface plot of flexural strength (FS) as a function of MWCNT and bioactive glass (BG) contents (wt%).

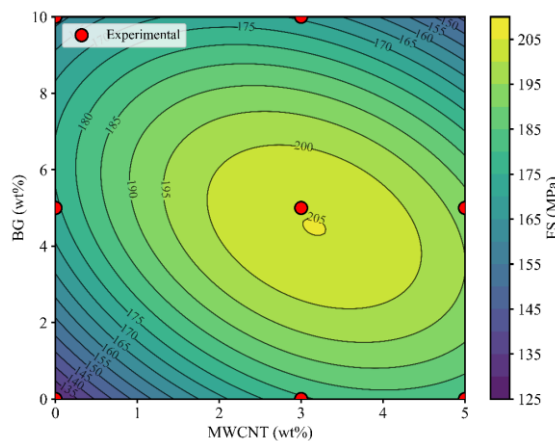


Fig. 2. Contour map of flexural strength (FS) as a function of MWCNT and bioactive glass (BG) contents (wt%). The color gradient represents the predicted FS values from the full quadratic regression model, with contour lines indicating iso-strength levels.

This area matches very well with the PC3G5 group, where the highest flexural strength (209.47 MPa) was shown in experimental work. As we move away from the marked optimum radially, the iso-strength lines are slowly decreasing in the order of (200, 195, 190, 185, 180 MPa, etc.), making it clear that flexural strength is very sensitive to the deviations from the optimal filler composition.

The contour map clearly indicates an asymmetrical format concerning the BG axis. Namely, the spacing between the iso-strength lines becomes denser as the BG content increases, showing a sharper decrease in the flexural strength as the concentration of BG increases. This asymmetry shows a graphical representation of the negative coefficient of the quadratic term BG^2 ($\beta = -0.717$) as well as the negative interaction term $MWCNT \times BG$ ($\beta = -0.583$) in the regression model. In physical meaning, it means that the BG particles, due to their ceramic and brittle nature, have a greater tendency to agglomerate with increasing loadings than MWCNTs, which are fibrous in their nature. As shown in the SEM micrographs in [18], at 10 wt% loading of BGs, the phenomenon of agglomeration takes place, creating stress concentrating points and reducing the carrying capacity of the composite that resulted in the decrease of the flexural strength.

Conversely, the distances between the contours of the response surface model in the MWCNT direction are larger at lower

concentrations (0–3 wt%), which suggests a slower but continuous increase in flexural strength with the increase in the MWCNT content due to the efficient load transfer mechanism between the strong nanotubes and the PEEK matrix. On the contrary, the contours start to bend down for the sample containing 5 wt% MWCNT, indicating the process of MWCNT entanglement and lower transfer efficiency, which is corroborated with the results of the previous observations based on SEM in [18]. In addition, the agreement between the experimental values and contours is good enough to support the efficiency of the quadratic model. For instance, the group PC3G10, which contained 3 wt% MWCNT and 10 wt% BG, falls on the contour with an approximate strength of 170 MPa, which is close to its experimental value of 167.73 MPa. Also, the group PG10, which contained 0 wt% MWCNT and 10 wt% BG, is placed near the contour strength of 160 MPa, which correlates with its experimental strength of 158.88 MPa.

In contrast to the pronounced curvature observed for flexural strength, the three-dimensional response surface of the E-modulus (Fig. 3) exhibits a nearly planar geometry, consistent with the reduced linear model adopted for this response. The model, expressed as $E = 3.645 + 0.094(MWCNT) - 0.014(BG)$, yielded a coefficient of determination of $R^2 = 0.646$, which is lower than that of the flexural strength model but appropriate given the narrow experimental variance of the stiffness values (ranging from 3.5 to 4.2 GPa) and the deliberate exclusion of higher-order terms to prevent statistical overfitting.

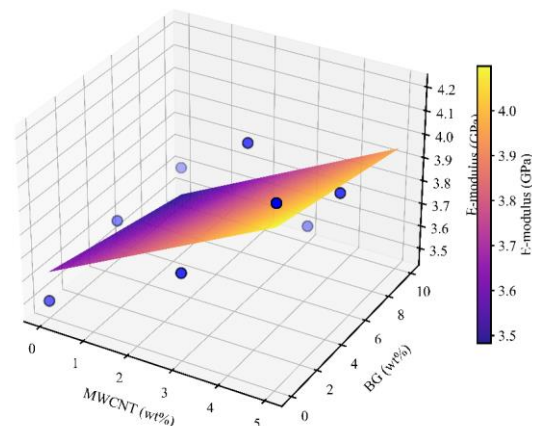


Fig. 3. Three-dimensional response surface plot of the elastic modulus (E-modulus) as a function of MWCNT and bioactive glass (BG) contents (wt%).

The response surface shows two specific and important physical characteristics. First, there is a very mild upward slope along the axis. So, when moving from 0 wt% MWCNT to 5 wt% MWCNT, we can observe an increase from about 3.5 GPa to 4.2 GPa. The slope is determined by the linear coefficient of 0.094 GPa per wt% MWCNT, which has a confidence interval of [0.001, 0.160], indicating that the precise incorporation adds stiffness to the matrix. The reason for that can be found in the high modulus of elasticity of MWCNTs (which is known to be in the range from 32 to 1470 GPa). The effective transfer of the load happens from the polymer matrix to the rigid nanotubes if there is enough proper adhesion established. In addition, and most importantly, the responses along the axis of BG are almost flat. The linear coefficient of BG is -0.014 GPa per wt% BG, and it is evident from the confidence interval of 95%, [-0.065, 0.036], that zero is included in this range. This means that the use of bioactive glass in this concentration interval, from 0 to 10 wt%, does not affect the elastic modulus of PEEK composites. The results

obtained here mathematically correspond to the experimental results shown in [18] above, where the binary PEEK-BG groups of PG5 and PG10 have the E-modulus values of 3.6 GPa, similar to that of pure PEEK (3.5 GPa). The flat characteristics of the response surface and the random arrangement of the data points vertically support the argument that the E-modulus of the materials depends entirely on MWCNT content, while the contribution of BG content is limited to a function of bioactive filler. The process of separating mechanical stiffening (caused by MWCNTs) from bioactivity (caused by BGs) is an important consideration for implant designs for particular patients, as it indicates that bioactive portions of the implants can be optimized independently of mechanical load-bearing requirements if, of course, the correct amount of MWCNTs is maintained in the material.

It is important to indicate that the PC3G10 class (3 wt% MWCNT, 10 wt% BG) achieved a value of E-modulus equal to 3.5 GPa, being the same as that of pure PEEK, which varies from the linearity predicted by the model. The reason for the deviation can be seen in the agglomeration of BG particles noticed at a high concentration, which, as it was mentioned while discussing flexural strength, can impede the efficiency of load transfer in the MWCNT structure and reduce their stiffening effect. However, the general linear model well describes the existing trend and demonstrates a simple representation of E-modulus behavior.

In order to specify the relative effect of MWCNT and BG contents on the elastic modulus of different PEEK composites, the three-dimensional response surface was projected onto the two-dimensional contour map (Fig. 4). The color gradient in this presentation represents the expected values of the E-modulus, whereby the violet color corresponds to the expected E-modulus equals to about 3.44 GPa (at the lower MWCNT concentrations), and the yellow color corresponds to about 4.08 GPa (at 5 wt% of MWCNT), while the black contour lines show the points of similar overall stiffness (iso-stiffness lines). The experimental points are shown on the map as blue circles for better comparison with the theoretical calculations.

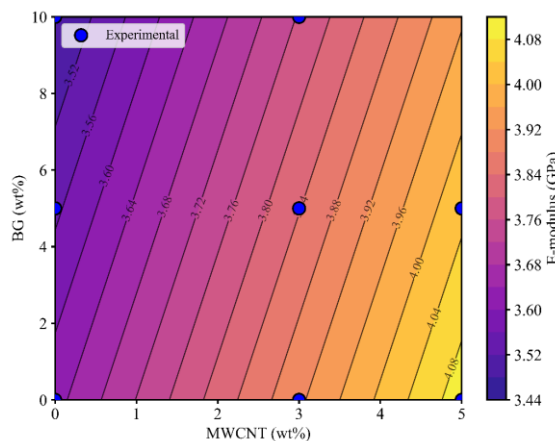


Fig. 4. Contour map of the elastic modulus (E-modulus) as a function of MWCNT and bioactive glass (BG) contents (wt%).

The contour graph shows an interesting geometrical feature with a significant physical meaning: the iso-stiffness lines are practically straight, parallel, and almost perpendicular to the MWCNT axis. It indicates that the system behaves according to the rule where only one independent variable (MWCNT content) defines the dependent variable (E-modulus), with the second variable (BG content) having a minimal effect.

Numerically, the iso-stiffness lines are moved by 0.04 GPa per 1 wt% of MWCNT content, i.e., the value that matches with the linear coefficient of 0.094 GPa per wt% MWCNT from the

simplified linear model. On the contrary, moving vertically up and down the BG axis (from 0 to 10 wt% BG) at a given level of MWCNT concentration does not result in any noticeable variation in the E-modulus value, as shown by the almost horizontal position of the iso-stiffness lines.

This graphical evidence shows clearly that bioactive glass at the concentrations being studied (0-10 wt%) does not serve as a structural stiffening agent for the PEEK matrix. This is consistent with the experimental results shown in [18], in which the E-modulus for the binary PEEK-BG formulations (PG5 and PG10) was determined to be 3.6 GPa, which is almost the same as that of pure PEEK (3.5 GPa). The non-significant value of the BG parameter (95% CI: $[-0.065, 0.036]$, note that this interval includes zero) further validates this conclusion.

The close match of the experimental data points (blue circles) with the predictive contour lines proves that the reduced linear model is valid. For instance, the PC5 group (5 wt% MWCNT, 0 wt% BG) lies on the ~4.08 GPa contour line, where it is equal to the experimental value of 4.2 GPa, while P (0 wt% MWCNT, 0 wt% BG) is close to the contour line of 3.52 GPa and is compatible with the measured value of 3.5 GPa. The small difference that occurs in some data points, for example, PC3G10, which is at 3.5 GPa, being lower than the expected ~3.80 GPa contour line, is likely related to the aggregation of BG particles at large concentrations that undermine the efficiency of load transfer in the MWCNT network and counteract their stiffening influence.

The separation of mechanical hardness (caused by MWCNTs) and bioactivity (caused by BGs), as illustrated in the present contour diagram, gives a unique insight in the field of engineering individualized prosthesis.

It makes it possible to refine the bioactive component in isolation from load-bearing conditions, as long as the concentration of MWCNTs remains appropriate for getting the necessary stiffness. This freedom of choosing components is especially beneficial in creating implants to be used in particular medical cases such as craniofacial reconstructions of low-stress nature where both bioactivity and matching stiffness are necessary. To assess the statistical robustness of the developed regression models and to quantify the uncertainty associated with the estimated coefficients, a non-parametric bootstrap resampling technique was employed.

Given the limited experimental sample size ($N=8$), conventional parametric assumptions for confidence intervals may not be fully reliable. Therefore, 2000 bootstrap samples were generated by random sampling with replacement, and the distribution of the resulting coefficients was used to construct the 95% confidence intervals (CIs), as illustrated in Fig. 5. For the flexural strength model (left panel of Fig. 5), the mean bootstrap estimates for the linear terms (MWCNT and BG) are positive, reflecting their initial reinforcing contribution. Crucially, the mean coefficients for the quadratic terms ($MWCNT^2$ and BG^2) and the interaction term ($MWCNT \times BG$) are consistently negative. It is important to note that the 95% CIs for these higher-order terms include zero (e.g., $[-4.896, 5.165]$ for $MWCNT^2$). This is an expected statistical artifact arising from the limited sample size relative to the number of model parameters, which inherently inflates the variance in resampled datasets.

However, the persistent negative directionality of the mean coefficients provides sufficient mathematical evidence to support the physical observation of filler agglomeration and stress concentration at higher loadings, as visually confirmed by the SEM micrographs.

For the E-modulus model (right panel of Fig. 6), the bootstrap analysis yields highly conclusive results. The linear coefficient for MWCNT is positive (mean = 0.094), and its 95% CI $[0.001, 0.160]$ lies entirely above zero. This confirms, with high statistical

confidence, that MWCNT incorporation has a significant stiffening effect on the PEEK matrix. Conversely, the coefficient for BG is near zero (mean = -0.014), and its 95% CI [-0.065, 0.036] clearly encompasses zero.

This statistical result provides quantitative proof that the incorporation of bioactive glass, within the investigated concentration range, does not exert a meaningful influence on the elastic modulus of the composites. This mathematical finding is in perfect agreement with the experimental observations [18], where binary PEEK-BG groups exhibited E-modulus values nearly identical to pure PEEK, confirming that BG acts primarily as a bioactive filler rather than a structural stiffener in this specific matrix. To further validate the predictive capability of the developed regression models, the mean predicted values from the 2000 bootstrap iterations were plotted against the corresponding experimental measurements (Fig. 6).

For the flexural strength (left panel), the data points cluster closely around the ideal line of perfect agreement ($y=x$), confirming that the full quadratic model successfully captures the complex, non-linear relationship between the filler contents and the mechanical response. The 95% confidence intervals (CIs) associated with the predictions are relatively wide, which is an

inherent consequence of the limited sample size ($N=8$) and the high number of parameters in the quadratic model. Nevertheless, the experimental values consistently fall within or very near the predicted confidence bands, demonstrating the model's robustness in estimating the flexural strength across the investigated compositional space.

For the elastic modulus (right panel), the predicted values also align well with the experimental data along the ideal line. The 95% CIs for the E-modulus predictions are noticeably narrower than those for the flexural strength.

This reflects the lower experimental variance and the simpler, linear nature of the E-modulus model. The close agreement between the predicted and experimental E-modulus values further corroborates the conclusion that the stiffness of the composites is predominantly governed by the MWCNT content, with the reduced linear model providing a reliable and parsimonious description of the data.

Overall, the bootstrap-based validation confirms that despite the small dataset, the developed models possess strong predictive accuracy and can be confidently used to guide the design of PEEK-MWCNT-BG composites for patient-specific implant applications.

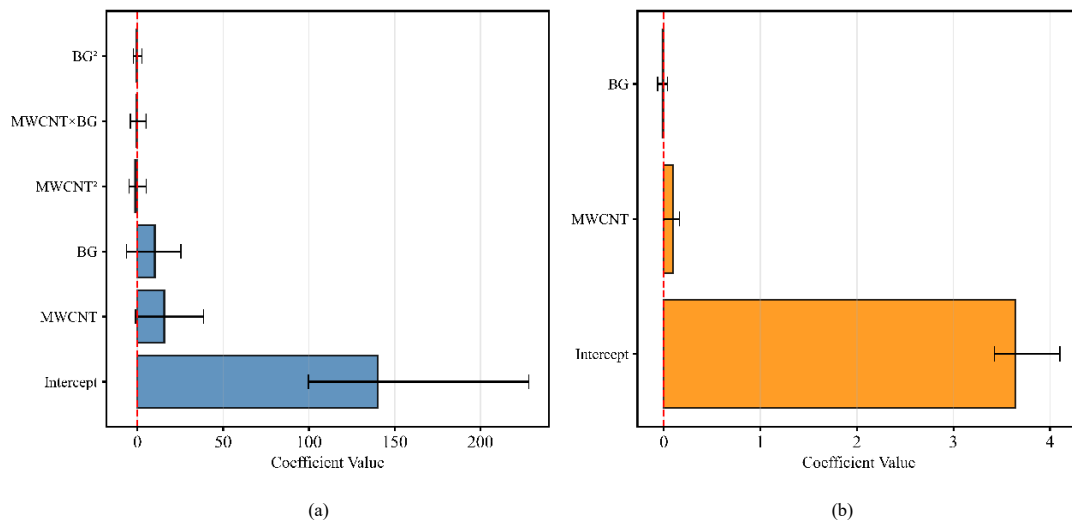


Fig. 5. Bootstrap regression coefficients and their 95% confidence intervals (CIs) for the flexural strength (a) and E-modulus (b) models.

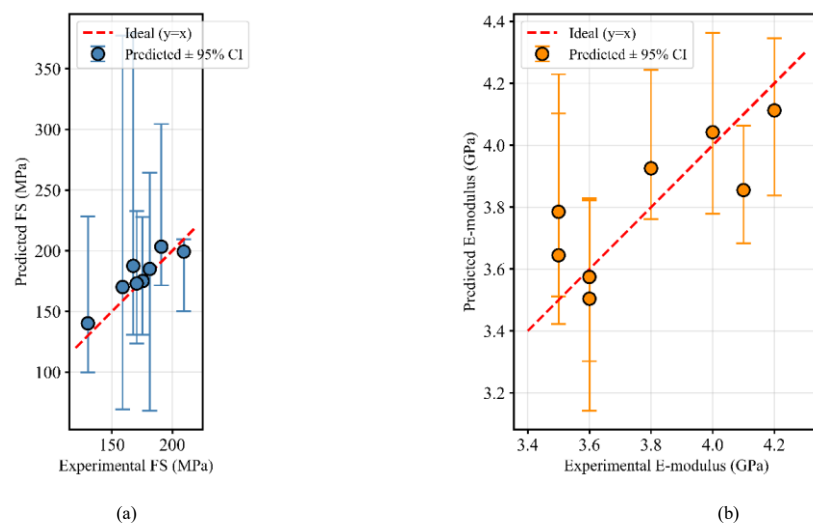


Fig. 6. Predicted versus experimental values for (a) flexural strength (FS) and (b) elastic modulus (E-modulus).

4. Conclusion

This research has accomplished the achievement of creating a dependable, effective predictive framework based on data for optimizing mechanical properties of ternary PEEK-MWCNT-BG composites by keeping in mind the specific requirements of dental and orthopedic implants of an individualized nature. It is accomplished with the help of the Response Surface Method (RSM) along with nonparametric bootstrap resampling, through which the complexity and non-linear relation between reinforcing filler materials and PEEK matrix have been analyzed, thus achieving the desired goals of design of the biomaterials. Based on flexural strength, which is an important factor for withstanding chewing forces in dental prosthesis and load being placed on bones in biomechanical scaffolds, the full quadratic regression method has turned out to be a perfect fit, having been achieved with the R-squared coefficient of the determined value lying within the scope of 0.9851. Thus, it was defined that around 3% MWNT and 5% of BG help complete the composition with the corresponding flexural strength valued at 209.47 MPa that signifies 60.9% improvement as compared to pure PEEK being used before. In addition, the Bootstrap analysis mathematically confirmed the physical limits of filler loading by detecting the critical threshold at which agglomeration compromises structural integrity.

More importantly, the elastic modulus was successfully characterized by a simple reduced linear model ($R^2=0.6460$). In addition, the uncertainty analysis proved the decoupling of mechanical stiffening from bioactivity: while MWCNTs produced a significant stiffening effect (95% CI: [0.001, 0.160]), bioactive glass had a statistically insignificant effect on the stiffness (95% CI: [-0.065, 0.036]). This is very important for the dental and orthopedic field because it shows that the osteoconductive BG can be introduced into the material to achieve osseointegration without influencing the properties of the PEEK material in terms of its stiffness. In conclusion, this strategy has given birth to a powerful mathematical tool helping customize the PEEK composite composition, allowing it to bring load-bearing capacity and osteointegrative nature to the optimum separately. The most effective components identified during this research, and especially the PC3G5 group, could be used in the production of patient-specific dental and bone products and require a thorough in vitro and in-vivo study.

Author contributions

Mehdi Khanmohammadi: Conceptualization, Writing – original draft, Writing – review & editing; **Reyhaneh Nasr Azadani:** **Reyhaneh Nasr Azadani:** Writing – original draft, Writing – review & editing.

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Conflict of interest

The authors confirm that no competing interests are associated with this work.

Data availability

No datasets were produced or utilized in the present study.

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