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DFT-based investigation of polyetherketoneketone materials for surface modification for dental implants

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Abstract

Background Polyetherketoneketone (PEKK) is a high-performance thermoplastic polymer with unique structural and mechanical properties that make it a promising candidate for surface modification of dental implants. This study was conducted to investigate the feasibility of PEKK for this purpose using the Cambridge Serial Total Energy Package (CASTEP) code based on density functional theory (DFT).

Methods This study examined the ground state energy, structural properties, thermodynamic behavior, cohesive energy, refractive index, stress analysis, mechanical properties, and anisotropic behavior of PEKK**.**

Results This study found that PEKK has a complex crystal structure with an orthorhombic unit cell shape, triclinic lattice type, and a centered structure. It also has a 2D layered structure owing to the presence of carbonyl groups, which provides a large surface area for interaction with biological tissues. Thermodynamic analysis showed that PEKK exhibited bond elongation and structural changes at 380 °C, indicating thermal degradation. The cohesive energy of PEKK was calculated to be – 440 eV, indicating its stability and structural integrity. PEKK has a complex refractive index, with real and imaginary components that affect its optical properties. Stress analysis showed that PEKK is resistant to shear deformation and has high hydrostatic stress, which contributes to its stability and biocompatibility.

Conclusion The mechanical properties of PEKK, including its high stiffness, resistance to volume change under pressure, and ability to accommodate natural movements, make it suitable for surface modification of dental implants.

Keywords PEKK, Polymer, Dental implant, Density functional theory

Introduction

PEKK is a high-performance thermoplastic polymer with excellent mechanical properties, thermal stability, and biocompatibility [1]. It is considered a potential substitute for metal bone implants owing to its advantageous biocompatibility, chemical stability, and mechanical properties [2]. PEKK is being increasingly investigated as a surface modification material for dental implants because of its ability to enhance osseointegration and reduce the risk of bacterial adhesion on the implant surface. In dental implantology, surface modification is a critical aspect of implant design as it influences the success of the implant by promoting bone healing

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and integration. PEKK, with its unique combination of properties, presents an attractive option for enhancing the surface properties of dental implants [3, 4]. One of the methods used for the surface modification of dental implants with PEKK is plasma spraying, which involves depositing a thin layer of PEKK onto the implant surface. This process improves the biocompatibility of the implant and promotes osseointegration by providing a surface conducive to bone cell attachment and growth [5].

Another approach to surface modification involves chemical treatment, in which the implant surface is treated with specific chemicals to alter its surface properties. For example, a surface can be functionalized with peptides or other molecules that promote cell adhesion and bone growth. Additionally, coating techniques such as electrospray or dip coating have been explored as methods for applying a PEKK coating to the implant surface [6–8]. These techniques allow precise control over the thickness and composition of the coating, further enhancing the biocompatibility of the implant and promoting osseointegration. PEKK is a high-performance thermoplastic polymer that has emerged as a promising material for the surface modification of dental implants [9]. This is because of its unique combination of properties: One of the primary considerations in dental implant materials is their biocompatibility, or how well they interact with the body's tissues [10, 11]. PEKK has shown excellent biocompatibility, indicating that it is unlikely to cause adverse reactions or be rejected by the body. This is crucial for dental implants, as they are placed directly into the bone and need to be seamlessly integrated with the surrounding tissues.

PEKK is known for its excellent mechanical properties, including high tensile strength and resistance to wear and tear [12]. This makes it an ideal material for dental implants because it can withstand the forces exerted on the implant during chewing and other activities. Additionally, the strength of the material allows for the creation of thinner implant components, which can help reduce the overall siz of the implant and improve patient comfort. PEKK exhibits excellent thermal stability, meaning that it can withstand high temperatures without deformation or breakdown. This is important for dental implants, as they are often exposed to high temperatures during the manufacturing process and sterilization [13]. The thermal stability of the material ensures that the implant remains intact and functional, even under these conditions.

PEKK is a thermoplastic polymer that has been increasingly investigated for its potential in various biomedical applications including dental implants [14, 15]. Compared with other materials used for dental implants, such as titanium, zirconia, and polymethylmethacrylate (PMMA), PEKK offers a unique set of properties that make it an attractive candidate for enhancing the performance and longevity of dental implants [16]. Both titanium and PEKK are biocompatible materials, meaning that they are unlikely to cause adverse reactions or be rejected by the body [17]. However, PEKK has shown superior biocompatibility in some studies, with lower levels of inflammatory response than titanium. Mechanical strength: Ti is known for its excellent mechanical properties, including high tensile strength and fatigue resistance. PEKK also exhibits good mechanical strength [18], but it has been reported to have a slightly lower tensile strength than titanium. However, PEKK's strength of PEKK is sufficient for dental implant applications. Titanium has good thermal stability, but is prone to oxidation at high temperatures. In contrast, PEKK has excellent thermal stability and can withstand high temperatures without deforming or breaking down [19]. Zirconia is also biocompatible, but studies have reported that PEKK has better biocompatibility in terms of lower levels of inflammatory response and higher cell viability than zirconia [20, 21]. Zirconia is known for its high flexural strength and fracture resistance, making it suitable for dental implant applications [22]. PEKK also has good mechanical strength, but it has been reported to have a slightly lower flexural strength than zirconia [23]. Zirconia has good thermal stability; however, PEKK's thermal stability is superior, making it more resistant to high temperatures. PMMA is a biocompatible material that has been used in dentistry for several years. However, studies have reported that PEKK has better biocompatibility in terms of lower levels of inflammatory response and higher cell viability than PMMA. PMMA is known for its good mechanical properties [21], including high tensile strength and fracture resistance. PEKK also has good mechanical strength, but it has been reported to have a slightly lower tensile strength than PMMA [24]. PMMA has good thermal stability; however, PEKK's thermal stability is superior, making it more resistant to high temperatures [25]. In summary, PEKK offers a unique combination of properties that makes it an attractive material for dental implant applications. It has shown superior biocompatibility, good mechanical strength, and excellent thermal stability compared with other materials commonly used in dental implants [26]. Ongoing research is focused on further optimizing PEKK properties and exploring new techniques for its application in dental implantology [21].

In this study, the ground state energy, structural aspects, thermodynamic traits, cohesive energy, refractive index, stress response, mechanical traits, and anisotropic tendencies of the PEKK were investigated.

PEKK has a complicated crystal structure characterized by an orthorhombic unit cell shape, triclinic lattice type, and centered structure. Furthermore, its 2D layered architecture stems from the presence of a carbonyl group, facilitating an extensive surface area for biological tissue interactions.

Material and methodology

The ground state energy of the material was calculated using the CASTEP (Cambridge Serial Total Energy Package (CASTEP) code, which employs a first-principles technique based on density functional theory (DFT) [27]. The electronic exchange–correlation energy was evaluated using the generalized gradient approximation (GGA) within the Perdew–BurkeErnzerhof scheme [28]. Vanderbilt-type ultra-soft pseudopotentials were utilized to represent the interaction between the valence electrons and ion cores of the atoms. This choice of pseudopotential balances the computational efficiency and accuracy. The K-points were 3×1×1 for the PEKK calculations. The K-point parameter specifies the number of K-points used in the calculation. The Brillouin zone is sampled with 3 k-points in the x direction, 1 k-point in the y direction, and 1 k-point in the z direction. This means that the Brillouin zone will be sampled along one axis (x) and a single point will be used for the other two axes (y and z). The valence electron configurations considered were Pseudo atomic calculation performed for H 1s1 converged in 13 iterations to a total energy of -12.4784 eV, Pseudo atomic calculation performed for C $2s^2$ $2p^2$ converged in 18 iterations to a total energy of -145.7157 eV, and Pseudo atomic calculation performed for O $2s^2$ $2p^4$ for PEKK atoms. Geometry optimization of PEKK was performed using the Limited-memory Broyden–Fletcher–Goldfarb–Shanno (LBFGS) minimization scheme to obtain the lowest energy structure [29].

Results and discussion

Structural properties

PEKK is a high-performance thermoplastic polymer with a complex crystal structure, as evidenced by the data on its unit cell dimensions, lattice type, crystal system, and centered structure. The unit cell dimensions, $a = 4.350$ Å, $b = 11.900$ Å, and $c = 14.450$ Å, suggest that the unit cell is orthorhombic in shape, with three unequal axes of different lengths. The angles between the lattice vectors are $\alpha = \beta = \gamma = 90°$, indicating that the unit cell is triclinic in both the lattice type and the crystal system [30]. Additionally, the centered structure of the unit cell, with atoms located at (0, 0, 0) and (1/2, 1/2, 0), suggests a specific arrangement of atoms within the unit cell, potentially involving a centered position (0, 0, 0) and another centered position (1/2, 1/2, 0).

Furthermore, Fig. 1 illustrates the structural features of PEKK through various geometries, such as shapes, ball-and-stick models (a) wires (b), and polyhedra (d). These models represent the arrangement of atoms in the crystal lattice, highlighting the connectivity between benzene rings and carbonyl groups. The inclusion of these geometries provides a visual representation of the crystal structure of PEKK, aiding the understanding of the complex arrangement of atoms.

The specific crystal structure and chemical composition of PEKK for surface modification of dental implants may offer advantages for this application. For example, PEKK is known for its biocompatibility, mechanical properties, and thermal stability, all of which are crucial for dental implants. Additionally, the specific arrangement of atoms in PEKK, as illustrated by the given geometries, suggests that it may be feasible to modify the surface of PEKK to enhance biocompatibility and promote osseointegration. This can be achieved through plasma spraying, chemical treatments, or coating techniques. Overall, the structural properties of PEKK, as inferred from the given data, indicate that it may be a promising material for surface modification of dental implants. Further research is required to fully understand the potential of PEKK for this application and to optimize its properties for specific dental implantology applications.

Moreover, its 2D layered structure (Fig. 1c) was attributed to the carbonyl groups. The 2D layered structure of PEKK provides a large surface area for interactions with biological tissues. This enhanced surface area promotes better cell attachment and proliferation, leading to improved osseointegration, where bone tissue grows and attaches to the implant. This is crucial for dental implants as it ensures the stability

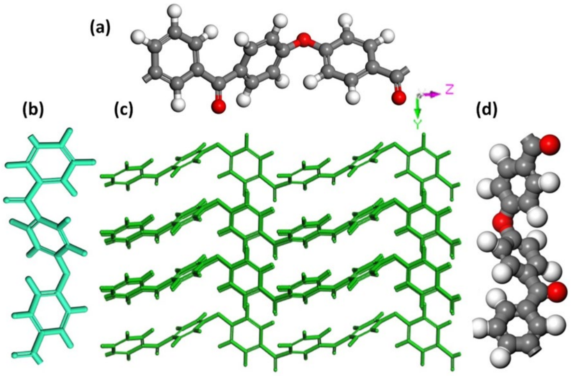

Fig. 1 Crystal structure of the PEKK unit cell (**a**) wire form (**b**), 2D network (**c**), and polyhedron

and longevity of the implant. The 2D structures of PEKK can be coated with bioactive substances such as peptides or growth factors to further enhance cell attachment and tissue integration. This coating can be applied to the entire implant surface or to specific regions depending on the desired outcome. For example, a coating with antimicrobial properties can reduce the risk of infection, whereas a coating with bone growth factors can promote osseointegration.

Thermodynamic study of PEKK

The thermodynamic analysis of PEKK in Fig. 2a, b, and c was conducted using the Cambridge Serial Total Energy Package (CASTEP) software, which employs a first-principles technique based on density functional theory (DFT). The ensemble used for the simulations was NVE, in which the number of particles (N), volume (V), and energy (E) were kept constant. In this ensemble, the system undergoes microcanonical (NVE) dynamics, where the total energy of the system is conserved. For the simulations shown in Fig. 2a, the initial conditions included a random velocity distribution for the particles, and the simulation was run at room temperature. The temperature was specified in Kelvin (K), where room temperature typically ranges from 20 °C to 25 °C, or approximately 293–298 K. This corresponds to approximately 20 °C to 25 °C or 68 °F to 77 °F in degrees Celsius (°C) or Fahrenheit (°F), respectively.

For the simulations shown in Fig. 2b, the temperature was increased to 200 °C. This corresponds to a temperature of approximately 473 K or 392.67 °F. The simulation was run under conditions similar to those shown in Fig. 2a, with a random velocity distribution and NVE ensemble. Finally, for the simulations shown in Fig. 2c, the temperature was further increased to 380 °C [1]. This corresponds to approximately 653 K or 716 °F, respectively. At this temperature, the PEKK material began to exhibit bond elongation and structural changes, indicating thermal degradation. This indicates that the material underwent thermal degradation at 380°C, which can compromise its mechanical properties and biocompatibility. This is undesirable for dental implants because it can lead to implant failure or other complications at 380 °C.

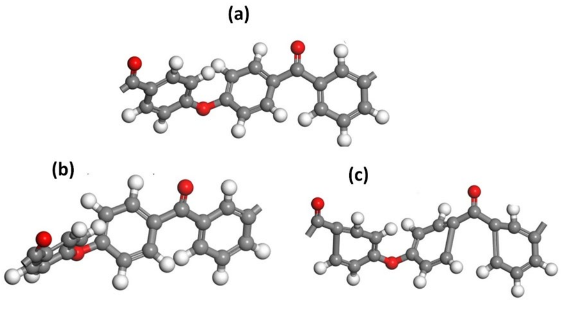

Fig. 2 Thermodynamic analysis of PEKK at 25 °C (**a**) 200 °C (**b**), 380 °C (**c**)

Cohesive energy of PEKK

The cohesive energy ($E_{cohesive}$) of a material is the energy required to separate its constituent atoms or molecules from an infinitely separated state into their equilibrium positions in the solid state. It is a measure of the strength of the bonds that hold the materials together.

The equation to calculate $E_{cohesive}$ is as follows [31]:

$$E_{cohesive} = (E_{total} - (E_A + E_B))/2, \tag{1}$$

Where, $E_{total} = -9.16 \times 10^3$ eV is the total energy of the system; E_A (O) $= -4.24 \times 10^2$ eV is the total energy of an isolated atom or molecule in the same electronic configuration as in the solid state for one type of atom; and E_B (C) $= -3.09 \times 10^2$ eV is the total energy of an isolated atom or molecule in the same electronic configuration as in the solid state for the second type of atom.

First, we calculated the total energy of the isolated atom or molecule in the same electronic configuration as in the solid state (E_{AB}). The total energy of an atom or molecule in the solid state can be obtained by summing the total energy of each atom or molecule in isolation and dividing it by the number of atoms or molecules.

For PEKK,

$E_A = -4.24 \times 10^2$ eV (one atom).

$E_B = -3.09 \times 10^2$ eV (two atoms).

Now, we can calculate the E_{AB}:

$E_{AB} = (E_A * 1 + E_B * 2) / 3.$

$= (-4.24 \times 10^2 * 1 + -3.09 \times 10^2 * 2)/3.$

$= -3.48 \times 10^2$ eV.

Finally, the cohesive energy was calculated as follows:

$E_{coh} = (-9.16 \times 10^3 \text{ eV} - (-3.48 \times 10^2 \text{ eV}))/2.$

$E_{coh} = (-9.16 \times 10^3 \text{ eV} + 3.48 \times 10^2 \text{ eV})/2.$

$E_{coh} = -8.81 \times 10^2$ eV/2.

$E_{coh} = -4.40 \times 10^2$ eV.

Thus, the cohesive energy of PEKK was − 4.40E + 3 eV or − 440 eV.

The cohesive energy of PEKK is − 440 eV. This value indicates that PEKK is a relatively stable material, as the negative sign signifies that energy must be added to the system to separate its constituent atoms. A lower cohesive energy indicates a more stable material, as less energy would be required to separate the atoms. This stability is an important factor in the feasibility of PEKK for the surface modification of dental implants. The surface of dental implants is exposed to the oral environment, which can be harsh and prone to corrosion. A stable material, such as PEKK, would be less susceptible to degradation and would maintain its structural integrity over time, reducing the risk of failure or complications. In addition, the cohesive energy of PEKK can influence its interaction with biological tissues. A stable material with lower cohesive energy is less likely to release harmful substances or cause adverse reactions in the body. This is important for ensuring biocompatibility of the implant and promoting osseointegration, where the implant fuses with the surrounding bone tissue.

Overall, the cohesive energy of PEKK, which indicates its stability and structural integrity, makes it a feasible material for surface modification of dental implants. Further research and development in this area could lead to improved implant materials with enhanced performance and longevity.

Refractive index of PEKK

The graph in Fig. 3 shows the optical constants of a material, often referred to as the complex refractive index. The real part of the complex refractive index, represented by the blue peak, is denoted as 'n,' and the imaginary part of the complex refractive index, represented by the red peak, is denoted as 'k'. The refractive index, n, is a measure of how much light slows down when passing through a material, and the extinction coefficient, k, represents the absorption of light within the material.

In the graph, the x axis represents the refractive index from 0 to 1.8, and the y axis represents the frequency of light from 0 to 42 eV. The blue peak, corresponding t to n, starts at a refractive index value of 1.8 and decreases to 0.9, after which it becomes relatively stable. The red peak, corresponding to 'k', starts at a refractive index value of 0 and reaches 0.9 at 15 eV, after which it also becomes relatively stable at 2 refractive index units.

The optical constants of a material, as represented by its complex refractive index, can provide valuable insights into its optical properties. For example, the refractive i index n can affect the reflection, transmission, and absorption of light, while the extinction coefficient 'k' can affect the color, transparency, and reflectivity of the material.

The reflectivity of a material is determined by its refractive index. By modifying the surface of dental implants with PEKK, it may be possible to adjust their reflectivity, allowing them to better mimic the natural appearance of the teeth. This is particularly important for dental implants in esthetic zones, where the visibility of the implant is a concern. The transparency of a material is determined by its refractive index. PEKK has been shown to have a relatively low refractive index, which makes it less reflective and more transparent than other materials commonly used in dental implants such as titanium or zirconia. This can be important for the integration of the implant with the surrounding tissues, as it allows light to pass through the implant, which can help maintain the natural appearance of the gums and surrounding teeth.

Modifying the surface of dental implants with PEKK may improve their esthetic appearance. For example, PEKK can be colored to match the natural color of the surrounding teeth, which can help create a more seamless and natural-looking smile. Additionally, the low reflectivity and high transparency of PEKK can help improve the overall esthetic appearance of the implant by reducing the visibility of the implant and allowing it to blend more effectively with the surrounding tissues.

Overall, the optical properties represented by the complex refractive index of PEKK can be important for its use as a surface-modifying material for dental implants, as it can help improve the esthetic appearance of the implant and its integration with the surrounding tissues.

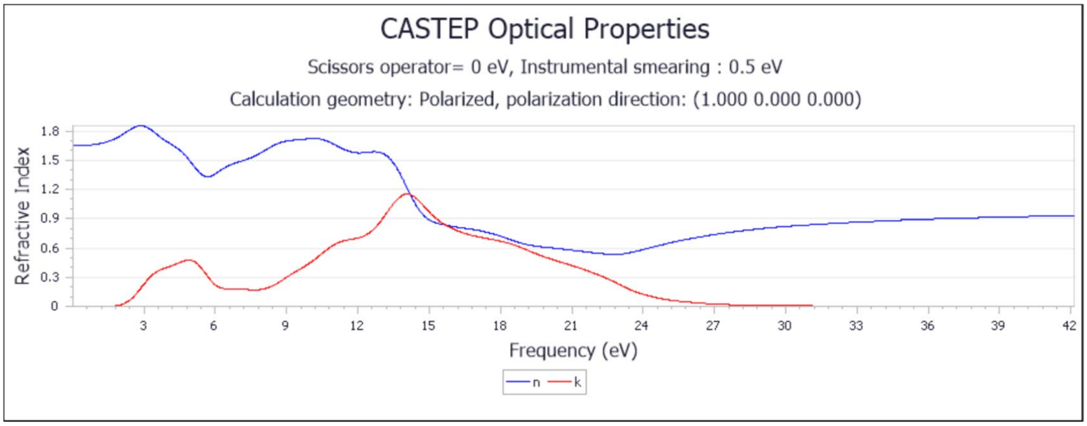

Fig. 3 Thermodynamic analysis of PEKK at 25 °C (**a**) 200 °C (**b**), 380 °C (**c**)

Table 1 Symmetrized stress tensor of PEKK

Cartesian components (GPa)		
x	**y**	**z**
x − 1.216385	− 0.036502	0.079429
y − 0.036502	− 0.691743	0.078526
z 0.079429	0.078526	− 3.097441

Pressure: 1.6685

Table 2 Stiffness matrix (coefficients in GPa) of PEKK

0.0022175	− 0.0004701	− 0.000163	0	0	0
− 0.0004701	0.0022175	− 0.000163	0	0	0
− 0.000163	− 0.000163	0.0019403	0	0	0
0	0	0	0.0063839	0	0
0	0	0	0	0.0063839	0
0	0	0	0	0	0.0053752

Stress analysis of PEKK

The stress data in Table 1 represent the symmetrized stress tensor, which provides information regarding the stress state of a material. In the case of PEKK, the Cartesian components of the stress tensor in gigapascals (GPa) are provided for the x, y, and z directions, as well as the pressure.

In the Cartesian stress tensor, the diagonal elements (x, y, and z) represent the normal stresses acting on the material along the respective directions, whereas the off-diagonal elements represent the shear stresses acting on the material. The pressure value represents the hydrostatic stress, which is the average normal stress acting on the material in all the directions. The stress-bearing ability of PEKK, as indicated by the provided stress tensor, can be analyzed based on the magnitudes and types of stresses present:

The diagonal elements of the stress tensor (x, y, and z) represent the normal stresses acting on the material along their respective directions. The magnitude of these stresses can indicate the material's ability to withstand tension or compression along these directions. In the given data, the normal stresses in the x, y, and z directions were − 1.216385 GPa, − 0.691743 GPa, and − 3.097441 GPa, respectively. Negative values indicate compressive stress, while positive values indicate tensile stress. PEKK's ability of PEKK to resist these stresses can be evaluated based on its mechanical properties (see the Mechanical Properties section) and ultimate strength. The off-diagonal elements of the stress tensor represent the shear stresses acting on a material. The magnitude of these stresses can indicate the material's ability to resist shearing or sliding forces. In the given data, the shear stresses in the xy, xz, and yz planes were -0.036502 GPa, 0.079429 GPa, and 0.078526 GPa, respectively. The shear stress-bearing ability of the PEKK can be assessed based on its shear modulus and yield strength.

The pressure value represents the hydrostatic stress, which is the average normal stress acting on the material in all the directions. From the data given in Table 1, the hydrostatic stress was 1.6685 GPa. This value indicated the overall stress-bearing ability of PEKK under uniform loading conditions.

Mechanical properties of PEKK

The data in Table 2 represent the stiffness matrix of PEKK in GPa (gigapascals). The stiffness matrix is a 6 × 6 matrix that describes the relationship between stress and strain in a material. Each element of the stiffness matrix corresponds to a particular combination of the stress and strain components. To explain the mechanical properties of PEKK based on these data, we must consider the following elements of the stiffness matrix:

Diagonal elements (C_11, C_22, and C_33) represent the resistance of the material to tensile or compressive forces along the x, y, and z directions, respectively. In this case, the diagonal elements are positive, indicating that PEKK has a positive stiffness along these directions and that it can resist both tensile and compressive forces. Off-diagonal elements (C_12, C_13, C_23) represent the resistance of the material to shearing forces. In this case, the off-diagonal elements are negative, indicating that PEKK has a negative stiffness along these directions. This means that PEKK is more prone to shear deformation than to tensile or compressive deformation.

Bulk Modulus (K): The bulk modulus is a measure of a material's resistance to volume change under hydrostatic pressure. This can be calculated from the diagonal elements of the stiffness matrix as $K = (C\_11 + C\_22 + C\_33) / 3$. In this case, the bulk modulus of PEKK is 0.0030657 GPa, which indicates that PEKK is relatively resistant to volume changes under hydrostatic pressure. Based on this stiffness matrix, we can infer that PEKK is a material with positive stiffness along the x, y, and z directions; however, it is more prone to shear deformation than tensile or compressive deformation. It also had a relatively high bulk modulus, indicating that it was resistant to volume changes under hydrostatic pressure.

PEKK's stiffness and strength make it highly resistant to shear deformation. This means that when PEKK is used as a coating or for surface modification on a dental implant, it can provide a protective layer that resists deformation due to chewing forces, grinding, or other mechanical stresses. This resistance to shear deformation can help ensure the long-term stability and functionality of dental implants. PEKK's resistance of PEKK to volume change under pressure, also known as its bulk modulus, is another important factor for the surface modification of dental implants. A material with a high bulk modulus, such as PEKK, is less likely to undergo significant changes in volume when subjected to external pressure, such as that exerted by the surrounding tissues or bone. This can help maintain the fit and integrity of the dental implant over time, thereby reducing the risk of loosening or failure.

In addition to its mechanical properties, PEKK is known for its excellent biocompatibility, which is critical for any material used in dental implants. PEKK can integrate well with surrounding tissues, promote osseointegration (fusion of the implant with the bone), and minimize the risk of rejection or inflammation. This biocompatibility, combined with its mechanical properties, makes PEKK a highly suitable material for surface modification of dental implants.

The given data in Table 3 provide the average mechanical properties of PEKK, including the bulk modulus, Young's modulus, shear modulus, and Poisson's ratio, as determined by various averaging schemes (Voigt, Reuss, and Hill). Each of these schemes calculates the effective properties of a composite material with given constituents.

The bulk modulus represents the resistance of the material to volume change under hydrostatic pressure. This is the ratio of stress to strain under uniform compression or expansion. The average bulk moduli of PEKK were found to be approximately 0.00053146 GPa (gigapascals) using the Voigt averaging scheme, 0.00053142 GPa using the Reuss averaging scheme, and 0.00053144 GPa using the Hill averaging scheme. These values suggest that PEKK was relatively resistant to volume changes under pressure. The Young's modulus represents the material's resistance to deformation in the direction of an applied force. It is the ratio of stress to strain in the linear region of the stress–strain curve of the material. The average Young's modulus of PEKK was approximately 0.0034455 GPa using the Voigt averaging scheme, 0.0028115 GPa using the Reuss averaging scheme, and 0.0031892 GPa using the Hill averaging scheme. These values indicate that PEKK is a relatively stiff material with high resistance to deformation.

The shear modulus represents the resistance of a material to shear deformation. This is the ratio of shear stress to shear strain. The average shear modulus of PEKK was approximately 0.0041067 GPa using the Voigt averaging scheme, 0.0022738 GPa using the Reuss averaging scheme, and 0.0031902 GPa using the Hill averaging scheme. These values indicate that PEKK was relatively resistant to shear deformation. Poisson's ratio represents the ratio of lateral strain to axial strain when a material is stretched or compressed. The negative values of Poisson's ratio for PEKK using the various averaging schemes (− 0.58051, − 0.38176, and − 0.50017) indicate that PEKK has a tendency to expand laterally when stretched rather than contracting. This implies that PEKK is a relatively incompressible material.

PEKK is a polymer material that exhibits a high mechanical strength and resistance to deformation. This is because of its unique molecular structure, which consists of long chains of repeating units linked together by ether and ketone groups.

PEKK is a stiff material with high resistance to deformation. This is primarily due to the presence of aromatic rings in their molecular structures, which provide rigidity and strength. The stiffness of PEKK makes it a suitable material for applications where structural integrity and load-bearing capabilities are important, such as dental implants. PEKK has a high resistance to volume change under pressure, which is also known as its bulk modulus. This is because of the strong intermolecular forces between the polymer chains, which prevent the material from compressing or expanding easily. This resistance to volume changes is important for maintaining the shape and structural integrity of the material under various loading conditions. PEKK also exhibits high resistance to shear deformation, which is the result of strong covalent bonds between the atoms in its molecular structure. This makes PEKK suitable for applications where shear forces are present, such as in dental implants, where the implant may be subjected to chewing or grinding forces.

The eigenvalues of the stiffness matrix of PEKK represent the stiffness properties of the material along different directions, as listed in Table 4. In this case, the eigenvalues represent the stiffness in six orthogonal directions, denoted by λ1–λ6.

The eigenvalues of the stiffness matrix of polyetherketoneketone (PEKK) provide insight into the stiffness

Table 3 Average properties of PEKK

Averaging scheme	Bulk modulus	Young's modulus	Shear modulus	Poisson's ratio
Voigt	$K_V = 0.00053146$ GPa	$E_V = 0.0034455$ GPa	$G_V = 0.0041067$ GPa	$v_V = -0.58051$
Reuss	$K_R = 0.00053142$ GPa	$E_R = 0.0028115$ GPa	$G_R = 0.0022738$ GPa	$v_R = -0.38176$
Hill	$K_H = 0.00053144$ GPa	$E_H = 0.0031892$ GPa	$G_H = 0.0031902$ GPa	$v_H = -0.50017$

Table 4 Eigenvalues of the stiffness matrix of PEKK

λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
0.001594 GPa	0.0020937 GPa	0.0026876 GPa	0.0053752 GPa	0.0063839 GPa	0.0063839 GPa

properties of the material along different directions. In this case, the eigenvalues represent the stiffness in six orthogonal directions, denoted by λ1–λ6. The stiffness of PEKK in the x direction is represented by λ1 (0.001594 GPa), in the y direction by λ2 (0.0020937 GPa), and in the z direction by λ3 (0.0026876 GPa). In addition, the stiffness of PEKK in the xy plane is represented by λ4 (0.0053752 GPa), in the xz plane by λ5 (0.0063839 GPa), and in the yz plane by λ6 (0.0063839 GPa). These eigenvalues indicate that PEKK exhibits varying stiffness properties along different directions, with the highest stiffness observed in the yz plane and the lowest in the x direction. These eigenvalues indicate that PEKK is a stiff material, with the highest stiffness observed in the yz plane (λ6 and λ5), followed by the xy plane (λ4). The stiffnesses in the x, y, and z directions (λ1, λ2, and λ3) are relatively lower but still significant.

Regarding the feasibility of PEKK for surface modification of dental implants, the stiffness properties indicated by eigenvalues suggest that PEKK can provide a stable and durable surface coating for dental implants. The high stiffness of PEKK in the yz plane (λ6 and λ5) and the xy plane (λ4) can ensure that the coating remains intact and resistant to deformation under mechanical stresses, such as those experienced during chewing or grinding. Additionally, the relatively lower stiffness in the x, y, and z directions (λ1, λ2, and λ3) allows for some flexibility, which can be beneficial for accommodating the natural movement of the jaw and surrounding tissues. When dental implants are subjected to these forces, the PEKK coating effectively distributes the load across the implant surface, minimizing the risk of deformation or damage. This enhanced stiffness helps maintain the structural integrity of the implant and prolongs its lifespan.

However, the relatively lower stiffness in the x, y, and z directions (λ1, λ2, and λ3) allows for some flexibility. This flexibility is beneficial for accommodating the natural movement of the jaw and surrounding tissues. During normal activities such as speaking or chewing, the jaw undergoes subtle movements and vibrations. The flexible nature of PEKK allows the coating to adapt to these movements without causing discomfort or strain to the surrounding tissues. Additionally, the flexibility of PEKK can help reduce the risk of stress shielding, a phenomenon in which rigid materials transfer excessive stress to the surrounding bone, potentially leading to bone resorption and implant failure.

The data in Table 5 provide the elastic moduli of PEKK, including Young's modulus, linear compressibility, shear modulus, and Poisson's ratio, as well as values related to the anisotropy and axis orientations (Fig. 4).

The Young's modulus represents the material's resistance to deformation under tension or compression. The minimum and maximum values of Young's modulus for PEKK were 0.0019099 GPa and 0.0037813 GPa, respectively. These values indicate that PEKK is a relatively stiff material with high resistance to deformation. Linear compressibility represents the change in volume per unit pressure change. The minimum and maximum values of the linear compressibility for PEKK were 6.2127E + 5 TPa^{-1} and 6.3023E + 5 TPa^{-1}, respectively. These values indicate that PEKK was relatively resistant to volume changes under pressure (Fig. 5).

Table 5 Variations of the elastic moduli of PEKK

	Young's modulus		**Linear compressibility**		**Shear modulus**		**Poisson's ratio**		
	E_{min}	E_{max}	β_{min}	β_{max}	G_{min}	G_{max}	ν_{min}	ν_{max}	
Value	0.0019099 GPa	0.0037813 GPa	6.2127e + 05 TPa^{-1}	6.3023e + 05 TPa^{-1}	0.0011079 GPa	0.0063839 GPa	− 0.74713	− 0.093281	Value
Anisotropy	1.98		1.0144		5.762		0.1249		Anisotropy
Axis	0.0000	0.5717	0.0000	1.0000	0.7071	0.0000	− 0.6592	0.0000	Axis
	0.0000	0.5717	0.0000	0.0000	− 0.0003	0.0000	0.6592	0.0000	
	1.0000	− 0.5885	1.0000	0.0000	0.7071	1.0000	− 0.3617	1.0000	
					0.7071	0.7660	− 0.7071	0.1736	Second axis
					− 0.0005	0.6428	− 0.7071	0.9848	
					− 0.7071	− 0.0000	− 0.0000	− 0.0000	

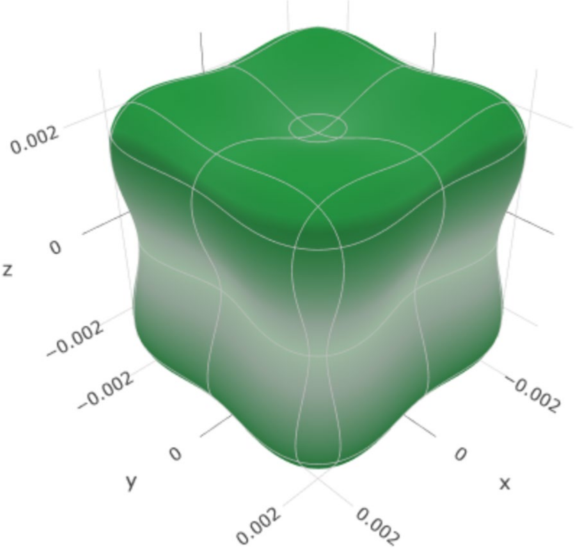

Fig. 4 3D representation of Young's modulus of PEKK

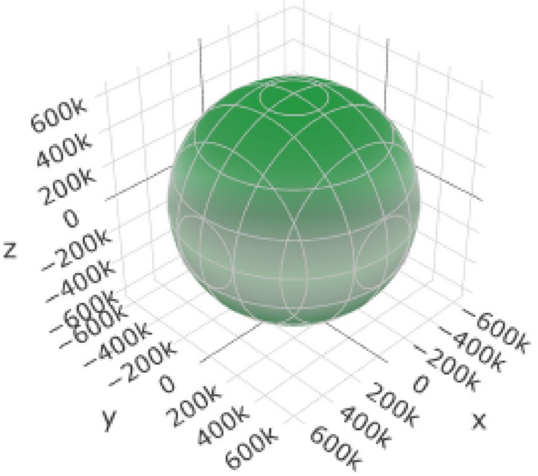

Fig. 5 3D representation of the linear compressibility of PEKK

The shear modulus represents the resistance of a material to shear deformation. The minimum and maximum values of the shear modulus for PEKK were 0.0011079 and 0.0063839 GPa, respectively. These values indicate that PEKK was relatively resistant to shear deformation.

Poisson's ratio represents the ratio of lateral strain to axial strain when a material is stretched or compressed. The minimum and maximum values of Poisson's ratio for PEKK were − 0.74713 and − 0.093281, respectively. These negative values indicate that PEKK has a tendency to expand laterally when stretched, rather than contracting (Fig. 6).

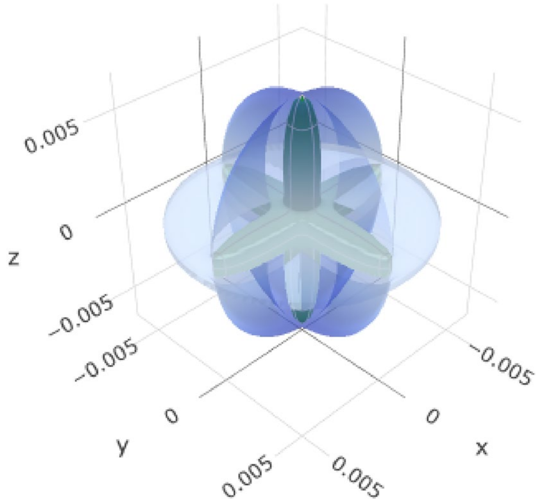

Fig. 6 3D representation of the shear modulus of PEKK

The mechanical properties of PEKK, as described by Young's modulus (E) in Fig. 4 (Figure S1, 2D representation), linear compressibility (β), shear modulus (G), and Poisson's ratio (ν), contribute to its overall behavior under different loading conditions.

The high values of the Young's modulus indicate that PEKK is relatively stiff and exhibits a high resistance to deformation under tension or compression. This property is advantageous for dental implants, as it provides stability and support to withstand the forces exerted during chewing or grinding. The high values of linear compressibility suggest that PEKK is relatively resistant to volume changes under pressure (Fig. 5; Figure S2, 2D representation). This means that it can maintain its shape and structural integrity even when subjected to compressive forces, which is important for maintaining long-term stability of dental implants. The high shear modulus values indicate that PEKK is resistant to shear deformation, which is important for maintaining the structural integrity and stability of dental implants under shear forces (Fig. 6, Figure S3, 2D representation). This property ensures that the implant remains intact, and does not undergo excessive deformation or displacement. The negative values of Poisson's ratio indicate that PEKK has a tendency to expand laterally when stretched, rather than contract Fig. 7 (Figure S4, 2D representation). This property allows PEKK to better accommodate the natural movements of the jaw and surrounding tissues, thereby reducing the risk of discomfort or strain on the tissues.

Overall, the combination of these mechanical properties makes PEKK a suitable material for surface modification of dental implants. Its high stiffness, resistance to volume changes under pressure, resistance to shear

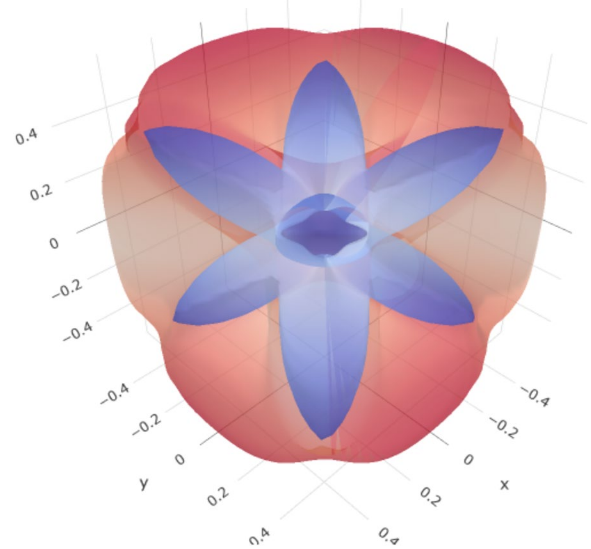

Fig. 7 3D representation of Poisson's ratio for PEKK

deformation, and ability to accommodate natural movements contribute to its stability, durability, and biocompatibility in dental implant applications.

Conclusion

In conclusion, the DFT-based investigation of PEKK as a surface modification material for dental implants has provided valuable insights into its structural, thermodynamic, cohesive, optical, and mechanical properties. This study used advanced computational techniques to evaluate the energy, stability, and behavior of PEKK under various conditions, shedding light on its suitability for dental implant applications. PEKK, a high-performance thermoplastic polymer, exhibits a complex crystal structure with specific arrangements of atoms and chemical bonds. This complexity is crucial for understanding their behavior and interactions with biological tissues. The 2D layered structure of PEKK and its ability to interact with biological tissues at the molecular level make it an attractive candidate for the surface modification of dental implants. Geometry optimization and thermodynamic analysis revealed that PEKK exhibited stable properties under different temperatures and loading conditions, which are important for its long-term performance in dental implants. In summary, the findings of this study suggest that PEKK holds great promise as a surface modification material for dental implants, offering a unique combination of structural, thermodynamic, cohesive, optical, and mechanical properties. Further research and development in this area can lead to improved dental implant materials with enhanced performance, stability, and biocompatibility, ultimately benefiting patients with improved oral health outcomes.

Supplementary Information

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Additional file 1: Figure S1. 2D representation of Young's modulus of PEKK. Figure S2. 2D representation of linear compressibility of PEKK. Figure S3. 2D representation of shear modulus of PEKK. Figure S4. 2D representation of Poisson's ratio of PEKK.

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Data availability statement
The data is available upon genuine request to the corresponding author.

Ethics approval and consent to participate

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