MD Analysis of TEGDMA Reinforced with Ag Nanoparticles: Insights into Swelling, Solubility, Contact Angle and physical Properties

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***Abstract*— In the context of biomaterials, TEGDMA (Triethylene glycol dimethacrylate) is a widely used monomer in dental composites due to its mechanical strength and versatility.**

Incorporating silver (Ag) nanoparticles into TEGDMA can enhance its performance, particularly in medical and dental applications. Silver is extensively used in dentistry due to its biocompatibility, antimicrobial properties, and non-toxicity. In this study, we investigate the influence of Ag nanoparticles on the physical and mechanical properties of TEGDMA using molecular dynamics (MD) simulations. We examine key liquid-like properties, including swelling, solubility, contact angle, density, and elastic properties, at varying Ag nanoparticle concentrations (0%, 3%, 4%, and 5%). The findings provide insights into the optimization of TEGDMA-Ag composites for enhanced dental applications. Additionally, we compare our results with existing literature to high- light the structural, thermal, and functional improvements achieved through nanoparticle incorporation.

I. INTRODUCTION

Triethylene Glycol Dimethacrylate (TEGDMA) was first synthesized for use in dental composite materials to enhance mechanical properties and durability [1]. However, TEGDMA-based composites face challenges such as water absorption, polymerization shrinkage, and a low degree of conversion, which can affect their long-term stability. To overcome these limitations, nanoparticles have been incorporated into TEGDMA to improve its mechanical, chemical, and biological performance.

Silver nanoparticles (AgNPs) have been widely used in dental applications, including as nano-sealers in dental fillings [2] and as antimicrobial agents in orthodontic adhesives [3]. Their biocompatibility, electrical conductivity, and chemical stability make them valuable for dental materials. Other nanoparticles, such as platinum [4] and titanium dioxide (TiO) [5], have also been explored to enhance adhesive properties in dental composites. Additionally, gold nanopar- ticles (AuNPs) have been used to improve drug delivery systems by reducing intracellular degradation [6]. Silvana et al. (2015) reported an enhanced degree of polymerization in methacrylate-based composites with the incorporation of AgNPs [7]. Similarly, research on gold nanorods in TEGDMA composites has demonstrated signifi- cant improvements in mechanical and optical properties [8, 9]. Recent studies have also employed molecular dynamics (MD) simulations to investigate the in- teractions between nanoparticles and the polymer matrix at the atomic level, providing deeper insights into the material's structural and functional enhancements [10].

In this study, we focus on the incorporation of silver nanoparticles in TEGDMA and analyze their effects on key properties such as swelling, solubility, contact angle, density, and elastic behavior using MD simulations. The findings will contribute to the optimization of TEGDMA-Ag composites for improved dental applications.

II. PROPERTIES OF TEGDMA-AG COMPOSITES

2.1 Mechanical Properties

Silver nanoparticles (AgNPs) significantly enhance the mechanical properties and antimicrobial efficacy of TEGDMA-based composites. Studies have shown that the addition of AgNPs improves compressive strength, hardness, and wear resistance. Furthermore, AgNPs inhibit bacterial colonization and biofilm formation, making these composites highly suitable for dental applications [11].

Molecular dynamics (MD) simulations indicate that AgNPs improve cohesive energy, tensile strength, and the degree of conversion due to enhanced nanoparticle-polymer interactions. Additionally, AgNPs maintain the biocompatibility of TEGDMA, making them a safe and effective choice for clinical applications[12].

2.2 Contact angle

The contact angle of TEGDMA with Ag/Au nanoparticles provides critical in- sights into the material's surface properties, which influence adhesion, mechanical behavior, durability, and biocompatibility. These properties are essential for optimizing its application in dentistry and other biomedical fields.

The presence of Ag or Au nanoparticles can alter the hydrophilicity or hydrophobicity of composite materials, affecting their interaction with biological environments. Studies on Boron Nitride/Silver nanocomposite-enhanced poly-methyl methacrylate (PMMA) resins have demonstrated improvements in mechanical and antibacterial properties, emphasizing the significance of nanoparticle incorporation in dental applications [13].

2.3 Optical Properties

The UV-Vis and IR spectra of TEGDMA composites with AgNPs serve as essential tools for:

Characterizing the nanocomposite.

Evaluating chemical interactions and stability.

Optimizing photocatalytic, mechanical, and aesthetic properties.

Infrared (IR) spectroscopy reveals changes in functional groups and bond vibrations due to the addition of nanoparticles [14]. Furthermore, UV-Vis studies on gold nanoparticles have highlighted their role in bioimaging and diagnostics [15].

2.4 Swelling properties

Swelling reflects water uptake, which directly impacts the hydrolytic stability of the composite. Excessive swelling can lead to structural degradation, reducing the mechanical and aesthetic durability of the material over time.

In the moist oral environment, dental composites must resist excessive swelling to ensure longevity and stability [16,17]. The incorporation of nanoparticles has been explored to mitigate these effects, enhancing the composite's overall performance.

2.5 Solubility

Low solubility is crucial for ensuring the durability and longevity of dental composites. Excessive solubility can result in the leaching of resin components, weakening the material and compromising its mechanical strength over time.

The addition of Ag and Au nanoparticles can modify the chemical matrix, improving resistance to solubilization in aqueous environments such as the oral cavity [18].

2.6 Viscosity and Surface tension

Viscosity is a measure of a material's resistance to flow, which directly impacts its handling and performance in dental applications. Low viscosity is essential for:

Easy mixing, dispensing, and application of the resin. Proper nanoparticle dispersion to prevent agglomeration.

AgNPs can affect viscosity by:

Increasing it through interactions with the polymer matrix. Providing a thixotropic effect, where viscosity decreases under shear stress during handling. Surface tension, the cohesive force at the liquid interface, influences wetting, adhesion, and curing behavior. It determines how well the resin adheres to tooth structures.

High surface tension results in poor wetting and adhesion. Ag nanoparticles can modify surface tension, improving wetting and bonding to hydrophilic surfaces like enamel and dentin.

Balancing viscosity and surface tension is crucial for:

Ensuring proper flow and spreading during application, Achieving high- quality adhesion without compromising mechanical strength Maintaining uniform nanoparticle distribution for consistent material properties [19].

III.MOTIVATION

Our recent Molecular Dynamics (MD) study on TEGDMA with 0%, 3%, 4%, and 5% Ag demonstrated significant changes in its mechanical, thermal, and op- tical properties [10]. These results emphasize the potential of AgNPs to enhance the performance, durability, and biocompatibility of TEGDMA composites for dental applications.

Furthermore, gold nanoparticles exhibit a high surface charge density, en- abling them to neutralize cancerous cells, as reported in our experimental work [20,21]. This highlights their potential beyond dental applications, extending into biomedical and therapeutic fields.

IV.MATERIALS AND METHOD

Materials and Methods

Generation of Molecular Structures

A Python program was developed to generate SMILES representations for 1%, 3%, and 4% silver (Ag) in TEGDMA and subsequently convert them into atomic fractional coordinates in .pdb format. The following script illustrates the process for 3% Ag in TEGDMA:

```
from rdkit import Chem
from rdkit.Chem import AllChem from rdkit.Geometry import Point3D
# Define TEGDMA structure
smiles =
"CC(=C)C(=O)OCCOCCOCCOC(=O)C(=C)C"
mol = Chem.MolFromSmiles(smiles) mol =
Chem.AddHs(mol)
AllChem.EmbedMolecule(mol,
AllChem.ETKDG())
AllChem.UFFOptimizeMolecule(mol)
pdb_block = Chem.MolToPDBBlock(mol)
# Define and add silver atoms silv_1 =
Chem.MolFromSmiles("[Ag]") silv_1 =
Chem.AddHs(silv_1)
silv_2 = Chem.MolFromSmiles("[Ag]")
silv_2 = Chem.AddHs(silv_2)
combined_1 = Chem.CombineMols(mol,
silv_1) combined_2 =
Chem.CombineMols(combined_1, silv_2)
# Adjust silver atom positions conf =
combined_2.GetConformer()
silv_idx_1 = combined_2.GetNumAtoms() -
2 silv_idx_2 = combined_2.GetNumAtoms()
- 1
conf.SetAtomPosition(silv_idx_1,
Point3D(5.0, 5.0, 5.0))
conf.SetAtomPosition(silv_idx_2,
Point3D(-5.0, -5.0, -5.0))
# Define box and save as PDB box = """
CRYST1     10.000  10.000  10.000  90.00
      90.00  90.00  P 1     1
"""
pdb_block_combined =
Chem.MolToPDBBlock(combined_2)
pdb_file_content = box +
pdb_block_combined
with open("molecule_with_silv.pdb",
"w") as file: file.write(pdb_file_content)
print("PDB file saved to
molecule_with_silv.pdb")
```

The molecular weight of TEGDMA is 254 g/mol. The required number of Ag atoms was calculated using:

Solving for n, we obtain n = 0.024. Since a fraction of an atom is not physically meaningful, we round to the nearest whole number. This results in:

1 Ag atom for 3

2 Ag atoms for 4

3 Ag atoms for 5

For structure generation, .pdb files were created, sometimes using obabel for format conversion. The methodology for incorporating Au atoms follows our previously published work [10].

Molecular Dynamics (MD) Simulations

MD simulations were conducted using LAMMPS following procedures in [22,23]. The Visual Molecular Dynamics (VMD) software [24] was used to pre- process and visualize molecular structures, employing its ”Tkconsole” feature for interfacing with LAMMPS [25]. The OPLS-AA force field was employed for modeling interactions within the TEGDMA matrix and the embedded Ag nanoparticles. Simulations were performed for Ag concentrations of 0%, 3%, 4%, and 5%, and the following properties were computed:

- Swelling and solubility
- Density
- Viscosity
- Surface tension
- Mechanical and physical properties
- Contact Angle Computation

To determine the contact angle, an MD simulation was executed using LAMMPS, generating dump.lammpstrj and dumpfinal.lammpstrj files. The fol- lowing LAMMPS script was used:

```
# Define groups group surface type 1 group droplet type 2

# Define potentials pair_style lj/cut 12.0
    pair_coeff2 2 0.1 3.4 # Surface
    pair_coeff1 1 0.1 3.4 # Droplet
    pair_coeff1 2 0.1 3.4 # Surface-droplet
                            interaction
# Fix surface atoms
tfix 1 surface setforce 0.0 0.0 0.0
# Minimize and equilibrate min_style cg
minimize 1e-4 1e-6 100 1000
velocity all create 300.0 12345
fix 2 all nvt temp 300.0 300.0 100.0
run 200000
# Output trajectory
dump 1 all atom 100 dump.lammpstrj
write_dump all atom dump_final.lammpstrj
```

The contact angle was then computed using the following Python script:

```
import MDAnalysis as mda import numpy as np
import matplotlib.pyplot as plt
u = mda.Universe("tegag.data",
"dump_final.lammpstrj",
format="LAMMPSDUMP") droplet =
u.select_atoms("type 1 or type 2 or type 3")
positions = droplet.positions z_coords =
positions[:, 2]
r_coords = np.sqrt(positions[:, 0]**2 +
positions[:, 1]**2)
bins = np.linspace(z_coords.min(),
z_coords.max(), 100)
r_avg = [np.mean(r_coords[(z_coords >
bins[i]) & (z_coords <= bins[i + 1])])
for i in range(len(bins) - 1)]
plt.plot(bins[:-1], r_avg,
label='Droplet Profile')
plt.xlabel('Height (z)')
plt.ylabel('Radius (r)') plt.legend()
plt.show()
z_contact = bins[np.argmax(r_avg)]
r_contact = r_avg[np.argmax(r_avg)]
angle = np.arctan(r_contact / z_contact) *
180 / np.pi print(f"Contact Angle:
{angle:.2f} degrees")
```

Swelling Computation

For swelling calculations, the molecular volume at 600K was compared with that at room temperature (300K). The .pdb files from MD simulations were analyzed using the following Python script:

```
import MDAnalysis as mda
def compute_volume(pdb_file): u =
mda.Universe(pdb_file) coords =
u.atoms.positions
x_min, y_min, z_min = coords.min(axis=0)
x_max, y_max, z_max = coords.max(axis=0)
volume = (x_max - x_min) * (y_max -
y_min) * (z_max - z_min)
print(f"Volume: {volume:.3f} Å ")
return volume
volume_300K =
compute_volume("structure_300K.pdb")
volume_600K =
compute_volume("structure_600K.pdb")
swelling_ratio = (volume_600K -
volume_300K) / volume_300K * 100
print(f"Swelling Ratio:
{swelling_ratio:.2f}%")
```

This approach provided quantitative insights into the swelling behavior of the TEGDMA-Ag composite at elevated temperatures.

Viscosity and surface tension were computed for TEGDMA with Ag nanopar- ticles at 0%, 3%, 4%, and 5% using MD simulations, following the procedure outlined in our earlier paper [10]. Additional physical parameters such as dipole moment, lattice energy, electronegativity, density, specific heat, Young's mod- ulus, S-wave and P-wave velocities, and self-energy were calculated using the General Utility

Lattice Program (GULP) [26]. GULP employs classical force fields to analyze the structural and energy characteristics of materials. Further- more, UV-Vis and IR spectra simulations for Ag nanoparticle-doped TEGDMA systems were performed using WebMO [27], applying the Hartree-Fock method with the PM7/PM6 basis set

V.RESULTS AND DISCUSSIONS

For varied composition of Ag nanoparticles in TEGDMA, physical parameters computed from the fractional coordinates of atoms are given in Table 1. Swelling in dental composites affects adhesion to the tooth surface, and this holds true for Ag nanoparticles, as shown by the values in Table 1. Swelling remains below 1% in all cases except for 3% Ag, where it reaches 9.98%. This contributes to the material's hydrolytic stability and helps reduce microleakage at the interface.

We have also extended our computation of swelling (in %) to TEGDMA with Au nanoparticles. The results show values of 0.0006%, 99.4%, and 0.0005% for 3%, 4%, and 5% Au, respectively, indicating that 4% Au nanoparticles in TEGDMA is not feasible.

Table 1: Physical parameters of TEGDMA with varied percentage of Ag

Physical parameters	0% of Ag	3% of Ag	4% of Ag	5% of Ag
Swelling(%)	-0.0002	9.98	-0.0005	-0.0005
Density(g/cm^3)	0.0005	0.0006	0.0004	0.0004
Viscosity(Pa.s)T=300K	3.0xE−8	1.23E^{-9}	1.54E^{-8}	8.3E^{-10}
Surface tension(N/m)T=300K	0.0039	0.0011	0.009	0.0009
Contact angle(Deg)	100	51.38	50.79	67.49
Solubility(g/L)	0.0000002	0.0000015	0.0000012	0.0000003
Lattice energy(eV)	-0.80	-0.89	-3.56	3.56
Electronegativity(eV)	6.43	6.39	6.39	6.39
Specific heat(Cv in J/mol-K)	71.4	92.7	95.9	101.2
Dipole moment(Debye)	0.82	2.97	3.76	14.34
Bulk Modulus(Voigt)(Ga.P)	0.106	0.0011	0.0011	0.0011
S-wave velocity(km/s)	2.156	0.37	1.36	1.36
P-wave velocity(km/s)	2.877	0.68	1.71	1.71
IR peak(cm^{-1})	1855.4	1841.1	1855.4	1683.3
UV (peak nm)	139.8	157.2	236.0	221.3
Self enegy (eV)	-0.80	-0.78	-3.14	-3.14
Entropy(cal/mol-K)	169.3	200.5	217.0	178.8
Zero point energy(eV)	0.411	0.011	0.044	0.044

The variation in density with increasing Ag nanoparticle content remains nearly constant, suggesting improved crosslinking, which mitigates the adverse effects of swelling and ensures uniform distribution.

Viscosity, which measures the material's flow properties, remains low even in the presence of Ag nanoparticles. A similar viscosity trend was reported for TEGDMA with Au nanoparticles [10].

Surface tension values from Table 1 indicate that increasing Ag nanopar- ticle content leads to a decrease in surface tension. We believe this promotes void formation during curing, a behavior also observed in TEGDMA with Au nanoparticles [10].

Contact angle computations yielded the droplet profile distribution for each sample, as shown in Figure 1. Table 1 reveals that the contact angle for pure TEGDMA is 100 , while for different Ag nanoparticle concentrations, it varies from 50 to 67 . For Au nanoparticles, the contact angles are 44 , 54 , and 52 for 3%, 4%, and 5% Au, respectively. Overall, the presence of nanoparticles lowers the contact angle. Lower contact angles typically indicate better wet- ting, which enhances bonding. By fine-tuning nanoparticle concentrations, the desired material properties can be achieved

Solubility values from Table 1 indicate that it remains below 1 for all concen- trations of Ag in TEGDMA. We extended these computations to

Au nanopar- ticles in TEGDMA and found solubility values of 0.0000014 g/L (3%), 0.000015 g/L (4%), and 0.0000014 g/L (5%), which are comparable to those for Ag nanoparticles. These low solubility values ensure the material's durability and structural integrity.

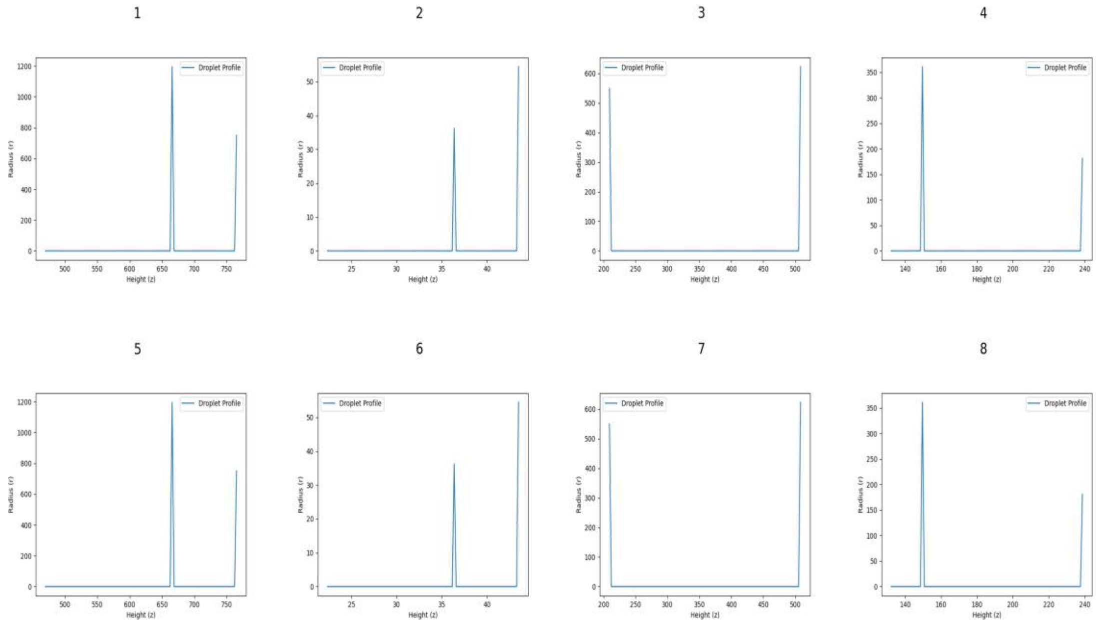

Figure 1: Variation of droplet profile to compute contact angle for TEGDMA in (1)0% , (2) 3%, (3)4% and (4) 5% of Ag and (5)0% , (6) 3%, (7)4% and (8) 5% of Au nanoparticles.

The impact of Ag nanoparticles on the internal structure—and consequently, the thermodynamic stability—of TEGDMA is assessed in terms of lattice energy. As shown in Table 1, lattice energy increases with the percentage of Ag nanoparticles. The electronegativity of metals does not undergo significant charge transfer and therefore remains nearly constant.
Specific heat increases with the addition of Ag nanoparticles, while zero- point energy remains constant, highlighting the importance of energy storage and transfer in thermal management applications. Dipole moment, which measures molecular polarity, indicates the material's interaction with electromagnetic fields, making it relevant for electrical and optical applications

Mechanical properties such as linear modulus, Poisson's ratio, shear mod- ulus, and Young's modulus exhibit variations both in magnitude and spatial distribution with the presence of Ag nanoparticles in TEGDMA. This is illus- trated in Figure 2, generated using the ELATE [28] online program, which uses computed 36 elastic constants with GULP software by considering symmetry operations and excluding rotational deformations[10].

ELATE, an advanced computational tool available at https : progs.coudert.name/elate, facilitates detailed analysis of second-order elastic tensors in anisotropic materials. It computes essential elastic properties such as Young's modulus, Poisson's ratio, linear modulus, and shear modulus while providing directional analysis to identify unique mechanical behaviors, including negative compress- ibility and auxetic properties. By utilizing interactive 2D and 3D visualizations, ELATE allows researchers to explore spatial variations in elastic properties, of-

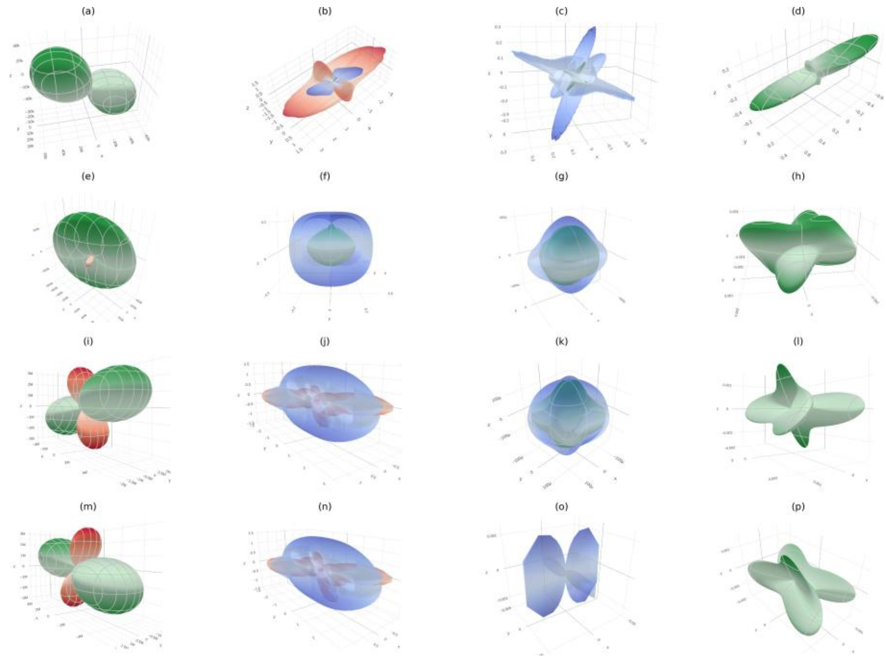

Figure 2: Spatial variation of linear modulus, Poisson's ratio, Shear modulus and Youngs' modulus for TEGDMA with (1)0% , (2) 3%, (3)4% and (4) 5% of Ag nanoparticles(from the top).

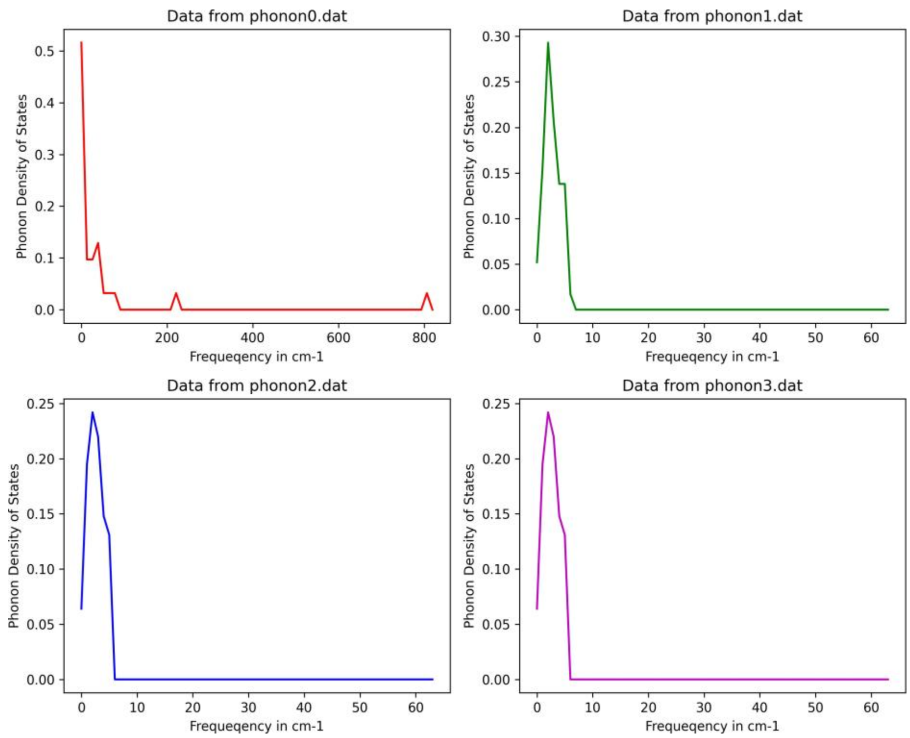

Figure 3: Variation of phonon density of states with phonon frequencies for TEGDMA with (phonon0)0% , (phonon1) 3%, (phonon2)4% and (phonon3) 5% of Ag nanoparticles(from the top).

fering deeper insights into material behavior [29]. The bulk modulus (GPa) decreases with increasing concentrations of Ag nanoparticles. Similarly, for Au nanoparticles in TEGDMA, the bulk modulus values—0.0015 GPa (3%), 0.0005 GPa (4%), and 0.0015 GPa (5%)—also de- crease compared to pure TEGDMA. This suggests that the reinforcing effect of Ag nanoparticles can be optimized to maintain better performance under oral stresses. Experimentally, it has been observed that flexural strength initially increases and then decreases with the addition of Ag nanoparticles [30].

Figure 3 illustrates the variation in the phonon density of states (DOS) with phonon frequencies. In a crystal lattice, each frequency in the phonon DOS cor- responds to a distinct vibrational mode. Peaks in the DOS indicate frequencies where multiple phonon modes exist within the material. The position of these peaks represents vibrational frequencies, with those on the lower end of the spectrum (left side) typically associated with acoustic phonons. These phonons involve atomic vibrations that are in phase and play a crucial role in thermal conductivity.

In contrast, peaks appearing at higher frequencies (on the right side of the

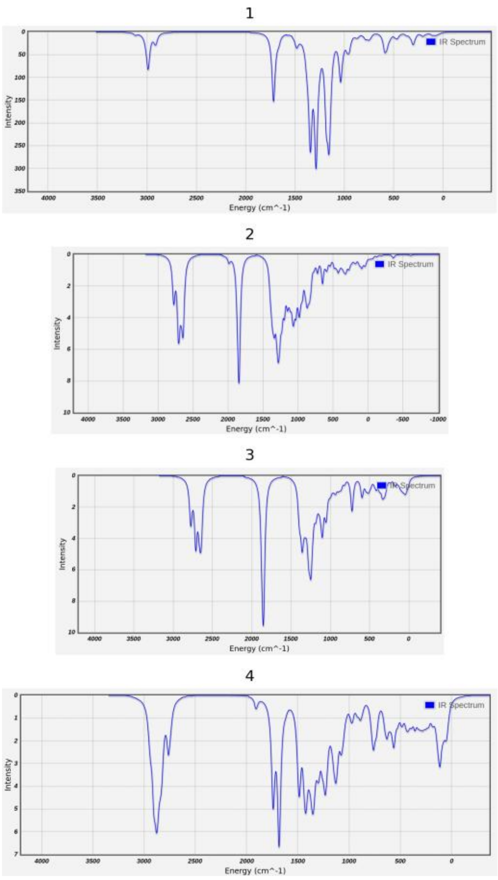

Figure 4: Simulated IR spectra for TEGDMA with (1)0% , (2) 3%, (3)4% and (4) 5% of Ag nanoparticles(from the top).

spectrum) correspond to optical phonons. These are higher-energy modes in which atoms within a unit cell vibrate out of phase, significantly affecting the material's specific heat, especially at elevated temperatures. A pronounced peak indicates a high density of phonon states at that frequency, while a sharp, well- defined peak is often associated with specific atomic bonds or interactions.

Significant modifications in the phonon spectra are observed when Ag is introduced into TEGDMA. Experimentally, key vibrational modes include O–C stretching at approximately 1150 cm , C=O stretching around 1700 cm , and peaks near 100 cm associated with nanoparticle interactions [31]. Figure 4 presents the IR spectra of Ag nanoparticle-doped TEGDMA, highlighting its optical properties within this frequency range. Furthermore, experimental observations for Ag nanoparticles in dental composites show O–H (3345 cm),

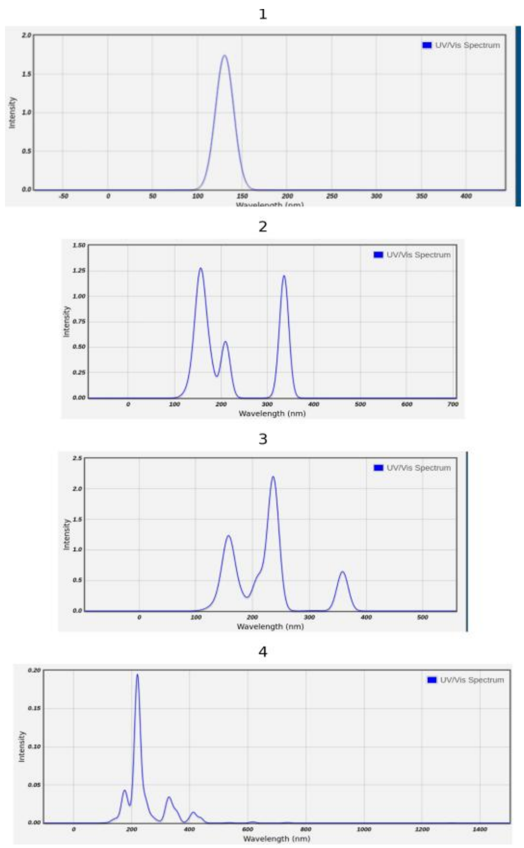

Figure 5: Simulated UV spectra for TEGDMA with (1)0% , (2) 3%, (3)4% and (4) 5% of Ag nanoparticles(from the top).

C=O (1636 cm), and C–C (666 cm) stretching modes [18], which are in agree- ment with Figure 4. The UV-Vis spectra of Ag in TEGDMA are shown in Figure 5, with peak positions has shifted from 140cm-1 to above 200 cm-1 which is due to the presence of Ag nanoparticles which influence both self- and zero-point energies, indicating the materials internal energy landscape in agreement with the experimental reports[32].

VI.STOCHASTIC ANALYSIS OF THE DATA

We present correlation surfaces and mean plots for Swelling, Solubility and Density, obtained using the Functional Principal Component Analysis (FPCA) package (available at http://www.stat.ucdavis.edu/PACE/) in MATLAB (The MathWorks Inc., Natick, MA, USA) [33]. Figure 5 illustrates the correlation surfaces and mean values corresponding to different Ag concentrations in the TEGDMA matrix.

The advantage of FPCA lies in its ability to analyze trends and variations across parameter spaces, even in regions with unobserved concentrations. This stochastic approach provides deeper insights into the interplay between material properties, enabling us to infer the influence of Ag nanoparticles on solubility, swelling, and density beyond the directly measured data points. By leveraging this statistical framework, we can better understand broader material behavior and predict trends in unexplored parameter ranges.

The 3D correlation plots illustrate the dynamic relationships among the stud- ied parameters across the observed Ag concentrations. The oscillatory nature suggests periodic or structured variations in the properties, likely influenced by nanoparticle interactions within the polymer matrix. Higher correlations indicate consistent and predictable trends in material properties, whereas lower correlations suggest regions where additional stochastic effects or nonlinear in- fluences play a role.

The Fraction of Variance Explained (FVE) curves quantify how well the principal components represent the data. A small number of principal components (PCs) capture over 95% of the variance, indicating that the material proper- ties are dominated by a few key underlying factors. The rapid convergence to high variance explained suggests that the system's behavior is governed by low- dimensional stochastic effects, reinforcing the efficiency of FPCA in reducing complexity while retaining significant information.

The mean plots depict the continuous variation of key material properties with increasing Ag nanoparticle (NP) percentage:

Swelling (3%): Exhibits a non-monotonic trend, peaking at an interme- diate Ag NP concentration. This suggests an optimal dispersion effect, where Ag NPs initially enhance swelling before leading to a stiffening ef- fect at higher concentrations.

Solubility (6%): Decreases with increasing Ag NP concentration, indi- cating enhanced stability of the TEGDMA-Ag composite, likely due to reduced hydrophilic interactions.

Density (9%): Increases with Ag NP content, which aligns with expecta- tions since Ag has a higher atomic mass than the polymer matrix.

VII.CONCLUSION

The incorporation of Ag nanoparticles into TEGDMA significantly influences its swelling, solubility, density, viscosity, surface tension, contact angle, and mechanical properties, impacting both structural integrity and functional performance.

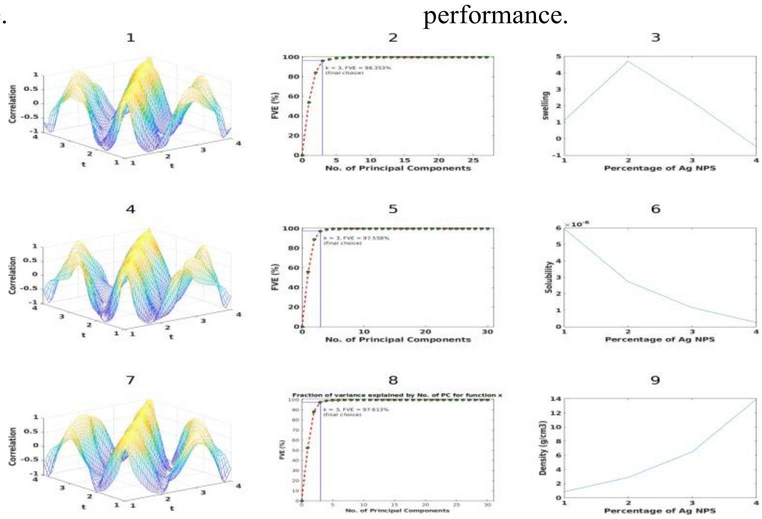

Figure 6: Stochastic analysis of correltaion, principal components and mean of Swelling, solubility and Density for TEGDMA (with 3%, 4% and (3) 5% of Ag nanoparticles horizontally)from the top.

Swelling: Swelling remains below 1% across all Ag concentrations except at 3%, where a significant increase (9.98%) is observed. This suggests that an intermediate Ag NP concentration may disrupt the polymer network, while higher concentrations promote stability by enhancing crosslinking.

Solubility: Extremely low solubility values (〈 1 g/L) indicate that Ag- doped TEGDMA retains high durability and structural integrity. Similar trends are observed for Au nanoparticles, reaffirming the stability of nanoparticle-reinforced composites.

Density: The density remains nearly constant with increasing Ag NP con- tent, suggesting improved crosslinking within the polymer matrix. This stabilization mitigates adverse effects of swelling and ensures a more uni- form distribution of nanoparticles.

Viscosity: The presence of Ag nanoparticles does not significantly im- pact viscosity, confirming that the material maintains favorable flow prop- erties essential for dental applications. Similar trends are reported for TEGDMA-Au composites.

Surface Tension: A decreasing trend in surface tension with increasing Ag NP concentration suggests that nanoparticles influence polymeriza- tion dynamics, potentially promoting void formation during curing. This behavior aligns with previous observations in TEGDMA-Au composites.

Contact Angle: Contact angle measurements reveal a reduction from 100 (pure TEGDMA) to 50°-67° (TEGDMA-Ag) and 44° -54° (TEGDMA-
Au), indicating enhanced wettability. Lower contact angles improve adhe- sion and bonding, highlighting the potential for fine-tuning nanoparticle concentration to achieve desired interfacial properties.

Mechanical Properties: The introduction of Ag nanoparticles alters Young's modulus, Poisson's ratio, shear modulus, and linear modulus, with spa- tial variations mapped using ELATE. The bulk modulus decreases with increasing Ag concentration, which can be optimized to enhance resilience under oral stress.

Physical Properties: Lattice energy increases with Ag NP concentration, reflecting improved thermodynamic stability. Electronegativity remains nearly constant, while specific heat shows a slight increase, influencing energy storage and thermal performance. The phonon density of states and IR/UV-Vis spectra indicate nanoparticle interactions, particularly in the O-C, C=O, and O-H stretching regions, reinforcing the structural modifications induced by Ag.

The stochastic approach provided by FPCA allows us to predict trends in unobserved regions, enhancing our understanding of how Ag nanoparticles influence TEGDMA's mechanical and physical properties. The ability to analyze the correlation structures, dominant principal components, and mean property variations highlights FPCA's strength in handling complex, multi-parameter systems in nanocomposite research.

Ag nanoparticle incorporation into TEGDMA enhances mechanical stabil- ity, reduces solubility, improves wettability, and maintains favorable viscosity while slightly lowering bulk modulus. However, the anomalous swelling at 3% Ag suggests a concentration-dependent balance between polymer-nanoparticle interactions. These findings provide critical insights for optimizing nanoparticle- reinforced dental composites to achieve improved durability, adhesion, and per- formance under clinical conditions. The stochastic approach provided by FPCA allows us to predict trends in unobserved regions, enhancing our understanding of how Ag nanoparticles influence TEGDMA's mechanical and physical prop- erties. The ability to analyze the correlation structures, dominant principal components, and mean property variations highlights FPCA's strength in handling complex, multi-parameter systems in nanocomposite research.

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Author contributions B.N.A: Computation and investigation; H.S: resources, writing review; B.C.M: investigation; M.B.N: investigation; R.S: supervision, re- sources, writing, conceptualization.

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