Novel Antimicrobial and Remineralizing Resin-Based Clear Aligner Attachment Orthodontic Materials

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Abstract

Introduction: Clear aligner orthodontic treatment provides a more hygienic and esthetic alternative to fixed appliances. Attachments play a crucial role in clear aligner therapy, but prolonged use is associated with plaque accommodation and white spot lesions.

Objectives: **(1)**Develop a novel resin-based antibacterial and remineralizing clear aligner attachment material to reduce white spot lesions during treatment **(2)** Investigate the material mechanical and physical properties, and antimicrobial capabilities on *Streptococcus mutans* (*S). mutans.* ***Materials and*** **Methods:** The resin-based clear aligner attachment material was formulated by adding triethylene glycoldivinylbenzyl ether (TEG-DVBE) and urethane dimethacrylate (UDMA), denoted as (UV), along with 3% of the antibacterial monomer dimethylaminododecyl methacrylate (DMADDM), nano-amorphous calcium phosphate (NACP) and glass fillers at different mass fractions (45%,50%,55%). Transbond LV and Vitremer were selected as commercial controls. Flexural strength, elastic modulus, degree of conversion (DC%) and microhardness, Enamel shear bond CFU, MTT and Lactic acid were evaluated. **Results:** The experimental groups with glass fillers at 45%,50% and 55% exhibited flexural strength from (109.2±8.6)MPa to (96.4±8.2)MPa, exceeding the ISO standard for resin-based materials. Degree of conversion for all experimental groups ranged from (53.4±2.3)% to (68.3±0.9)% significantly higher than the commercial control (37.1±4.1)% ($p<0.05$). Enamel shear bond shows no statistical significance difference between all the experimental and the commercial control I. The antibacterial effectiveness for experimental groups with 3% DMADDM showed 6-log CFU reduction and 95% reduction of metabolic activity and 92% lactic acid production. **Conclusion:** The modified resin based clear aligner attachment material demonstrated excellent antimicrobial activity and remineralizing potential while maintaining good physical and mechanical properties. These qualities may offer enhanced protection against white spots lesions during clear aligner therapy.

Introduction

- Clear aligner orthodontic therapy is a popular alternative to traditional fixed appliances due to its enhanced aesthetics and improved oral hygiene. However, prolonged use of attachments can contribute to plaque accumulation and white spot lesions (WSLs) formation due to bacterial biofilm activity and reduced saliva flow, leading to enamel demineralization[1].
- The development of a resin-based clear aligner orthodontic attachment with antibacterial and remineralizing properties is crucial for enhancing protection against WSLs during orthodontic treatment.

Figure 1. Thermoplastic clear aligner loaded with Resin attachment material.

Figure 2. WSL around removed attachment.

- This study synthesized a novel resin-based attachment orthodontic material by incorporating nano-sized amorphous calcium phosphate (NACP) for ion release and dimethylaminododecyl methacrylate (DMADDM) for antibacterial effects.
- **Antibacterial Monomer:**
- DMADDM has an alkyl chain length of 12 (Fig 3) and it was synthesized via a modified Menschutkin reaction, in which a tertiary ammonium group was reacted with organohalide as prescribed previously [2].
- DMADDM is a potent cationic antibacterial agent with good biocompatibility.
- It was shown to exhibit strong antibacterial activity against several oral pathogens and their biofilms [3].

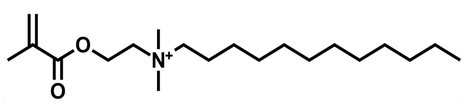


Figure3 : Dimethylaminododecyl Methacrylate (DMADDM) chemical structure.

Amorphous Calcium Phosphate Nanoparticles (NACP):

- Advantageous due to its small size/high surface area. Synthesized via a spray-drying technique and incorporated into resin. composite [4].
- ACP is a non-crystalline form of calcium phosphate that releases supersaturated concentrations of calcium and phosphate ions in proportions similar to naturally-occurring hydroxyapatite.
- Attachment with nanoparticles of amorphous calcium phosphate (NACP) neutralized acid attacks, whereas commercial controls failed to neutralize the acids [5].
- NACP attachment effectively reduced caries in enamel in a human *in situ* study [6], and remineralized enamel tooth lesions *in vitro* [7].

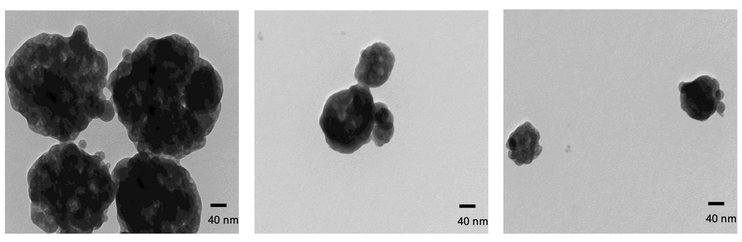


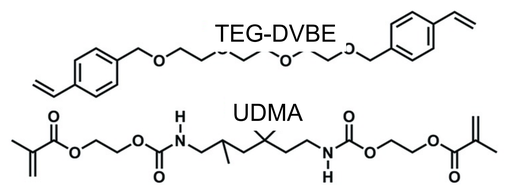
Figure 4. TEM images of amorphous calcium phosphate nanoparticles.

Objective

- The aims of this research were to **(1)** Develop a novel resin-based antibacterial and remineralizing clear aligner attachment material to reduce WSLs; **(2)** Evaluate the effects of nano-sized amorphous calcium phosphate (NACP) and dimethylaminododecyl methacrylate (DMADDM) on mechanical, physical, and antibacterial properties against *Streptococcus mutans*.

Materials and Methods:

- **Resin-Based Clear Aligner Attachment Formulations**
- The resin-based clear aligner attachment material was formulated by incorporating triethylene glycol divinylbenzyl ether (TEG-DVBE) and urethane dimethacrylate (UDMA), denoted as (UV), along with 3% of the antibacterial monomer dimethylaminododecyl methacrylate (DMADDM), nano-amorphous calcium phosphate (NACP) and Silanized barium boroaluminosilicate glass particles with an average size of 1.4 µm were used as a co-filler for mechanical reinforcement.



- The experimental groups were formulated as follows:

Group Name	Resin-base clear aligner attachment material composition
Commercial control I	Transbond supreme LV (3M Unitek, Monrovia, CA)
Commercial control II	Vitremer™(3M ESPE, St. Paul, MN, USA)
Experimental group 1 (packable material)	UV + 3% DMADDM + 20% NACP + 45% glass
Experimental group 2 (Flowable material)	UV + 3% DMADDM + 20% NACP + 45% glass
Experimental group 3 (flowable material)	UV + 3% DMADDM + 20% NACP + 45% glass
Experimental group 4 (packable material)	UV + 3% DMADDM + 20% NACP + 45% glass

- **Mechanical Testing:** A three-point flexural test with a span of 10 mm was used to fracture the specimens at a crosshead speed of 1 mm/minute on a computer-controlled Universal Testing Machine Flexural strength, S, and Elastic modulus, E, were recorded.
- **MTT Viability Assay:** MTT(3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay was performed according to previous study [8].
- Larger absorbance values indicate increased production of the formazan product that is correlated to increased cell viability.
- **Lactic Acid Production and CFU Counts:** 48-h biofilms were assayed for lactate concentration and CFU counts and culture plates, containing 15% sucrose, was used to determine total streptococci [8].
- **Enamel shear bond (MPa):** Was conducted using Universal testing machine that is connected to chisel tip (n = 15) An occluosgingival load (1kN; speed=0.5 mm/min) was applied between the enamel surface and the resin-based attachment.
- **Microhardness (GPa):** The Vickers indentation was performed at a load of 980.7 mN and a dwell time of 10 s using resin-based attachment bars (n = 12).
- **Degree of conversion (DC%):** The degree of conversion (DC) of each group (n = 4) was measured via FTIR-ATR. The intensity of the aliphatic carbon-carbon double bond (1637 cm−1) and the aromatic carbon-carbon double bond (1583 cm−1) were measured using the following formulation.

$$DC(\%) = (1 - \frac{(A_{1637}/A_{1583})_{post\ cure}}{(A_{1637}/A_{1583})_{before\ cure}})X100$$

- Data were analyzed using one-way ANOVA with Tukey's post hoc test for multiple comparisons (α = 0.05).

Results

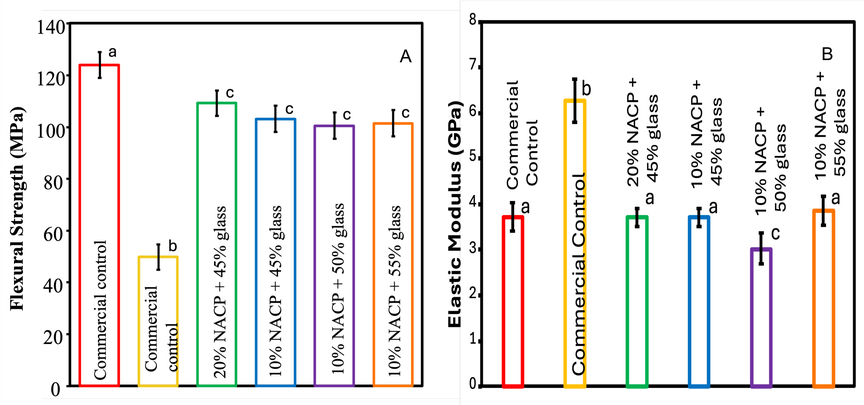


Figure 3. (A) Flexural strength (mean ± SD; n = 6). The experimental groups resulted values exceeded ISO and the commercial control 2 ($p < 0.05$). (B) elastic Modulus (mean ± SD; n = 6). The experimental groups shows values comparable to control I.

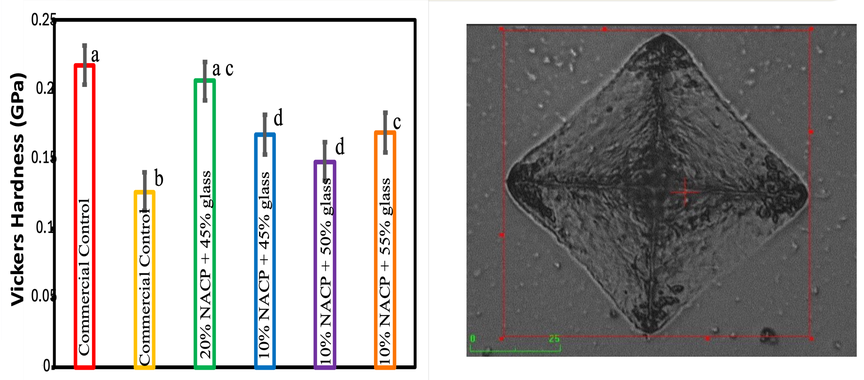


Figure 5.A The Vickers Microhardness (GPa) (mean ± SD; n = 12). Different letters indicate statistically significant differences between the groups ($p < 0.05$). **B** Vickers indentation on the surface of resin-based attachment.

Results (Continued)

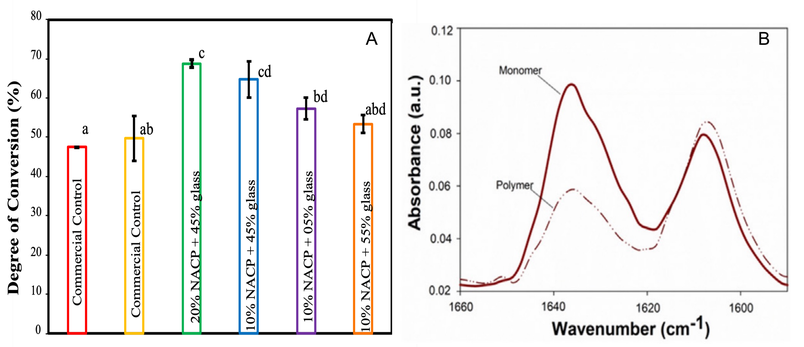


Figure7. A Degree of conversion % (mean ± SD; n = 3) Experimental groups showed statistically significant differences compared to commercial control I &II ($p < 0.05$). **B** The graph show the FTIR spectra of DC from monomer to polymer for the experimental groups; illustrates peaks high, which was used to calculate the DC.

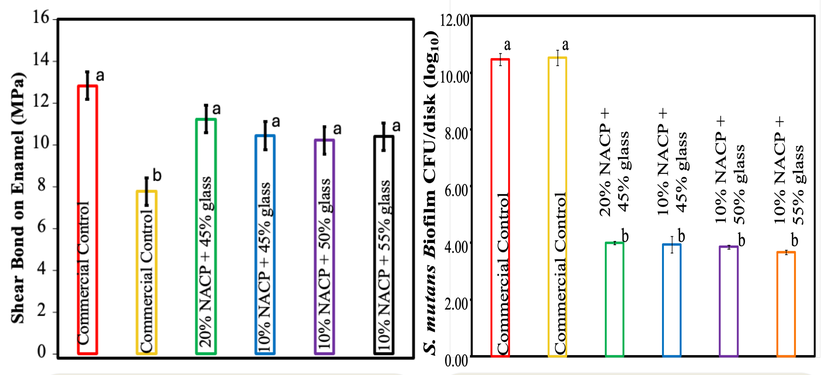


Figure 6. Enamel shear bond strength(mean ± SD; n = 20). Experimental groups showed values comparable to control I.

Figure 8. The incorporation of DMADDM into a novel resin attachment with NACP significantly reduced CFUs count for *S. mutans* compared to the control ($p < 0.05$).

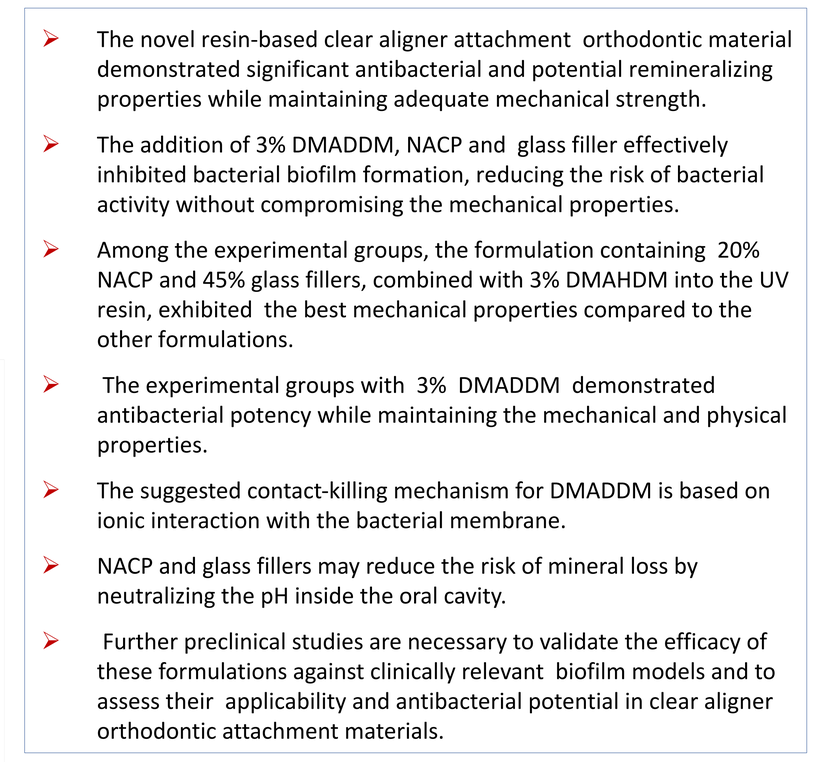


Figure 9. Viability of 2-day biofilms on attachment disks. **(A)**Biofilm metabolic activity (MTT), **(B)** lactic acid production (mean ± SD; n = 6). The incorporation of DMADDM into the novel UV resin-based attachment containing NACP had the lowest lactic acid production and metabolic activity compared to commercial control ($p < 0.05$).

Discussion

- The novel resin-based clear aligner attachment orthodontic material demonstrated significant antibacterial and potential remineralizing properties while maintaining adequate mechanical strength.
- The addition of 3% DMADDM, NACP and glass filler effectively inhibited bacterial biofilm formation, reducing the risk of bacterial activity without compromising the mechanical properties.
- Among the experimental groups, the formulation containing 20% NACP and 45% glass fillers, combined with 3% DMAHDM into the UV resin, exhibited the best mechanical properties compared to the other formulations.
- The experimental groups with 3% DMADDM demonstrated antibacterial potency while maintaining the mechanical and physical properties.
- The suggested contact-killing mechanism for DMADDM is based on ionic interaction with the bacterial membrane.
- NACP and glass fillers may reduce the risk of mineral loss by neutralizing the pH inside the oral cavity.
- Further preclinical studies are necessary to validate the efficacy of these formulations against clinically relevant biofilm models and to assess their applicability and antibacterial potential in clear aligner orthodontic attachment materials.

Acknowledgment

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