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Saud khalil Al hauly
College of Science, University of Mosul, Mosul, Iraq

Mazin Ahmed
College of Science, University of Mosul, Mosul, Iraq.

Sarmad S. S. Al Qassar
Assistant Professor, Department of Pedo Ortho Prevention, College of Dentistry, University of Mosul, Mosul, Iraq.

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ORIGINAL STUDY

Impact of Orthodontic Adhesive Magnets on Degree of Conversion and the Kinetics of Polymerization

Saud khalil Al Healy [a], Mazin Ahmed [a], Sarmad S.S. Al Qassar [b,*]

[a] College of Science, University of Mosul, Mosul, Iraq
[b] Department of Pedo Ortho Prevention, College of Dentistry, University of Mosul, Mosul, Iraq

Abstract

The purpose of this study was to investigate the effects of storing uncured photopolymerized dental adhesive in a magnetic field on their kinetics of polymerization and degree of conversion (DC%). Method: Vage Ortho Uv orthodontic adhesive was used in this experiment. Under constant frequency (50 Hz), the applied magnetic field was used at two different intensities (fixed at 0.01 T and 0.05 T) for 5 min each. Using Fourier transform infrared spectroscopy (FTIR-ATR), the degree of conversion (DC%) and polymerization kinetics were assessed. Results: There was a clear improvement in the results when compared to the control, the DC% mean tends to increase as MF increases starting at 0.05 T. Conclusions: The DC% of the Vega ortho Uv assessed orthodontic adhesive is influenced by the MF. Uncured orthodontic adhesive that has been exposed to MF for five minutes improves the changed bond angles or causes bond elongations, both of which would cause molecular deformation.

Key words: Polymer, Degree of conversion, Magnetic field, Orthodontic adhesive, Polymerization kinetics

1. Introduction

Magnets are all around us, but what exactly are magnets and magnetism? Any object that creates its own magnetic field and interacts with other magnetic fields is a magnet [1,2]. Since the time of Faraday, magnates have been recognized to affect diamagnetic materials. The effects of magnetic fields on non-magnetic materials (organic, inorganic, and macromolecular) have recently received attention. Advances in superconductivity technology and the availability of strong magnetic fields play an important role here. As a result, it is now possible to observe how magnetism affects biological objects, including polymers, wood, water and living organisms [3].

The induced mobility of electrons in the presence of a magnetic field (MF) is the primary cause of diamagnetis [4,5]. Using a bisphenol-A a glycidyl methacrylate (Bis-GMA) resin and acid etching in order to directly bond orthodontic brackets, was initially utilized by Silverman et al. [6] and Weisser [7]. Since when Bis-GMA resins were first used as adhesives in clinical orthodontic practice, the acid etched/composite technique quickly gained popularity. This bonding method has many benefits, including easy handling, strong adhesion, lessened gingival sensitivity, improved aesthetics, and a decrease in caries [8,9].

The Vega Ortho Uv (DFL, Brazil) is a light-cured orthodontic adhesive resin and the most popular photosensitizer for dental composite resins that are visible light cured is camphoroquinone (CQ). Technologies for curing light have advanced in recent years. Rapid polymerization has been demonstrated with light emitting diode (LED) curing lamps with distinct halogen light absorption spectra [10].

Polymerization of glycidyl methacrylate and bisphenol-A gives bis-GMA. In addition to being a resin component of dental sealants and composite restorative products, it is also used as an implant bonding material. For more than ten years, Bis-GMA has been the main component of most dental fillings [11]. The photocatalytic process results from a redox reaction that produces light-induced h+ (hole) and e (electron) on top of the incentive. Active

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* Corresponding author.
E-mail address: Iraq.sarmadsobhi@uomosul.edu.iq (S.S.S. Al Qassar).

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radicals such as hydroxyl (*OH) and superoxide (*O2) are produced during the reaction between the h+ and the e, as well as safe byproducts [12,13].

The amount that monomers react to form polymers, or the proportion of C=C double bonds that are transformed into C−C single bonds, is referred to as the degree of conversion (DC%) [14]. The DC% has a significant impact on the physical characteristics of the resulting cross-linked polymers. The mechanical strength, modulus, and hardness increase with increase conversion of double bonds [14,15]. Resin composites typically have DC% values between 52% and 75% [16,17]. The currently most popular experimental technique to measure the degree of conversion is Fourier transform infrared spectroscopy (FTIR) [18,19].

The relative band ratio approach is commonly used to calculate the DC. In this method, the intensity drop of vinyl bond vibrations caused by polymerization is measured in comparison to vibrations that do not directly participate in the reaction of polymerization (internal standard). The amount of absorption of the reference vibrations in the monomer and polymer is assumed to be equal [20]. The aromatic C=C stretching vibration at 1609 cm^{-1} is utilized as an internal standard [20]. In certain studies, where resins do not contain aromatic rings, the C=O stretching vibration at 1720 cm^{-1} is utilized as a standard. The results of that procedure may be erroneous, and many scientists dismiss the C=O band as a valid standard [21].

Numerous factors, including the kind of matrix, the presence of fillers, the kinetic of polymerization, the degree of conversion, and the modulus of elasticity, affect the amount of generated polymerization stress [22]. The pressure applied to the adhesive and the surrounding tooth structure through the process of polymerization is known as shrinkage stress [14]. Although there has long been interest in experimental evidence for the influence of magnetic fields (MFE) on the kinetics of chemical reactions, a field that we might call "magnetokinetic", an impressive advancement in the field, comes not only in before the late 1960s, when the phenomena of nuclear spin polarization and electrons in chemical reactions were discovered and understood. The so-called radical torque mechanism underlying these phenomena has turned out to be a very useful key for methodically assigning MFEs to chemical efficiencies and kinetics [23].

Influence of irradiance (mW/cm^2) − often erroneously referred to as light intensity (I_o) − on polymerization kinetics. It has been shown that increasing irradiance increases not only the rate of polymerization but also the conversion of double bonds, resulting in a much higher degree of polymerization. This effect was explained by the increase in sample temperature with higher irradiance, which is due to both the increased heat output of the lamp and the higher curing heat generated in the short curing time, resulting in higher mobility and hence higher conversion [24]. A new study published in 2021 [25] examined the impact of keeping orthodontic adhesives that had been exposed to light in a static magnetic field (MF) on the conversion degree (DC%) of the monomer. They applied a static magnetic field continuously for 48 h with a setting of 0.0225 T. It was determined that the orthodontic adhesive's DC test was impacted by the static magnetic field. After being exposed to the magnetic field, they observed a noticeable improvement. Their research concentrated on the (DC%) evaluation, and they only used static magnetic fields (SMF) with only one magnitude MF intensity (0.0225 T) over a lengthy exposure time (48).

Up to date, according to our knowledge, this is the first study conducted to search the effect of exposure of light curing Orthodontic Adhesives to different intensities of the magnetic field, specifically on the Degree of Conversion and kinetics of polymerization. The aim of the study was to calculate the degree of conversion of the material (VEGA ORTHO UV orthodontic adhesives) under the influence of the magnetic field at different intensities and to measure the polymerization kinetics.

2. Materials and methods

The research ethics committee (REC) of the College of Science at the University of Mosul examined and approved the study protocol (no. 4S/918 on 6/4/2022). According to (Table 1), Vega Ortho UV Orthodontic Adhesive was employed in this investigation.

2.1. Sample preparation for DC% testing

The 5 mm in diameter and 1 mm in breadth dental resin specimen disks that were used to calculate the DC% were created using a clear mold. A thin, 0.5 mm-thick layer of Mylar was placed on a piece of

Table 1. Chemical composition of the natural orthodontic UV adhesive utilized in this study

Orthodontic adhesive	Chemical Structure	Lot. No
VEGA ORTHO UV	Bisphenol A-Diglycidyl ether methacrylate (Bis-GMA),silica, barium glass, comphorquinone, diurethane dimethacrylate resin, fluorine, dimethylaminoethy methacrylate, inhibitor and pigments.	**21010047**

glass. A glass slide and another Mylar strip were used to cover the substance's surface after it had been overfilled into the mold and set on a surface with a yellow background that had a reflectivity of 70%. Using an LED curing unit (Raydent - LC device - Piece, USA) in standard mode at a distance of 0 mm with a light intensity of 1700 mW/cm^2, all of the composite specimens (n = 10/group) were light-activated. On the top side, 20 s. After that, samples were stored in distilled water for a day at room temperature (22 ± 2 C^o) to account for any post-curing effects. After 24 h, the specimens were removed from the molds.

2.2. DC% testing

The DC% of the polymerized sample was determined. To determine the discs initial (DC%), a total reflectance that has been attenuated was employed. Fourier transforming infrared spectroscopy (FTIR/ATR Alpha II, Platinum, Bruker Optic, Germany) was carried out in the absorbance mode following a period of 24 h in distilled water. For calculating DC%, several methods have been devised. The degree of polymerization of monomer molecules can be determined using the precise and straightforward Fourier transform infrared (FTIR) method, a spectral technique based on the interaction of light and material. Aliphatic C═C bonds are present in conventional methacrylate-based compositions (analytical peak, 1637 cm^{-1}), and these bonds are destroyed during polymerization to produce C−C bonds. However, since the reaction doesn't affect the aromatic C−C bonds (1610 cm^{-1}), they can be used as an internal reference peak without the need to be aware of the precise component concentrations. The DC% will be calculated using the following equation:

$$DC\% = [1 - \text{cured } (1639\ cm^{-1}/1609\ cm^{-1})/\text{uncured } (1639\ cm^{-1}/1609\ cm^{-1})] \times 100\%$$

2.3. Polymerization kinetics

In this test, you did not prepare the samples as in DC%, but the preparation and measurement of the samples was directly on the device, after exposing the material to the magnetic field at the intensity of 0.05 T for 5 min, after which the FTIR/ATR device was programmed to perform the test Where the range was specified between only (1580 cm^{-1} _ 1750 cm^{-1}). We put a small sample on the lens of the (FTIR/ATR) device, and then we display the material to a light curing LED for the polymerization process to occur, and then we start the measurement process, where we take 5 scans for one sample, with 3 min between each scan, and then we calculate the DC% value as done.

2.4. Statistical analysis

One-way ANOVA was performed to test the DC% data for the two tested groups, with a significance limit of $\alpha = 0.05$. The post hoc Tukey test in SPSS (version 22) was used to assess the statistical difference between groups.

3. Result

Fig. 1 displays the complete overlaying spectra of the FTIR/ATR chart for the drug (Vega Ortho Uv) with MF exposure. The graph of the material showed that the absorbance of the control and magnetic field groups increased in the 400 to 1200 cm^{-1} (fingerprint spectra) spectral range.

According to the formula above, the DC% for the control group was 66.74%. The DC% climbed to (69.62%) at the 5 min MF-0.05 T mark as shown in Table 2.

3.1. Polymerization kinetics

Results with a clear difference were obtained between the control and the magnetic field, where the effect of the field was significant. As shown in the Fig. 2.

4. Discussion

Since it has recently been discovered that magnetic flux has an effect on polymeric materials used in many fields, attention should be paid to the evolution of the magnetic field as well as its effect on with a variety of materials, including polymers. In this study, adhesives for fixing orthodontic appliances were investigated. Monomer materials are subjected to different magnetic field strengths before polymerization. The degree of conversion (DC%) is used to measure impacts.

Pulsed magnetic fields have been used to improve material properties as they provide non-contact reinforcement and protect the environment [26]. The results showed that the DC% values of composite materials cured with LEDs varied statistically significantly, and they also showed that the magnetic field has a great impact on the DC% of the composite materials. Diamagnetic particles were slightly arranged during the polymerization process, despite the fact that they lack permanent magnetic dipoles and therefore, aren't sensitive to the external magnetic field [27].

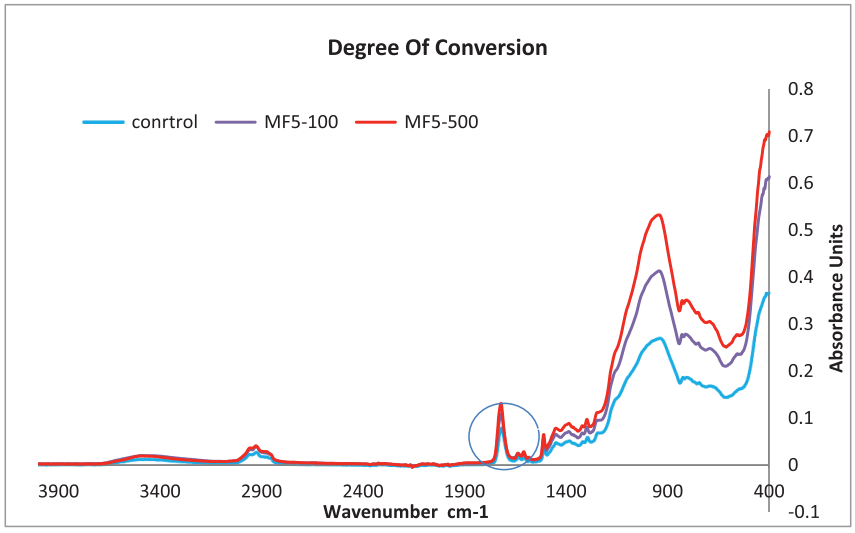

Fig. 1. Diagram showing the overlay of the complete spectrum of the VEGA ORTHO UV orthodontic adhesive for control group (blue line) and the different magnetic intensities (other lines).

Table 2. The means and standard deviations (SD) value of Degree of conversion (DC%)

adhesive	Mean DC%	SD	(*p*)value
MF- 0.00 T	66.74^{a,b}	±1.438	0.016
MF- 0.01 T	68.22^{a,b}	±1.613	
MF- 0.05 T	69.62^{b}	±1.466	

DC values are displayed as means ± standard deviations. Different lower-case superscript letters indicate values that differ significantly (Tukey HSD test, $p \leq 0.05$).

FTIR has been recognized as a powerful technology and suitable analysis and is often used as an effective method among a variety of methods because it detects vibrations caused by C=C stretching before and after hardening the material [28–30].

Accordingly, the effect of a strong magnetic field on the molecular alignment will improve the light transmittance of the adhesive, thereby increasing the DC% of the orthodontic composite to that of the small molecule composite [31,32]. It is believed that 5 min of exposure to the MF would be sufficient to modify the molecules of the unset orthodontic adhesive. In this study, the composite of the control group's C=C double bonds had a DC% of 66.74%, which indicates that 33.26% of the C=C double bonds were "uncured." Leaching of the uncured

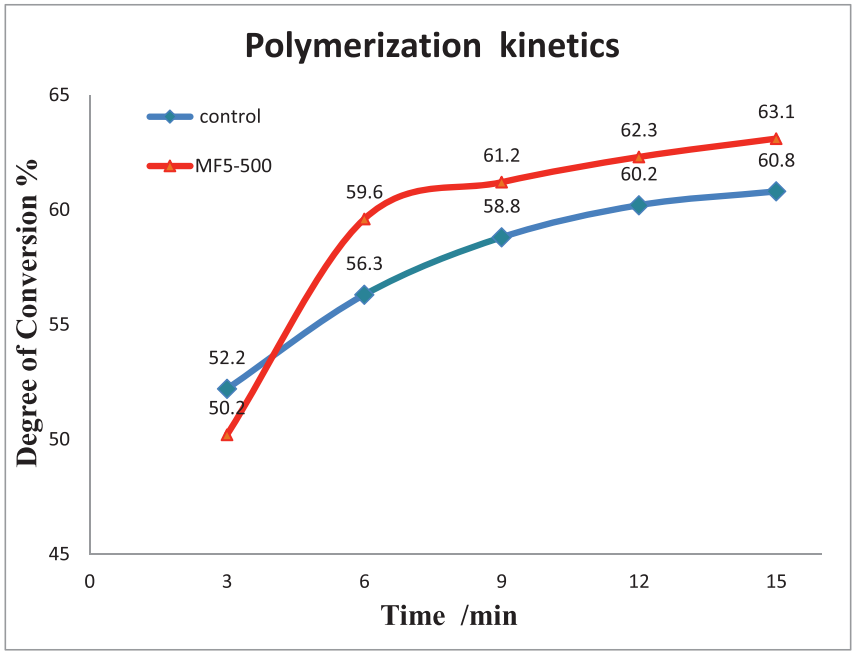

Fig. 2. The chart shows polymerization kinetics for vega ortho uv orthodontic adhesive in the control group (blue line) and the magnetic field (red line).

monomer may result in a reduced ratio of aliphatic to aromatic C=C double bonds in the effect magnetic state compared to the cured state in the control group, as previously mentioned.

It is clear from the magnetic orientation of aliphatic and aromatic polymers that the magnetic anisotropy of the individual monomers is not as strong. The alignment is influenced by the packing of the crystal, the secondary structure of the polymer chain, and the magnetic anisotropy of the monomer [33]. Numerous factors can affect the magnetic orientation of aliphatic and aromatic polymers. 1. Molecular structure: The existence of conjugated systems increases electron delocalization and strengthens the magnetic bonds in aromatic polymers. In comparison to aliphatic polymers, this may result in higher order and magnetic bonding. 2. Magnetic Anisotropy of Monomers: The propensity of monomers to align their magnetic dipole moments along a specific direction is referred to as magnetic anisotropy. Due to the molecular structure or electronic distribution of some monomers, they naturally exhibit magnetic anisotropy. The polymer chains may preferentially align if this anisotropy is preserved throughout polymerization. 3. External magnetic field: When used during polymerization or after curing, an external magnetic field can cause bonding in the polymer. The arrangement happens when the polymer chain's magnetic dipoles align themselves parallel to the field. The alignment's degree and direction can be affected by the field's strength and direction [33–35].

When an external magnetic field acts to generate a pair of free radicals, a certain magnetic behavior of the substance over time can be expected. The operation can start in the case of a root pair and eventually turn into a triple. Two free radicals will join to form a bond by recombination [36,37].

Due to the suppression of the magnetic field of the triplet–single transition, there is an increase in free radical production [23,38]. The molecular orientation generated by the magnetic field is mainly responsible for the kinetic magnetic effects in the production of conductive polymers [39].

Magnetic fields are capable of distorting molecules by changing the angle of chemical bonds in monomers with ionizable polar groups as well as intermolecular bond distances [40]. It should be noted that further research is needed to determine the quantitative relationship between microscopic mechanism and reaction kinetics. Several areas of research are required to develop a quantitative connection between reaction kinetics and micromechanics in the setting of magnetic fields: Advanced experimental techniques have been developed to accurately and precisely assess the effects of magnetic fields on microscopic and kinetic systems at high frequency. This could entail creating novel setups or changing tried-and-true methods. Theoretical models: Create theoretical models that can quantitatively explain how magnetic fields and micromechanics interact. This may entail integrating spin interactions and quantum mechanical effects into current reaction kinetic models. Research that is methodical: To comprehend broad trends and patterns relating to magnetic field effects, methodical examinations of a range of reactions and mechanisms should be conducted. The effects of various magnetic field intensities, directions, and frequencies may be studied in this regard. Comparison and verification by contrasting their predictions with experimental results, theoretical models and simulation techniques can be proven to be accurate. In explaining the relationship between micromechanics and response kinetics in the presence of magnetic fields, this can help to improve models and methodologies and establish their accuracy [36,41]. To the authors' knowledge, it is difficult to induce direct coincidence using magnetic fields.

5. Conclusions

The following conclusions can be drawn within the limitations of our in vitro research: The DC% of the Vega ortho Uv assessed orthodontic adhesive is influenced by the MF. The MF may have altered the bond angles or brought about bond elongations, which would result in molecular deformation. The magnetic field at an intensity of 0.5 T was sufficient to have a clear effect on the polymerization kinetics. The underlying radical pair process has proven to be the key to unlocking the kinetic properties of this phenomena.

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