STUDY OF THE COMPRESSIVE STRENGTH AND FLEXURAL MODELING OF NANOBIOCOMPOSITES

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Article History: Received: 24.01.2022 **Revised:** 25.02.2022 **Accepted:** 27.03.2022

Abstract

Rather than using Mineral Trioxide Aggregate, dentists can use Nano Fast Cement (NFC), a nanocomposite with a rapid curing time for filling root canals in teeth. The new tooth restorative material has poor workability and low compressive strength, which is a major drawback. In order to enhance its physical, mechanical, and biocompatibility features, NFC was modified in this study by adding polyvinyl alcohol (PVA), colloidal nano-silica, and hydroxyapatite nanoparticles. The strength-enhancing effects of all three compounds were analysed. The Taguchi method was used to create the experimental setup. Compressive and flexural strengths were maximised by finding the sweet spots for the three additions. The results demonstrated that polyvinyl alcohol is the most influential factor in determining the mechanical (compressive and flexural strength) qualities of NFC. Taguchi analysis shows that the best mechanical properties come from a mix of 6% PVA, 0.5% nano-silica, and 0% nano-hydroxyapatite.

Keywords: Nano Fast Cement (NFC), Hydroxyapatite Nanoparticles, colloidal nano-silica, Polyvinyl Alcohol, Optimization

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DOI: 10.31838/ecb/2022.11.01.011

1. Introduction

Composite materials with a phase size on the nanoscale scale are known as nanocomposites. As a result of their exceptional qualities, nanocomposites can be used as a replacement for microcomposites and monolithic materials. However, controlling the nanophase's elemental composition and stoichiometry presents difficulties in the nanocomposites' preparation methods. [1] One more exciting development in this field was the discovery of carbon nanotubes in 1991, which have since been used in the fabrication of nanocomposites. Nanocomposites are composites wherein nanosized filler components are added to the main material to enhance its qualities.

Because of the unique properties of the elements and the inhomogeneous distribution of the reinforcement, nanocomposites typically exhibit anisotropy (properties are directionally dependent. [5] Nanocomposites are replacing more traditional composite materials in many settings thanks to their superior performance. You can use sheets (like exfoliated clay stacks or graphene) or fibres (like aramids) to make up the reinforcing material (e.g., electrospun nanofibers).[17]

Nano-reinforced composites have an order of magnitude larger contact area compared to traditional composites [2] As a class of nanofiller materials, clays have seen widespread application in the production of nanocomposites with a polymer matrix. Recently, polymer/clay nanocomposites have garnered a lot of interest from both academics and businesses thanks to their superior qualities compared to those of traditional composites.[21] Layered silicates, of which clay minerals are a part, are distinguished by their layered structure. Puggal, Shivraj (2016) Because of their unique feature combinations and design practicality, polymer nanocomposites are finding widespread use in a variety of industries, including packaging, sports equipment, the automotive sector, and biomedical applications. Polymer nanocomposites have recently attracted increased attention in both the academic and commercial communities as a result of the advances in their properties. This research examines the numerous approaches to nanofiller dispersion, coating on fibres, and the enhancement of characteristics. Since only 1–5% of nanoparticles are loaded, the density is not altered like it would be with a composite material, but the improved attributes are still realised. Incorporating various nanoreinforcements into elastomers has been shown to improve the materials' modulus, strength, durability, toughness, and barrier to gases in comparison to conventional materials. These nanoreinforcements include layered silicate clays, carbon nanotubes, nanofibres, and silica nanoparticle nanocomposites. They add value to a home and are good for the planet. They have several positive applications, but producing them in a sufficient number and quality will be difficult.[24]

Numerous nanocomposites

Nanocomposites can be classified based on the reinforcement and matrix components they contain.[6] Based on the matrix material used, nanocomposites can be divided into three broad categories:

- Polymer Matrix Nanocomposites
- Nanocomposites in a Ceramic Matrix
- Metal matrix nanocomposites

Nanocomposites using a Polymer Matrix:

Materials with polymer matrices and nanoadditives for reinforcement are called polymer nanocomposites. [4] One-dimensional additives include nanotubes and fibers, but two- and three-dimensional additives can be created using layered materials such as clay (spherical particles).

Nanocomposites in a Ceramic Matrix

New generations of engineering materials, ceramic matrix nanocomposites with at least one phase of nano dimension, find widespread use in a variety of industries. Due to their exceptional microstructure, nanoceramic composites exhibit remarkable electrical and mechanical capabilities. [9]

Nanocomposites with a Metal Matrix

Reinforced by nanoparticles, metal matrix nanocomposites have a ductile metal or alloy matrix. [8]The physical, chemical, and mechanical properties of these nanoparticle-filled metal and alloy matrices are very different from those of the matrix material itself.[25]

Nanocomposites in polymers: their characteristics

Nanocomposite quality is affected not only by the characteristics of the constituent parts but also by the following factors: [7,12] Nanosized particles must be adequately dispersed and distributed in the matrix material in order to achieve enhanced nanocomposites properties; otherwise, particle agglomeration will occur, and the properties of nanocomposites will deteriorate.

(a) even dispersal, uneven distribution

(b) uneven dispersion and insufficient distribution,

c) uneven distribution but widespread impact, and

d) a broad and even distribution

The nanocomposite property improvement is also affected by the interface between the matrix and the filler ingredient. [9] Polymer matrix nanocomposites are characterised by the presence of a phase border between the matrix and the filler material and the formation of an interface layer between the two.

2. Materials And Method

The mechanical qualities (flexural compressive strength and workability) of samples that had three different additives added to Nano Fast Cement (NFC) were studied. These additions were polyvinyl alcohol (PVA; 0%, 3%), colloidal nano-silica (0.5, 1%), and hydroxyapatite nanoparticles (10, 20%).

Materials

The Nano Fast Cement (NFC) served as the primary material in this investigation; the presence phases in NFC were determined using the X-ray diffraction technique. Additives include Nano hydroxyapatite (NHA), Nano Silica Sol, and Polyvinyl Alcohol (PVA), and distilled water serves as the solvent. Sanat Avaran Vista Co. provides Nanosized NFC, which is supplied by the Iranian company Sanat Avaran Vista Co.In a precipitation process, we used calcium hydroxide ($Ca(OH)_2$, purity 99.0%; Sigma-Aldrich, USA) and phosphoric acid (H_3PO_4, purity 85.0%; Sigma-Aldrich, USA) to create nano hydroxyapatite particles (NHA).

Methods

Making Paste

Powdered polyvinyl alcohol (PVA) (molecular weight range of 146,000-186,000 g/mol, degree of hydrolysis> 99.0%; Aldrich, St. Louis, MO) was dissolved in water at 80°C with vigorous stirring to make PVA aqueous solutions. The nano-silica used was a commercially available aqueous colloidal solution with a nano SiO_2 content of 30%wt. When the solutions were ready, they were combined with the composite powder made of nano hydroxyapatite, nano-silica sol, and polyvinyl alcohol in the appropriate quantities. Next, the material was pressed into the desired shape using silicone moulds.

Design of Experiments

The Taguchi method was used to create the experiments. The composite was tested at three different concentrations of nano-hydroxyapatite, nano-silica sol, and polyvinyl alcohol. The L9 orthogonal matrix served as the basis for all experimental procedures. The outcome was examined with the help of the signal-to-noise ratio (S/N). It's important to remember that there are three distinct S/N ratios to consider when trying to optimise a given set of parameters. Taguchi, on the other hand, divided the S/N ratio into three groups based on the intended response type: smaller-is-better, larger-is-better, and nominal-is-better. The shorter the setting time, the better.

$$S/N_N = 10\,Log_{10}\frac{\frac{1}{n}\left(\frac{(\Sigma y_i)^2}{n} - \frac{\Sigma y_i^2 -}{n}\right)}{\frac{\Sigma y_i^2 - \frac{(\Sigma y_i)}{n}}{n-1}}$$

When it comes to strength, bigger is better:

$$S/N_S = -10\,Log_{10}\frac{1}{n}(\Sigma y_i^{\,2})$$

In support of the nominal:

$$S/N_B = -10\,Log_{10}\left(\frac{1}{n}\Sigma\frac{1}{y_i^{\,2}}\right)$$

Characterization

Compressive Strength

To determine the compressive strength of the final product, we used a universal testing equipment (Intron, Zwick, Germany) set to a crosshead speed of 1 mm/min. After 24 hours in silicone moulds, every sample was put to the test (4 mm in diameter and 6 mm in height). There were three separate attempts at each test. The force needed to break each specimen was used to figure out its compressive strength.

Stress-Resistant Flexibility

Beam-shaped samples were made and given 24 hours to cure. Then, the bending strength of each sample was measured by using a crosshead speed of 1 mm/min and a three-point bending test at room temperature.

3. Results

Table 1. Process Variables and Their Values

Parameters	Level 1	Level 2	Level 3
Nanohydroxyapatite (NHA)	0%	10%	20%
Colloidal nanosilica	0%	0.5%	1%
Polyvinyl alcohol (PVA)	0%	3%	6%

Table 2. Experimental design matrix

Test number	%HA	%Sio2	%Pva
1	0%	0%	0%

2	0%	0.50%	3%
3	0%	1%	6%
4	10%	0%	3%
5	10%	0.50%	6%
6	10%	1%	0%
7	20%	0%	6%
8	20%	0.50%	0%
9	20%	1%	3%

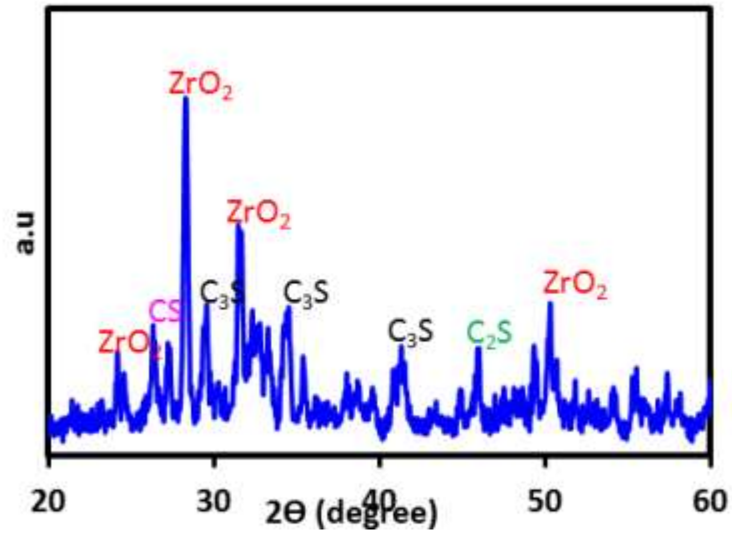

Fig 1. The priming powder XRD pattern

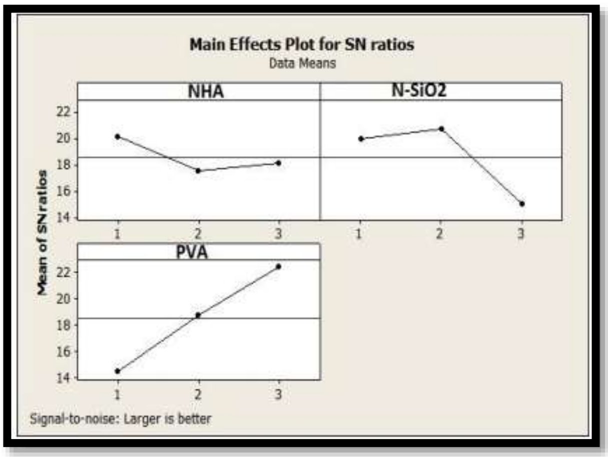

Fig 2. A schematic depicting the relationship between the S/N ratio and the compressive strength of a nanocomposite containing the additives (A) hydroxyapatite (B) nanosilica (C) polyvinyl alcohol.

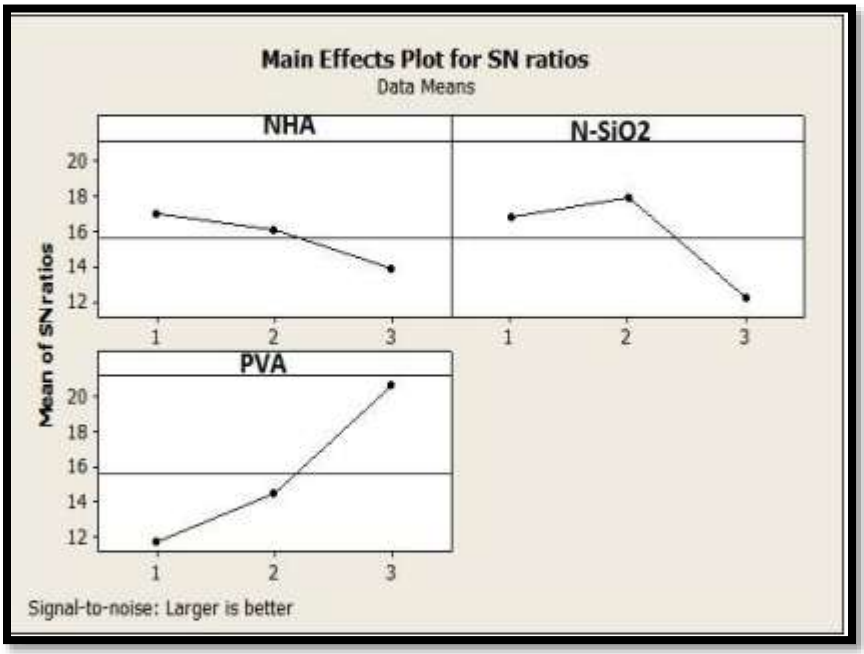

Fig 3. The S/N diagram shows how different additions (A hydroxyapatite, B nano-silica, and C polyvinyl alcohol) affect the flexural strength of a nanocomposite.

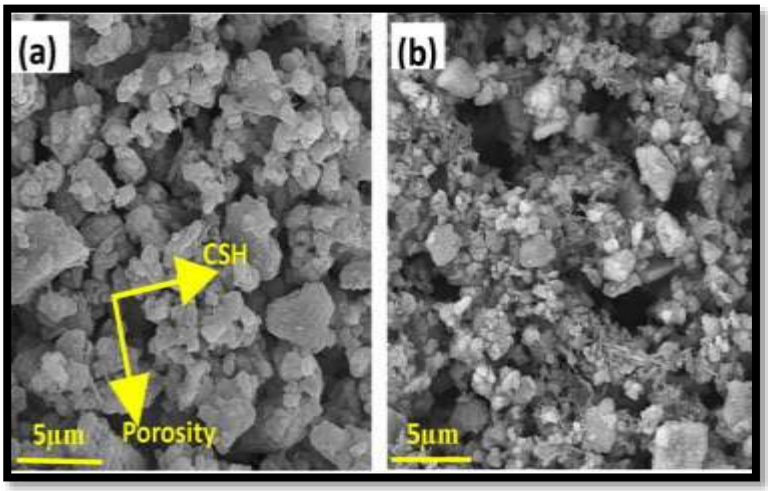

Fig. 4 shows scanning electron microscopy (SEM) images of the products of two different nanocomposite optimization

4. Discussions

The XRD analysis of NFC cement showed that the primary components of NFC cement are zirconium dioxide, tricalcium silicate (C_3S; Ca_3SiO_5), dicalcium silicate (C_2S; Ca_2SiO_4), and tricalcium aluminate (C_3A) ($Ca_3Al_2O_6$). Mechanical tests were conducted to determine the material's strength and evaluate its resistance to incoming functional stresses. [23] The capacity to withstand a given tension without breaking is the essence of strength. Both compressive and flexural strengths are crucial in endodontics. Here, we used compressive and flexural experiments to investigate the mechanical properties of the NFC/PVA nanocomposite. As expected, PVA is found to be the most influential factor in determining final tensile strength. [25] However, as can be observed, the S/N curve rises up to 0.5%wt of nano-silica and then gradually lowers. Since the value of S/N is highest at 0.5%, this concentration is chosen as the sweet spot for nano-silica content. Taguchi analysis shows that a combination of 6% PVA, 5% nano-silica, and 0% nanohydroxyapatite provides the maximum compressive strength. [27] As shown by the validation tests of the conditions, the projected value of 14 MPa is met at this condition. PVA's role in bonding between aggregates and the elimination of pores in NFC are credited with the increased compressive and flexural strength. [28]

5. Conlclusions

The physical and mechanical properties of a Nano Fast Cement (NFC) were investigated in this study, along with the additions of poly(vinyl alcohol), colloidal nano-silica, and nanohydroxyapatite. In order to create a liquid component for this nanocomposite, it is necessary to choose the ideal amount of nano-silica and PVA. [30] At 6% polyvinyl alcohol polymer and 0.5% nano-silica by weight, the resulting material has the perfect combination of stiffness and strength. As far as we can tell, the incorporation of hydroxyapatite nanoparticles into NFC does not significantly alter its mechanical or physical properties. [29]

6. References

Badawi A. "Characterization of the optical and mechanical properties of CdSe QDs/ PMMA nanocomposite films". J Mater Sci Mater Electron Vol 26, issue (1), Page 3450–7,2015.

Sirvastva R, "Synthesis and characterization techniques of nanomaterials", International Journal of Green Nanotechnology: Physics and Chemistry, 2012, Vol 4, issue (1), Page 1-11,2012.

ScheiffN. "Nanoscience and Nanotechnologies, The Royal Society & the Royal Academy of Engineering" 2004.

Xiang J. "Preparation and magnetic properties of SrFe12O19/ Ni0.5Zn0.5Fe2O4 nanocomposite ferrite microfibers via sol–gel process". Mater Chem Phys;vol 126, issue (1), Page 791–6,2011.

Luo JJ and Daniel IM, "Characterization and Modeling of Mechanical Behavior of Polymer/Clay nanocomposites", Compos. Sci. Technol., Vol 63, issue (1), Page 1607-1616,2003.

Thostenson E, "Review Nanocomposites in Context", Journal of Composites Science & Technology, Vol 65, issue (1), Page 491-516,2005.

. Schmidt D, "New Advances in Polymer/Layered Silicatenanocomposites, Current Opinion in Solid State and Materials Science", Vol 6, issue (1), Page 205-212,2002.

Alexandre M and Dubois P, "Polymer-layered Silicate Nanocomposites: Preparation,Properties and Uses of a New Class of Materials", Mater. Sci. Eng., Vol 28, issue (1), Page 1-63,2000.

Park C, "The Fabrication of SyndiotacticPolystyrene/Organophilic Clay Nanocomposites and Their Properties", Polymer, Vol 42, issue (1), Page 7465-7475,2001

Mehta R. "Glass Fiber reinforced polymer-clay nanocomposites: processing, structure and hygrothermal effects on mechanical properties". Procedia Chemistry. Vol 4, issue (1), Page 39–46,2012

M.T. Rahman, et al." Study on the mechanical, electrical and optical properties of metal-oxide nanoparticles dispersed unsaturated polyester resin nanocomposites", Results in Physics , Vol 13 , Issue (1), Page 1-9,2019

Abdallah S, Badawi A. "Characterization of optical, thermal and electrical properties of SWCNTs/PMMA nanocomposite films". Iran Polym J vol 23, issue (1), Page 437–43,2014.

Masuri AF, Kashif M. "Synthesis and Characterization of ZnOCNTs Filled PVA Composite as EM Detector". J Appl Sci vol 11, issue (1), Page 1303–8,2011.

Shivraj Puggal "A Review on Polymer Nanocomposites: Synthesis, Characterization and Mechanical Properties", Indian Journal of Science and Technology, Vol 9, issue (4),page 1-19,2016

Abdallah S, "Single wall carbon nanotube/titania nanocomposite photoanodes enhance the photovoltaic performance of cadmium selenide quantum dot-sensitized solar cells". Mater Sci Semicond Process , vol 26, issue (1), Page 162–8,2014

Azzam W. "Behavior of modified clay microstructure using polymer nanocomposites technique". Alexandria Engineering Journal. Vol 53, issue (1), page 143–50,2014.

Dobrzanski LA, "Polymer nanocomposites reinforced with montmorillonite". Archives of Materials Science and Engineering. Vol 53, issue (1), page 5–28,2012.

Khankrua R, Pivsa S, Thermal and mechanical properties of biodegradable polyester/silica nanocomposites. 10th Eco-Energy and Materials Science and Engineering Symposium", Energy Procedia. Vol 34, issue (1), page 705–13,2012.

Manoharan N, Cryogenic mechanical properties of PP/MMT polymer nanocomposites". Indian Journal of Science and Technology. Vol 7, issue (1), page 16–23,2014.

Chow W. "Water absorption of epoxy/glass fiber/organomontmorillonite nanocomposites". eXPRESS Polymer Letters, Vol 1, Issue (2), page 104–8,2007.

Tippur, H.V.: "Quasi-static and dynamic fracture behavior of particulate polymer composites: a study of nano-vs. micro-size filler and loading-rate effects", Composites Part B: Engineering, Vol 43, issue (8), page 3467-3481, 2012.

Bhowmik, "Optimization of mechanical properties of epoxy based wood dust reinforced green composite using Taguchi method", Procedia Materials Science, Vol 5, Issue (1), Page 688-696, 2014,

Kumari, "Synthesis and characterization of a Cu (II) Schiff base complex immobilized on graphene oxide and its catalytic application in the green synthesis of propargylamines", RSC Advances, Vol 6, Issue (1), Page 15340-15344, 2016.

Lengowski, E.C "Avaliação de métodos de obtenção de celulose com diferentes graus de cristalinidade.", Forest Sciences/Scientia Forestalis, Vol 41, Issue (1), Page 185-194, 2013

Marinelli, L.A "Desenvolvimento de compósitos poliméricos com fibras vegetais naturais da biodiversidade: uma contribuição para a sustentabilidade amazônica", Polímeros: Ciência e Tecnologia, Vol 18, issue (2), Page 92-99, 2008

Mishra, S "Studies on mechanical performance of biofibre/glass reinforced polyester hybrid composites", Composites Science and Technology, Vol 63, issue (10), Page 1377-1385, 2003

Mohanty, A.K "Surface modification of jute and its influence on performance of biodegradable jute-fabric/Biopol composites", Composites Science and Technology, Vol 60, Issue (7), Page 1115-1124, 2000

Yokozeki "Improved mechanical properties of carbon fiber/graphene oxide-epoxy hybrid composites", Composites Science and Technology, Vol 135, Issue (1), Page 28-38, 2016

Patnaik, A “Wear behavior of plant fiber (pine-bark) and cement kiln dustreinforced polyester composites using Taguchi experimental model”, Journal of composite materials, Vol 44, issue (5),Page 559-574

Porras, “Optimal tensile properties of a Manicaria-based biocomposite by the Taguchi method”, Composite Structures, Vol 140, Issue (1), Page 692-701, 2016.