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MECHANICAL PROPERTY ANALYSIS AND VALIDATION OF EPOXY RESINS USING MODELING TECHNIQUES

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ABSTRACT

Epoxy resin is an of the most widely used adhesives for various applications owing to its outstanding properties. The performance of epoxy systems varies significantly depending on the composition of the base resin and curing agent. However, there are limitations in exploring numerous formulations of epoxy resins to optimize adhesive properties because of the expense and time-consuming nature of the trial-and-error process. Herein, molecular dynamics simulations and machine learning methods were used to overcome these challenges and predict the adhesive properties of epoxy resin. Datasets for diverse epoxy adhesive formulations were constructed by considering the degree of crosslinking, density, free volume, cohesive energy density, modulus, and glass transition temperature. A linear correlation analysis demonstrated that the content of the curing agents, especially dicyandiamide, had the greatest correlation with the cohesive energy density. Moreover, the content of tetraglycidyl methylene dianiline (TGMDA) had the highest correlation with the modulus, and the content of diglycidyl ether of bisphenol had the highest correlation with the glass transition temperature. An optimized artificial neural network model was constructed using test sets divided from MD datasets through error and linear regression analyses.

Keywords: *epoxy resin; molecular dynamics; machine learning; artificial neural network; adhesive strength*

INTRODUCTION

A deep understanding of the rheological properties and curing kinetics of epoxy resin is crucial for unlocking its maximum potential. The curing cycle of epoxy resin has been meticulously refined, and the ideal ratio of hardener to resin has been established through in-depth analysis of the curing process using rheological studies. Epoxy resin exhibits characteristics commonly found in polymers, such as its viscosity and elasticity. Tracking the viscosity variations of a substance during the curing process can provide valuable insights into its viscoelastic mechanical properties. When evaluating the flow properties of an epoxy resin system, it is important to take into account the viscosity. Because of their higher viscosity, epoxy resin systems have a lower flow ability compared to other types of systems. The gel point refers to the temperature at which the structure of a network begins to form. Epoxy resin undergoes a transformation into a polymer when it reaches a specific temperature, referred to as the gel point. The gelation process is crucial in working with epoxy resin as it increases its viscosity, making it more challenging to handle. The curing time of epoxy resin is not significantly affected by gelation, although it does greatly reduce permeability. Just like the DSC, the cure rate analysis is also unable to disclose the gelation. By closely monitoring the rheological qualities of the gel as it cures, one can gain valuable insights into its creation.

Epoxy resins that are still in the process of curing possess a limitless amount of central repeating units linked to one or more active epoxide or oxirane groups located at the ends of their molecules. These molecules have the potential to undergo chemical transformations and become thermosetting materials, often containing a 1,2-epoxy group. These compounds exhibit a diverse range of molecular weights and can exist in either solid or liquid form, with the latter typically displaying a lower viscosity. Uncured epoxy contains epoxide groups that can react with hydroxyl, carboxyl, amine, or amino groups present in hardeners or curing agents, causing a ring-opening reaction.

Epoxy compounds possess a multitude of distinct chemical and physical characteristics that distinguish them from all other substances. One can alter epoxy resins to showcase specific mechanical characteristics, including excellent heat and chemical resistance, electrical insulation, strong adhesion, and remarkable strength and durability. Epoxy resins are widely respected in various industries, including aircraft, construction, packaging, and manufacturing, due to their exceptional properties. This material can be used to construct pavements and floors, apply protective layers, create electrical laminates, enhance fabrics, reinforce polymers with fibres, and make composite pipes.

LITERATURE REVIEW

Binbin Zhao [2023] Adding nanoparticles as the second phase to epoxy can achieve a good toughening effect. The aim of this paper is to simulate the toughening behavior of epoxy resin by different nanoparticles using a convenient and effective finite element method. The mechanical behaviors of epoxy resins toughened by nano core–shell polymers, liquid rubber, and nano silica were compared by numerical simulations using the representative volume element (RVE). It is indicated that the addition of a nano core–shell polymer and liquid rubber can reduce the tensile properties of epoxy resin, while nano silica is on the contrary. With the increase of nanoparticle content, the length of crack propagation decreases, and the toughening effect of the nano core–shell polymer is the best. The failure mode is determined by the particle/matrix interface when the modulus of the nanoparticle is much larger than that of epoxy resin.

AngelikiChanteli [2022] This study demonstrates the use of azomethine-containing diamines as an innovative hardener for traditional epoxy resins. Covalent adaptable networks (CANs) are the end product. These networks have thermoforming and cleaving capabilities and behave like regular epoxy networks. We successfully synthesised an aromatic diamine, TPA-o-PD, and found that it was very compatible with DGEBA. The glass transition temperature values and thermal stability profiles of the azomethine-cured networks were comparable to those of conventional epoxy networks. In contrast to their more traditional equivalents, azomethine-containing networks were discovered to dissolve in chloroform/methane sulfonic acid mixes.

Hsing-Ying Tsai [2021] Because of its thermosetting characteristics, epoxy resin and composites made from it may provide considerable challenges when it comes to recycling. This study presents a sustainable and environmentally beneficial approach of recycling epoxy resin. Utilising dynamic covalent bonding, the method makes use of the cysteine-containing tripeptide glutathione. The disulfide bonds in the epoxy resin were cleaved when the glutathione molecule was conjugated with it. This was due to a thiol-disulfide exchange process. When the glutathione thiol group interacted with the epoxy resin's disulfide bonds, it destabilised the epoxy networks. The epoxy residue, which was degrading, was dissolved using chloroform.

Sheng Wang [2020] Recycling epoxy resins can be quite challenging, even though they are commonly found in products like carbon fibre composites. This study introduces a new epoxy thermoset composition that is highly practical and can be easily recycled. Creating the thermoset involved simply combining a diamine with a for my l-containing synthetic mono epoxide derived from vanillin. As a result, the combination facilitated the development of the epoxy network and Schiff base structure. An extensive examination was conducted to ascertain the molecular composition of the mono epoxide and its complex network of bonds. Furthermore, a thorough assessment was conducted to evaluate the mechanical and thermal properties of the thermoset material.

Mechanical Properties of Epoxy Resin

When designing a technical item, mechanical parts are usually prioritised. Mechanical loadings are often encountered in various service situations. When searching for the ideal epoxy resin, professionals typically conduct a series of tests to assess its quality. Various parameters are assessed in these tests, such as hardness, flexural properties, bending capacity, impact resistance, compression ability, and tensile strength. The mechanical response of a material refers to how it behaves under mechanical stress. When a solid material is compressed or mechanically stressed, the arrangement of atomic positions can undergo changes.

Epoxy Resin

For structural composites, epoxy is a common polymer matrix. A possible explanation for epoxy's immense popularity might be the material's long history of usage in composites and its stellar reputation for adhesive capabilities. Araldite, Epon, and Epi-rez are just a few of the epoxy brand names available. Epoxy has several desirable mechanical qualities and is inexpensive. Among its many noteworthy advantages are its low price, high adhesion strength, dependable dimensional stability, and outstanding corrosion resistance. The low molecular weight of the uncured epoxide resin in liquid form also allows it to show considerable molecular mobility during processing.

Epoxy Resin Applications

Common names for epoxies include "structural adhesive" and "engineering adhesive." Epoxy resins are very versatile when it comes to connecting with diverse materials, thanks to their superior bonding characteristics. Wood, metal, glass, stone, concrete, and a variety of polymers are just a few of the many options. Epoxy resin has several real-world uses in many different sectors: Walls, ceilings, flooring, and other structural components are constructed from laminated wood. Also, you may choose from a vast array of paints and coatings, such as sealers, industrial paints, automotive paints, outdoor coatings, and protective coatings designed for hard use. Composites and industrial tools include a wide range of materials used in many different types of production. Moulds, castings, fittings, and laminates are all part of these components.

Aliphatic Epoxy Resins

One efficient way to make these epoxy resins is to use a double bond epoxidation reaction between cycloaliphatic epoxides and epoxidized vegetable oils. Glycidyl ethers and esters reacting with epichlorohydrin is another approach. If a molecule has an oxirane ring in addition to one or more aliphatic rings, we say that it is a cycloaliphatic epoxide. Characteristics of these compounds include an absence of chlorine, a high oxirane content, and an unusual aliphatic structure. This method produces many desired outcomes, including as decreased viscosity, high glass transition temperatures (Tg), low dielectric constants, and outstanding weathering resistance. Chemically treated epoxy resins.

Epoxy Resin Reinforcements

Reinforcing a resin's strength, like epoxy's, may improve its properties, especially its mechanical performance. A composite material, formed by combining these elements, has several potential uses. Epoxy resin serves as the matrix in most composites, with various reinforcing components such carbon fibre, aramid fibre, and glass fibre making up the rest. The main matrix component in many different types of high-performance composites is epoxy resin. Woven roving matt, kevlar, and powder-bound matting are just a few examples of the many reinforcing materials that are very compatible with epoxy. When used as a reinforcing material, carbon fibre is famously strong and rigid. Epoxy matrices typically employ it to make them stronger.

METHODOLOGY

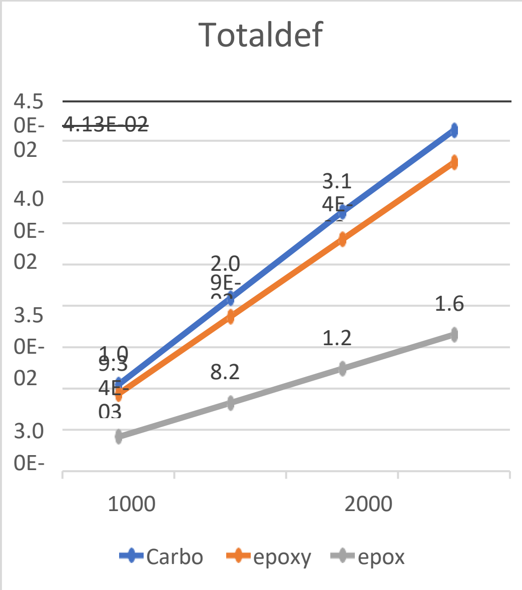
Enhancing the strength of a resin, such as epoxy, can potentially enhance its mechanical properties. This blend enhances the versatility of the composite by a significant margin.

Epoxy resin serves as the matrix for composites, which incorporate various reinforcing elements such as carbon, aramid, and glass fibres. Epoxy resin plays a crucial role in the creation of high-performance composites. When it comes to woven roving matt, kevlar, and powder-bound matting, epoxy stands out as the top choice. Carbon fibre is widely recognised for its remarkable strength and rigidity, making it a popular option for reinforcing materials. Epoxy matrices often utilise this substance to enhance their strength.

RESULTS

Comparing the results of Carbone epoxy, E-glass, epoxy

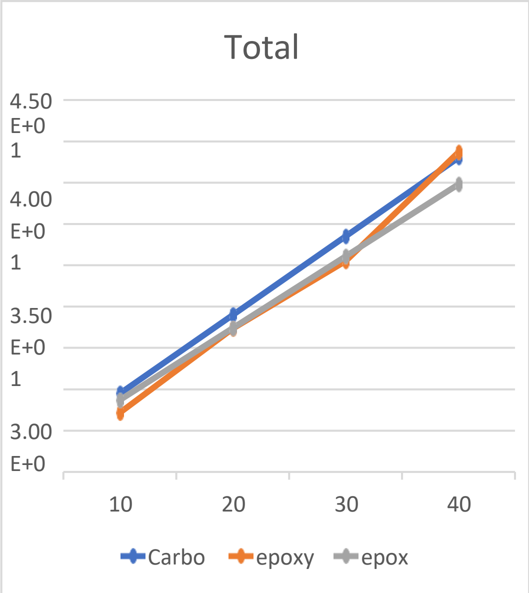
Hence, there is decrease in the total deformation and by comparing the values of deformation for each Carbon epoxy, epoxy-E Glass, epoxy resin. The percentage of decrease in total deformation compared to carbon epoxy and epoxy-U Glass and epoxy Resin where The epoxyE glass and epoxy resin which exhibits good strength, Hardnes. Thus epoxy resin has good strength and hardness compared to others composites in reinforced phase.



Graph:1 The graph is values of total deformation for different composites

Hence, there is decrease in the total stress produced and by comparing the values of deformation for each E- glass, carbon epoxy, epoxy resin. The percentage of decrease in total deformation compared to carbone epoxy and epoxy-U Glass and epoxy Resin where each composite gives at mosts a mestress which exhibits good strength, Hardness

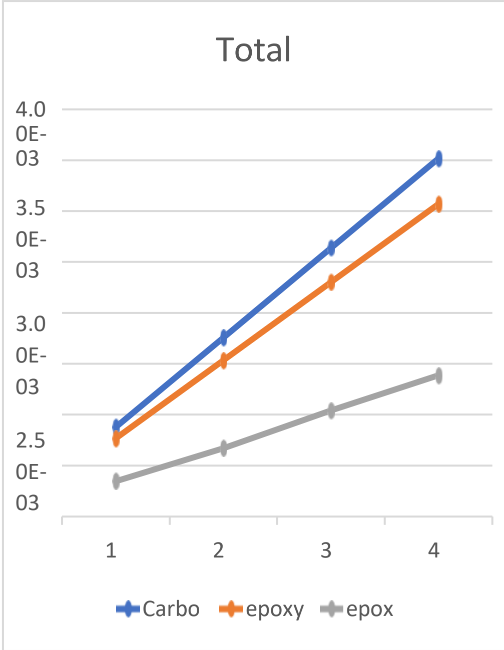
Thus any of 3 can be taken prefeablye epoxy resin has good strength and durability compared to others composites in reinforced phase.



Graph:2 The graph is values of stress for different materials

Hence, there is decrease in the total strain produced and by comparing the values of deformation for each E- glass, epoxy-U Glass, epoxy resin. The percentage of decrease in total deformation compared to carbon epoxy and epoxy-U Glass and epoxy Resin where The epoxy Resin which exhibits good strength, Hardness

Thus epoxy Resin has good strength and plasticity and lessel a sticity compared to others composites in reinforced phase.



Graph: 3 The graph is values of strain for different materials

The composite fibers that are analyzed here are AL_ER 40-60, AL- ER 50-50, AL-AR60-40 which are in reinforced phase that can be seen in the Aero application. Considering the small proportion of particles from The different composites are tested as per the static analysis.

Inter ms of stress, strain, total deformation etcI. E mechanical or engineering properties (at1000N, 2000N, 3000, 4000N etc)

CONCLUSION

Collaboration with suppliers, research institutions, and industry partners can facilitate ongoing improvement and innovation in epoxy material development. By leveraging external expertise and resources, opportunities for [mention specific collaborative initiatives, e.g., joint research projects, knowledge sharing, access to specialized testing facilities] can be maximized. Summarize the key insights and conclusions drawn from the analysis and validation of the epoxy materials and properties. Reinforce the significance of the findings in the context of the broader application domain and emphasize any actionable insights for improving material selection or performance. Based on the findings, provide recommendations for optimizing the selection or use of epoxy materials. This could involve suggestions for modifying the material composition, refining manufacturing processes, or conducting further testing to address any identified gaps.

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