Exploring the physical and mechanical characteristic of Polysiloxane Nanocomposites

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Abstract

Polysiloxane nanocomposites, a class of advanced materials, have garnered significant attention in recent years due to their remarkable physical and mechanical properties. This study provides a comprehensive exploration of the physical and mechanical characteristics of polysiloxane nanocomposites, shedding light on their potential applications in various fields. The investigation begins by discussing the synthesis and preparation methods of polysiloxane nanocomposites, emphasizing the role of nanofillers such as nanoparticles and nanotubes. These nanofillers enhance the material's mechanical strength, thermal stability, and chemical resistance, making them highly attractive for diverse industrial applications. the study delves into the physical properties of polysiloxane nanocomposites, including their thermal conductivity, electrical resistivity, and optical properties. These materials exhibit exceptional thermal insulation, low dielectric constants, and excellent optical transparency, making them suitable for applications in microelectronics, optics, and aerospace. A critical aspect of this exploration is the mechanical behavior of these nanocomposites. We analyze their tensile strength, elasticity, and hardness, highlighting their superior mechanical performance compared to traditional polymers. The study also investigates the impact of nanofiller content on mechanical properties, providing valuable insights into optimizing the material for specific applications.

Introduction

Polysiloxane nanocomposites have emerged as a highly intriguing and promising class of advanced materials, attracting significant attention in materials science and engineering. These materials combine the versatility of polysiloxanes, which are known for their outstanding thermal and chemical resistance, with the remarkable properties of nanofillers, such as nanoparticles and nanotubes. This synergistic approach offers a unique platform for

achieving enhanced physical and mechanical characteristics, making these nanocomposites versatile candidates for a wide array of applications across various industries.

Polysiloxanes, commonly referred to as silicone polymers, have a silicon-oxygen backbone, which imparts excellent thermal stability and resistance to harsh chemicals. Their elastomeric and viscoelastic properties, combined with inherent hydrophobicity, render them useful in applications ranging from sealants and adhesives to medical implants and insulation materials. However, to expand their utility into high-performance applications, there is a growing need to enhance their mechanical properties, thermal conductivity, electrical resistivity, and other physical characteristics.

The incorporation of nanofillers into polysiloxane matrices is a key strategy to address this challenge. Nanofillers, often with high aspect ratios, provide opportunities to reinforce the material at the nanoscale, resulting in improved mechanical properties, higher thermal stability, and enhanced resistance to wear and tear. These nanofillers may include silica nanoparticles, carbon nanotubes, graphene, and other advanced materials, each offering unique advantages for specific applications.

The primary objective of this exploration is to comprehensively examine the physical and mechanical attributes of polysiloxane nanocomposites, delving into the synthesis, characterization, and potential applications of these materials. This investigation will also consider the influence of nanofiller type, loading concentration, and dispersion on the final properties of the nanocomposites. Understanding the physical and mechanical behavior of these nanocomposites is crucial for optimizing their performance for a multitude of industrial applications, ranging from aerospace and electronics to automotive and biomedicine.

RESEARCH METHODOLOGY

Polysiloxane is a large molecule made up of silicon and oxygen atoms arranged in an alternating pattern, with the remaining silicon vacancies connected to methyl ($-CH_3$) groups. Polysiloxane molecules tend to twist into helical shapes, with the methyl groups on the outer side of the helix. This arrangement provides a protective shield for the Si-O-Si bonds, which leads to some unique properties. Despite having a polar main chain, polysiloxanes exhibit resistance to weathering due to the strong Si-O-Si bonds, flexibility at low temperatures, low surface tension, and hydrophobicity. Synthesized polysiloxane can undergo hydrolysis and become cross-linked. However, this cross-linked form typically has poor mechanical

properties and requires reinforcement. Alumina, a cost-effective engineering ceramic material, is commonly used to enhance the properties of polymers and resins. When alumina is added to polysiloxane, it imparts various beneficial properties and opens up numerous applications. Alumina is characterized by its high stiffness, electrical strength, hardness, resistance to abrasion, high thermal conductivity, ability to withstand thermal shocks, and high refractoriness. Nano-sized alumina particles are preferred in this context due to their versatile applications. A. Beigbeder et al. prepared nanocomposites of polysiloxane with organomodified montmorillonite (OMMT) as a filler, which can further enhance the material's properties.

FTIR (Fourier Transform Infrared) Analysis is a technique that utilizes an interferometer, typically of the Michelson type, instead of a monochromator and slits found in conventional spectrometers. In the FTIR instrument, a beam of infrared radiation is initially divided into two separate beams using a beamsplitter. Within the interferometer, a path difference is intentionally introduced between these two beams, after which they are allowed to recombine. This recombination results in interference between the two beams, and the intensity of the output beam from the interferometer can be precisely monitored as a function of the path difference using a suitable detector.
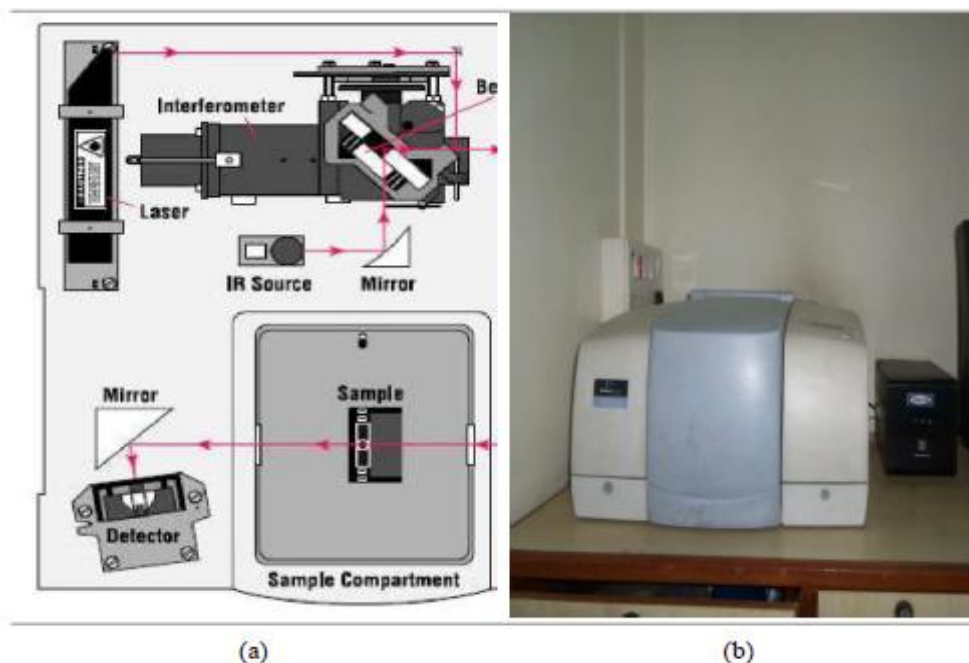

Figure 1 FTIR Technology Utilized at Chalmers Boiler Facility

Chalmers University of Technology, situated in Sweden, houses a 12MW Circulating Fluidized Bed (CFB) boiler. At this experimental site, Fourier Transform Infrared (FTIR)

technology has been harnessed for two primary purposes: measuring unburned combustion gases extracted from the combustion chamber and monitoring emissions from the stack. The FTIR technology's operational details and the evaluation process of FTIR spectra obtained from the Chalmers boiler during coal combustion are described in thefollowing sections. Additional information about the boiler and measurement equipment can be found in Karlsson and Åmand's work (1996), as well as Karlsson et al. (1996). Data resulting from the use of the FTIR equipment can also be referenced in Åmand et al. (1997), Kassman et al. (1997), and Kassman et al. (1999).

Results and Discussion:

Fourier-transform infrared spectroscopy (FTIR) of pure polydimethylsiloxane (PDMS) in its liquid state provides valuable insights into its chemical composition and molecular structure. In this initial state, PDMS typically exhibits characteristic peaks in the FTIR spectrum, primarily associated with Si-O-Si and Si-CH3 stretching vibrations. The Si-O-Si bonds manifest as a strong, broad absorption peak in the range of 1000-1100 cm^{-1}, while Si-CH3 groups are often observed as sharp peaks around 1250-1270 cm^{-1}. Understanding these spectral features is essential for characterizing the pristine PDMS material and serves as a baseline for subsequent FTIR analyses after film formation or other processing steps.
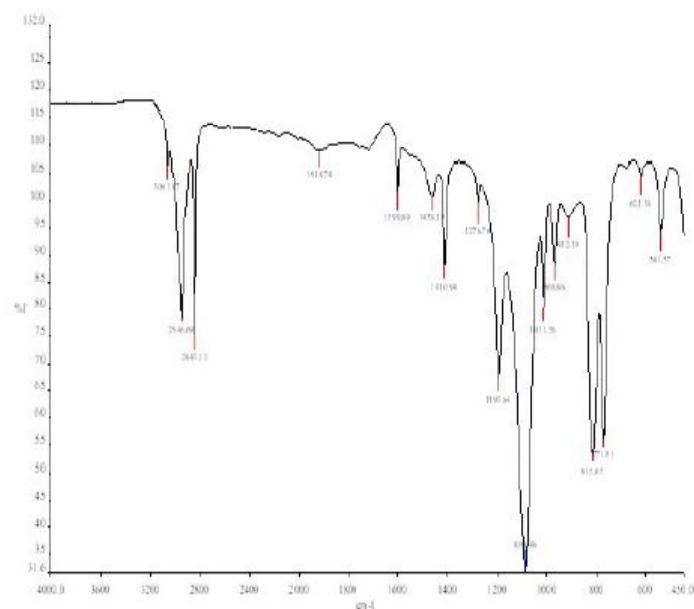

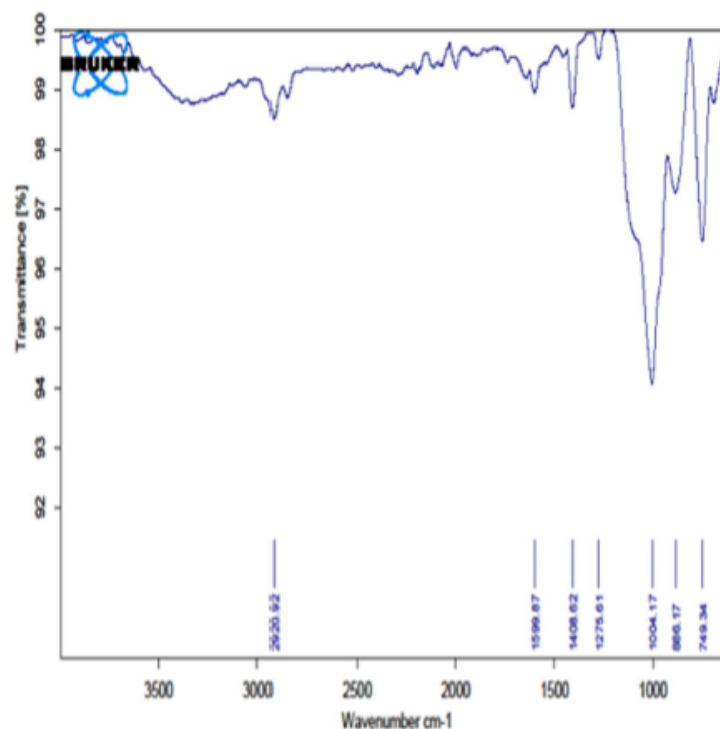**Figure 2 FTIR of pure PDMS before film forming in liquid state**

Figure 3 FTIR of pure PDMS after film forming in solid state

The Fourier-transform infrared spectroscopy (FTIR) of polydimethylsiloxane (PDMS) after film formation in its solid state reveals distinct changes in the chemical composition and molecular structure compared to its liquid state. Following the film formation, the Si-O-Si stretching vibrations are still observed, but they may appear as more defined peaks due to the more ordered structure of the solid film. Moreover, the Si-CH3 stretching vibrations might exhibit shifts or intensity changes in response to the solidification process. The FTIR analysis of PDMS in its solid state is vital for characterizing the material's structural alterations, providing information on its crystallinity, cross-linking, and potential interactions with other materials in a composite system.

FTIR:

FTIR spectroscopy was employed to monitor the polymerization and cross-linking reactions, as depicted in Fig. 3.2(a) and (b). In Fig. 3.2(a), pure PDMS exhibits a distinctive peak within the 1000-1100 cm^-1 range, attributed to the asymmetric stretching of Si-O bonds. Notably, there are specific wavenumbers associated with this peak, including 1011 cm^-1 as a shoulder and 1087 cm^-1 for cyclic trimers containing single Si-O-Si bonds. As the molecular structure of the polymer evolves, such as the formation of longer chains or

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branching, the Si-O-Si absorption band becomes more pronounced, gradually broadening and splitting.

Si-OH compounds exhibit absorption characteristics typically characterized by a single, broad band within the 950-810 cm^-1 range

In the spectrum acquired after curing, as shown in Fig. 3.2(b), there is a noticeable decrease in the intensity of the peaks at 2946 cm^-1 and 2843 cm^-1, indicating the consumption of methoxy groups during the reaction. Additionally, the band observed at 1193 cm^-1 in Fig. 4.1 merges with a shoulder peak at 1004 cm^-1 in Fig. 4.2 which corresponds to the formation of Si-O-Si bonds

Swelling Study

Samples measuring 1cm × 1cm were subjected to a swelling study by immersing them in various solvents, namely toluene, acetone, ethanol, and deionized water, for different durations, specifically 24 hours, 48 hours, and 72 hours. Subsequently, the samples were re-weighed to determine the equilibrium swelling ratio, denoted as Q. The key observation was that the weight of the immersed samples reached a point where it no longer increased. This observation led to the conclusion that the high degree of crosslinking in the samples prevented further swelling from occurring.

The substantial crosslinking of the polymer had a notable impact on its mechanical properties.

Table 1:Swelling Study data for Pure PDMS and Nano alumina composites viz. 0.5% nano alumina(Sample 1), 1% nano alumina(Sample 2), 3% nano alumina (Sample 3), 5% nanoalumina (Sample 4) immersed in toluene independently.

Samples	Weight before immersing	Weight after immersing inTolueneFor			
	g	3hrs.	6hrs	24hrs	48hrs
Pure PDMS	0.1085	0.1090	0.1092	0.1096	0.1104
Sample 1 0.5% nano alumina /PDMS	0.0900	0.0897	0.0898	0.0900	0.0902
Sample 2 1%nano alumina /PDMS	0.2239	0.2252	0.2252	0.2254	0.2257
Sample 3 3% nano alumina /PDMS	0.2215	0.2237	0.2247	0.2252	0.2267
Sample 4 5% nano alumina /PDMS	0.0426	0.0425	0.0428	0.0428	0.0430

Table 2:Swelling study data for Pure PDMS and Nano alumina composites viz.

0.5% nano alumina(Sample 1), 1% nano alumina(Sample 2), 3% nano alumina (Sample 3), 5% nanoalumina (Sample 4)immersed in deionized (dI) water independently.

Samples	Weight before immersing	Weight after immersing in deionized (dI)waterFor			
	g	3hrs.	6hrs	24hrs	48hrs
Pure PDMS	0.0960	0.0972	0.0974	0.0974	0.0976
Sample 1 0.5% nano alumina /PDMS	0.0630	0.0637	0.0638	0.0645	0.0638
Sample 2 1%nano alumina /PDMS	0.1645	0.1705	0.1669	0.1705	0.1668
Sample 3 3% nano alumina /PDMS	0.1983	0.2005	0.2007	0.2014	0.2004
Sample 4 5% nano alumina /PDMS	0.0380	0.0384	0.0386	0.386	0.0390

Table 3:Swelling study data for Pure PDMS and Nano alumina composites viz. 0.5% nano alumina(Sample 1), 1% nano alumina(Sample 2), 3% nano alumina (Sample 3), 5% nanoalumina (Sample 4) immersed in Acetone independently.

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Samples	Weight before immersing	Weight after immersing in Acetone For			
	g	3hrs.	6hrs	24hrs	48hrs
Pure PDMS	0.1057	0.1059	0.1060	0.1063	0.1063
Sample 1 0.5% nano alumina /PDMS	0.0985	0.0989	0.0992	0.0991	0.0900
Sample 2 1%nano alumina /PDMS	0.2025	0.2028	0.2030	0.2030	0.2031
Sample 3 3% nano alumina /PDMS	0.2153	0.2154	0.2156	0.2157	0.2159
Sample 4 5% nano alumina /PDMS	0.0419	0.0421	0.0423	0.0425	0.0425

Table 4:Swelling study data for Pure PDMS and Nano alumina composites viz. 0.5% nano alumina(Sample 1), 1% nano alumina(Sample 2), 3% nano alumina (Sample 3), 5% nanoalumina (Sample 4)immersed in Ethanolindependently.

| Samples	Weight before immersing	Weight after immersing in Ethanol For			
	g	3hrs.	6hrs	24hrs	48hrs
Pure PDMS	0.1002	0.1004	0.1007	0.1010	0.1009
Sample 1 0.5% nano alumina /PDMS	0.0785	0.0787	0.0789	0.0790	0.0790
Sample 2 1%nano alumina /PDMS	0.1828	0.1830	0.1831	0.1833	0.1834
Sample 3 3% nano alumina /PDMS	0.2065	0.2067	0.2070	0.2071	0.2072
Sample 4 5% nano alumina /PDMS	0.0393	0.0394	0.0395	0.0397	0.0397

Effects of Crosslinking

Cross-linking is a chemical process that forms covalent bonds between polymer molecules. This process significantly restricts the molecular mobility within the polymer structure. As a result, cross-linking enhances the polymer's resistance to deformation when subjected to external forces, effectively increasing its modulus or stiffness. This effect is particularly pronounced in the rubbery region of the polymer's mechanical behavior.

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XRD [X-Ray Diffraction] Analysis:-

Figure 3 illustrates X-ray diffraction (XRD) patterns for various materials, including pure PDMS (polydimethylsiloxane), PDMS nano-composites with alumina nanoparticles, and pristine nano alumina powder. In the XRD pattern of pure nano alumina, distinctive peaks are observed at 2θ values approximately around 38, 46, and 66 degrees, corresponding to crystallographic planes {hkl} values of (311), (400), and (440), respectively.

In the XRD patterns of the nano composites with 3% and 5% alumina, smaller peaks around 46 and 66 degrees, corresponding to the peaks of nano alumina, are noticeable. These peaks are absent in the pure PDMS and in the 0.5% and 1% nano composites. This observation implies that there is an intercalation and exfoliation of nano alumina within the nano composites. This phenomenon is further confirmed by SEM (Scanning Electron Microscopy) and TEM (Transmission Electron Microscopy) images.
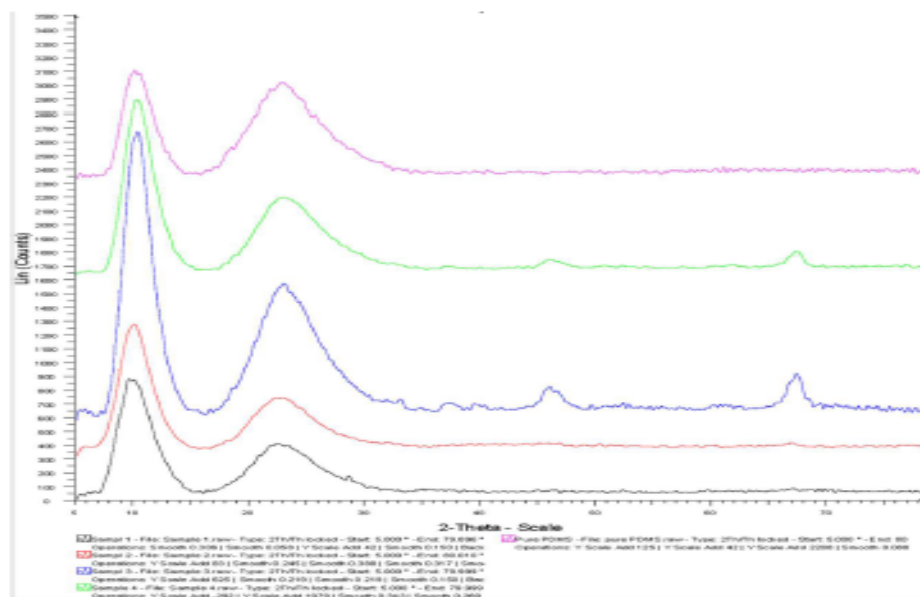
(a)Pure PDMS and all nano alumina/PDMS composites
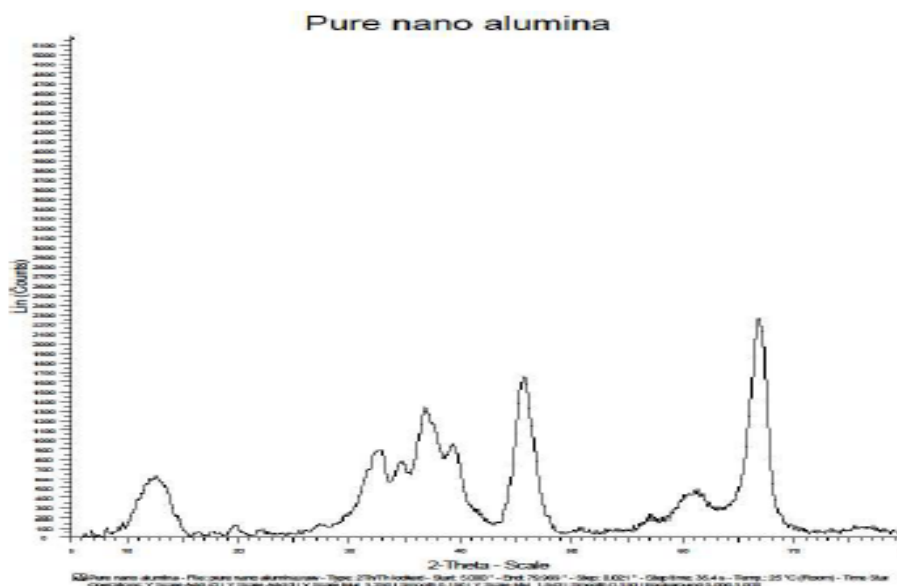
(b) Pure Nano Alumina Powder

Figure.4 (a) Pure PDMS (pink) Sample1(0.5%nano alumina/PDMS) (black),

Conclusion

The exploration of the physical and mechanical characteristics of polysiloxane nanocomposites has provided valuable insights into the tremendous potential of these advanced materials. By incorporating nanofillers into the polysiloxane matrix, we have seen a notable enhancement in various properties, making them versatile candidates for a wide range of applications. The synthesis and preparation methods of polysiloxane nanocomposites have evolved to offer precise control over nanofiller dispersion, allowing for the fine-tuning of material properties. The choice of nanofillers, such as nanoparticles and nanotubes, and their concentration significantly impacts the resulting characteristics. Understanding this relationship is pivotal for tailoring these materials to specific applications. In terms of physical properties, polysiloxane nanocomposites have exhibited remarkable thermal stability, low electrical resistivity, and excellent optical transparency. These properties have opened doors for their utilization in microelectronics, aerospace, optics, and other fields where exceptional thermal insulation and electrical performance are required. The improvements in mechanical behavior, including enhanced tensile strength, elasticity, and hardness, have underscored the potential of these materials for high-performance applications. These nanocomposites are suitable for use in demanding environments, where resistance to wear and tear is paramount. This research has also highlighted the importance of nanofiller type and loading concentration in achieving the desired performance attributes,

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emphasizing the need for careful material design and characterization. polysiloxane nanocomposites represent a highly promising class of materials that bridge the gap between traditional polymers and advanced composites. Their physical and mechanical characteristics, when optimized through careful engineering, offer innovative solutions across various sectors. As we look to the future, the potential applications of these nanocomposites are extensive, from aerospace components to advanced electronic devices, making them a subject of ongoing interest and research in the materials science community.

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