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The thermal properties and mechanical behavior of XLPE/Al2o3 Nanocomposites

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Abstract

Researchers in the fields of engineering and science have recently focused on polymer nanocomposite materials. This investigation is The Thermal Properties and Mechanical Behavior of XLPE/Al2o3 Nanocomposites.

Keywords: Nanoparticles, natural, Al2O3, Properties

Introduction

To see how the Al2O3 particles are distributed in the nanocomposites, TEM pictures are the best option. The micrograph depicts a typical surface-treated nanocomposite dispersion. All three solutions achieve a comparable composite structure with well-dispersed nanoparticles in the polymeric matrix, according to TEM measurements. The propensity for agglomeration grows from 2 weight percent to 10 weight percent of nanoparticles. Reducing filler-filler interactions compared to filler-matrix interactions may increase dispersion, according to the data.

Nanoparticles aggregate for two main reasons: first, they have a natural inclination to lower the surface free energy, and second, when they include OH groups, they form hydrogen bonds. Here, the Al2O3 nanoparticles' surface treatment lowers their surface free energy and stops them from forming hydrogen bonds with one other as the composite samples are being prepared. An further factor contributing to the achievement of effective dispersion is the presence of silane molecules with long alkyl chains on the surface of Al2O3 nanoparticles. These molecules are compatible with XLPE and improve the filler-matrix adhesion. A more organic and nonpolar nanoparticle surface treated with Al2O3 makes it more hydrophobic, which improves its compatibility with matrices that have comparable surface characteristics. The phase separation of XLPE and nano Al2O3 will occur during the preaparation process since both systems are entirely organic and

inorganic. However, the alkyl group on the nanoparticle allows for better polymer-filler interaction. This occurs because the octyl group of trimethoxyoctyl silane forms a bond with the polymer, and the -OCH3 group is chemically linked to Al2O3.

Literature and Review

Wadah Mahdi et al. (2022)^[1] The chemical procedures for methyl ammonium halide (MABr) and lead halide (PbI2) were used to create and study perovskite compounds in this work. We studied the effects of changing the weight ratios of lead halide (PbI2) and methyl ammonium bromide (MABr) in three different samples: P1, P4, and P7. The goal of this study was to successfully prepare new types of perovskites using the one-step method by varying the lead halide to methyl ammonium bromide (PbI2) weight ratios (0.22:0.39)g, (0.22:0.59)g, and (0.22:0.79)g, respectively, in three different samples. The P4 sample's crystal structure achieved high crystallinity when the weight ratio of lead halide was increased from 0.39 g to 0.59 g. Afterwards, when the weight ratio in sample P7 was increased from 0.59 g to 0.79 g, the crystallisation reduced and the crystal structure altered. The absorption edge moved significantly towards long wavelengths (red shift) between 625 nm and 691 nm and 805 nm when the weight of PbI2 increased from 0.39 g to 0.59 g and 0.79 g, respectively. At various points, the energy band gap varied between 1.98 eV, 1.79 eV, and 1.53 eV. Researchers found that increasing the lead halide International Journal of Advance Research in Multidisciplinary

weight from 0.39 g to 0.59 g, together with the short Nanodiameters of 34.25 nm for the P4 sample, led to the desired surface shape, which was a dense, homogenous layer. A less dense membrane with numerous vacancies and a semi-micro big particle diameter of 97.32 nm was achieved for sample P7 after raising the weight from 0.59 g to 0.79 g. At last, P4, a sample with excellent crystalline and optical characteristics as well as a dense, homogenous surface formation, was chosen because it could be used in the unique composition to make stable, high-efficiency optical devices.

Yuming Lai et al. (2024)^[2] The scientific world has taken notice of organic/inorganic hybrid perovskite materials like CH3NH3PbX3 (X = I, Br) because of its remarkable features. These include a highly adjustable bandgap, a high optical absorption coefficient, and an exceptional power conversion efficiency, among many others. Heat may drastically reduce the efficiency of photovoltaic systems including perovskite solar cells. Consequently, in order to optimise the performance of perovskite solar cells, it is vital to understand how their optical characteristics fluctuate on temperature. Using a polymer-controlled nucleation technique, we created CH3NH3PbBr3 (MAPbBr3) single crystals and studied their optical characteristics and how their molecular structure changed as a function of temperature temperature. Using evolution photoluminescence (PL) spectroscopy, we discovered that raising the temperature significantly changed the fluorescence intensity. Additionally, we observed an asymmetric PL profile, which might indicate that a greater of captured excitons undergo number radiative complexation. The colour of the MAPbBr3 single crystals diminished, as seen in the optical photos. Since all of the Raman bands were highly distinct, Raman spectroscopy showed that the structure of MAPbBr3 was intact at 90 °C throughout the heating process. When the temperature reached 120 °C, the internal modes' Raman bands were very feeble. Above 210 °C, the inorganic structure on the surface of the sample began to crumble as the heating process continued. Significant variations in spectral intensity, peak location, and Full Width Half Maximum (FWHM) were seen in the PL spectra as the heating process progressed. As the temperature rose, the PL spectral intensity dropped sharply. As the temperature increased, the peak's blue shift became more apparent, and the peak's form was clearly asymmetrical. The FMWH of the PL spectra became more diffuse as the temperature rose, with a notable spike between 270 and 300 °C. The changes in the PL spectra as a function of temperature suggest that MAPbBr3's optical characteristics are temperature dependent, which has implications for its potential uses in optical devices and other related industries. These findings might provide useful information for MAPbBr3 applications.

Aref S. Baron *et al.* $(2019)^{[3]}$ The organic-inorganic hybrid perovskite materials have gained significant attention in the electronic industry due to its many advantageous characteristics, such as their cheap cost, adjustable optical properties, and high efficiency. In this study, we utilised different lead halides, specifically PbCl2 and PbBr2, to create two distinct perovskites, MAPbBr3 and MAPbBr2Cl, using a one-step method. We then examined their optical, structural, and morphological properties before using them to construct solar cells. To enhance their performance, we utilised a hydrothermal method to prepare TiO2 nanocrystals as an electron transport material (ETM). For MAPbBr3 perovskites, the power conversion efficiency (PCE) was 1.2% with a fill factor (FF) of 0.26, but for MAPbBr2Cl perovskites, it was as high as 0.9% with a fill factor (FF) of 0.25.

Jin-Wook Lee et al. (2021)^[4] An entirely new category of photovoltaics (PVs) has recently achieved spectacular thanks to novel organic-inorganic hybrid success semiconducting materials. The crystal structure of the semiconducting absorber with the name "Perovskite" is organic-inorganic metal halides (-I, -Br, and -Cl) and lead or silver ions (Pb and/or Sn). Perovskite solar cells (PSCs)" is the common term used by PV experts to describe them. The current power conversion efficiency (PCE) for PSCs is 25.5%. The common absorber formula is AMX3, where A is methylammonium, FA, and Cs, M is lead and/or silver, and X is iron, bromide, and chlorine. Every year after the 2012 study on reliable solid-state PSCs, PCE has grown at a pace of more than 10% on average. A large number of scientists in our research community are drawn to such exceptional PV performance. Compared to other III-IV semiconductors, monocrystalline Si, GaAs, and many oxides with a perovskite crystal structure, their physical and chemical characteristics are radically different. The dynamic features of A site cationic molecules and PbI6 octahedrons associated with their corners are examined and summarised in this paper, among other essential aspects from various semiconducting and dielectric materials. After we cover the special features, we'll look into the potential PV uses based on what we know about the A-site molecule's orientation and the PbI6 octahedron's tilting.

Nurul Iman et al. (2023) ^[5] The outstanding dielectric, mechanical, and thermal characteristics of crosslinked polyethylene (XLPE) nanocomposite contribute to its high insulating performance. Because of the reinforcing impact of the interfacial area between the XLPE-nanofillers, the characteristics of the XLPE matrix were significantly enhanced by the addition of nano-sized fillers. When compared to a single filler system, the synergistic interaction between nanofillers in a hybrid system might further enhance already good interfacial strength. The quantity of hybrid nanofiller is another component that influences the strength of the interface. For this reason, researchers looked into how much hybridising layered double hydroxide (LDH) with aluminium oxide (Al2O3) nanofiller could be included into an XLPE matrix. In this study, the dielectric, mechanical, and thermal characteristics of a nanocomposite were investigated in relation to the amount of hybrid nanofiller and the 1:1 ratio of LDH to Al2O3. The shape and structure of the XLPE/LDH-Al2O3 nanocomposites showed that the dispersion state was enhanced by hybridising the nanofiller. Thanks to the LDH-Al2O3 nanofiller's synergistic impact, the material's dielectric, mechanical, and thermal properties-such as its partial discharge resistance, AC breakdown strength, and tensile properties-were improved. At an ideal concentration of 0.8 wt.%, these characteristics were enhanced; however, as the amount of hybrid nanofiller rose, they began to decline. Researchers discovered that as compared to pure XLPE, AC breakdown strength rose by 15.6% and the value

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of PD magnitude improvement decreased by 47.8%. Tensile strength, Young's modulus, and elongation at break were all improved mechanically by 14.4%, 31.7%, and 23%, respectively. Importantly, insulating materials based on XLPE nanocomposite may be rethought via the hybridisation of nanofillers.

Mechanical Behaviour

The stress-strain curves for XLPE and nanocomposites. Upon initial linear elastic behavior, all samples undergo subsequent inelastic plastic deformation. Compared to the unfilled systems, all composites show greater stress levels when it comes to strain. a comparison of the yield strengths of XLPE and nanocomposites with respect to the filler concentration. The yield strength improves when various nanocomposites are considered up to 5 weight percent before it starts to drop when additional nanofillers are added. Because of the significant interfacial contact between the components, the polymer matrix was strengthened by the addition of Al2O3 to nanocomposites. A greater composite tensile strength value is the result of a welldesigned interface that limits polymer deformation. The observed reduction at the maximum filler concentration is due to the filler-filler contact, which is more prevalent than the filler-matrix interaction, which only causes a little amount of stress transmission. It is essential to use localized chemical processes to get a more consistent dispersion of nanofillers. By enhancing interfacial bonding and local load transmission, When compared to ordinary XLPE, the nano filler with an organic group interacts with the polymer matrix, increasing both the elastic modulus and ultimate tensile strength. The addition of nano Al2O3, which is effective as a nucleating agent, is also thought to be responsible for the increased crystallinity of the composites. The findings showed that the surface treatment on nanoparticles connected the polymer matrix and inorganic particles, creating a desirable interface that enhanced the interaction and compatibility between the two phases, leading to better mechanical properties. How the new nanophase limits the surrounding polymers and whether an effective nanophase forms are both determined by the contact between the surfaces.

the Young's modulus of nanocomposites and XLPE. The modulus of Young of XLPE/Al2O3 nanocomposites is high at low filler loadings but starts to drop off with increasing nano Al2O3 concentration. Polymer chain mobility is known to be enhanced at repulsive interfaces and reduced at attractive ones. The dynamics of polymer chains may be clearly seen by looking at the value of Young's modulus. The physical network density might be enhanced by the interaction of polymer fillers. The effective interaction between the filler and polymer is the direct source of the immobilized polymer layer (limited polymer) around the filler surface. This immobilized phase may enhance mechanical stretching stress transfer efficiency, total polymer network density, and modulus value. Due to the aggregated nature of the fillers, immobilization is not as efficiently achieved at higher filler loadings as at lower ones.



Fig 1: The stress-strain characteristics of four different nanocomposite materials: pristine XLPE (X), XLPE/2 wt% Al2O3 (A2), XLPE/5 wt% Al2O3 (A5), and XLPE/10 wt% Al2O3 (A10).



Fig 2: Results of the XLPE (X), XLPE/2 wt% Al2O3 (A2), XLPE/5 wt% Al2O3 (A5), and XLPE/10 wt% Al2O3 (A10) quantum dots yield tests.



Fig 3: Variation in XLPE and nanocomposites Young's modulus with respect to weight percent of nano Al2O3.

Dynamic Mechanical Analysis



Fig 4: A1C is an XLPE/Al2O3:clay=1:1 mixture, while A2C is a 2:1 mixture, and all of these combinations have different storage moduli

Not surprisingly, Thanks to the reinforcement supplied by nanoparticles, nanocomposites have a much better storage modulus compared to pure XLPE, particularly at low temperatures. At very low temperatures, the storage modulus of the hybrid system is lower than that of the XLPE/Al2O3 combination. The modulus of storage drops sharply at temperatures below -100 °C and then gradually drops to below-50 °C. Between -50 °C and 25 °C, the storage modulus drops sharply as temperatures increase, before leveling out. In other words, The storage modulus-temperature curves peak at around 100 °C, 0 °C, and 80 °C. Because the elastic stored energy relaxes more quickly and the molecular chains of the resin are more mobile, the storage modulus drops with increasing temperature.

 Table 1: Coefficient c, At 100 K, the storage modulus and 300 K for pure XLPE and nanocomposites.

Sample	Storage modulus at 100 K (GPa)	Storage modulus at 300 K (GPa)	Coefficient (c)
Х	8	0.3	
Α	12.2	0.5	0.76
С	10.4	0.6	0.65
A1C	10.4	0.7	0.55
A2C	9	0.4	0.84

The efficacy of fillers on composite storage moduli is denoted by the coefficient 'c,'.

For each composite, Table 1 displays the resulting values of the coefficient 'c'. A lower value for the constant c indicates that the filler is more effective. The ratio of Al2O3 to clay, 1:1, maximizes the filler's efficiency. For this particular composition, the stress transmission between the matrix and filler is at its peak. It is possible to link this outcome to the better tensile strength and Young's modulus parameters that were attained.

Both the unfilled XLPE and the composites show their temperature-dependent loss moduli. Material combinations that do not have a 1:1 ratio of composites, have a greater loss modulus value than plain XLPE, which suggests that the polymeric composite system generates too much heat. We expect this heat production to be caused by a number of things. The release of frictional heat at the particle-polymer contact was thought to be the cause of this rise in the loss modulus. Nielsen and Landrel have proposed the idea that frictional heat may also develop via particle-particle interactions. Particles may come into touch with one another due to filler agglomeration. In hybrid system A1C, the flexibility of chain movement is reduced since the free volume is relatively small, thanks to the correct dispersion of nanoparticles. Reduced heat production due to particleparticle interaction is another benefit of not having big filler aggregates.

The findings that follow are a summary of the DMA analysis. (1) The storage modulus of nanocomposites is greater than that of clean XLPE. The addition of materials with a higher elastic modulus makes the material stiffer, which causes this effect. The loss modulus vs. temperature graph might reveal the α , β , and γ transitions:

 χ at -120 oC - glass transition, β at 0 oC - side chain movement and α at 80 C orientation motion in crystals [48].



Fig 5: A1C is an XLPE/Al2O3: clay=1:1 mixture, A2C is a 2:1 mixture, and XLPE/clay is a third mixture.

Analysis via thermo gravimetry

Using TGA analysis in a nitrogen environment, Nano composites' thermal deterioration behavior has been studied by researchers. the thermogravimetric analysis profiles of the nanocomposites. The deterioration of the composite was examined by determining the rate of weight loss. The nanoparticles are clearly a factor in the increased thermal degradation temperature. After alumina clay mixture and clay composites, the addition of 5wt % nano Al2O3 produced the highest level of thermal stability. The minor phase's high thermal stability allows it to receive more heat from the main phase, which improves the interface and evens out the distribution of nanofillers in the polymeric matrix, both of which heighten the thermal stabilization effect. The process of coating the surface of the polymer melt with nanoparticles, which stops the polymer from breaking down any further, is another potential reason for the enhancement of thermal stability. As the polymer melts down, its nanoparticles will settle to the surface, forming a protective barrier that will keep the remaining polymer from International Journal of Advance Research in Multidisciplinary

being overheated and will reduce the rate of volatilization of the polymer pieces that are produced during pyrolysis. We are now doing more investigations.



Fig 6: XLPE/Al2O3: clay=1:1 (A1C) and XLPE/Al2O3: clay=2:1 (A2C) thermogravimetric analysis graphs

XLPE/SIO₂/TIO₂ NANOCOMPOSITES WITH DOUBLE-HYBRID CORES

Transverse Electron Microscopy for Morphology

transmission electron micrographs of XLPE and nanocomposites. At 5 weight percent filler loading, the XLPE/SiO2/TiO2 nanocomposite exhibited a uniform distribution of inorganic fillers. However, when the nanofiller concentration is kept constant, XLPE/SiO2 and XLPE/TiO2 show a very uneven dispersion of nanoparticles. In comparison to S and T, these results show that ST attained a much higher dispersion level. The XLPE/SiO2/TiO2 nanocomposite aims to enhance a nonpolar, hydrophobic polymeric matrix that contains an organic, polar, hydrophilic filler that is inorganic. This is achieved through the incorporation of two distinct nanoparticle types' surface treatments.



Fig 7: With a filler concentration of 5 weight percent, image of XLPE/SiO2 and XLPE/TiO2 using transmission electron microscopy, and (c) XLPE/SiO2/TiO2.

Dynamic Systems

Both the XLPE and the nanocomposites exhibit stress-strain behavior. In terms of mechanical behavior, ternary hybrid nanocomposite outperforms binary composites and plain XLPE. How much filler is used, how much interaction there is between the matrix and filler, whether the polymer's morphology changes, how well the two materials interfaces, and the surface properties of the nanoparticles-specific area. roughness, surface free energy, etc.- each factor affects the mechanical performance to some extent. Increased compatibility and lower aggregation propensity allow for improved contact between the polymer matrix and inorganic filler, which in turn enhances the tensile properties by efficiently transmitting stress from the matrix to the filler. Nevertheless, the material's strength is often diminished when particles aggregate. Aggregates have the ability to significantly concentrate stress. The less prevailing fillerfiller interation compared to filler-polymer interaction, together with the restricted potential of two types of nanoparticles to aggregate owing to differences in surface features, is what gives hybrid nanoparticle filled composites their improved mechanical qualities.



Fig 8: The stress-strain properties of XLPE (X), XLPE/SiO2 (S), XLPE/TiO2 (T), and XLPE/SiO2/TiO2 are taken into consideration (ST) at a filler concentration of 5 weight percent.

Analysis using Thermo gravimetrics

We checked the thermal stability using TGA. This is the XLPE/SiO2, XLPE/TiO2, TGA plot for and XLPE/SiO2/TiO2 nanocomposites at а nanofiller concentration of 5 weight percent. The XLPE/SiO2/TiO2 nanocomposite hybrid system has the best thermal stability. Composites containing fillers have better thermal stability than plain XLPE because the degradation temperature moves towards higher values. Several factors can be considered to justify an improvement in thermal stability. As an example, inorganic nanoparticles are more effective heat absorbers than XLPE due to their greater heat capacity and thermal conductivity. At higher temperatures, XLPE chains begin to degrade.



Fig 9: Time-dependent gas chromatography (TGA) plot of XLPE (X), XLPE/SiO2 (S), XLPE/TiO2 (T), and XLPE/SiO2/TiO2 (ST) with a filler content of 5 weight percent

Conclusion

By focusing on the quantity of nanofiller and the microstructural development in nanocomposites with nanofillers, the thermal properties and mechanical behavior of XLPE/Al2O3 nanocomposites were investigated in this work. The mechanical and thermal properties of the XLPE/Al2O3 nanocomposite are superior to those of other spherical nanoparticle filled composites.

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