Flexible low-density polyethylene–BaTiO3 nanoparticle composites for monitoring leakage current in high-tension equipment. [Dataset].

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2021

Supporting Information

Flexible Low-Density Polyethylene-$BaTiO_3$ Nanoparticle Composites for Monitoring Leakage Current in High-Tension Equipment

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Section 1.

The prepared film sample is as shown in Figure 1 and the attachment of the copper electrodes is also shown.

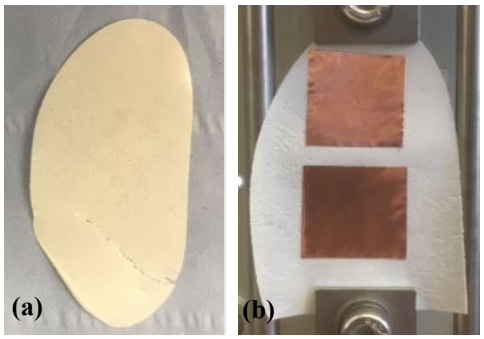

Figure 1. (a) Flexible film sample prepared for the electrical characterisation and (b) Attached with copper tapes (electrodes) for electrical displacement, current density, and current measurement with the applied electric field.

The effect of the silica coating is observed in the TEM images as compared below:

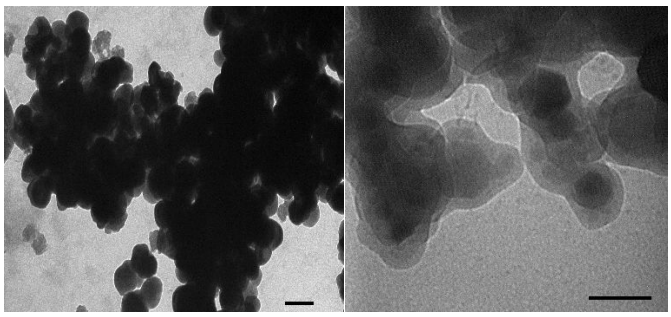

Figure 2. TEM images of uncoated (Left) and silica coated (Right) $BaTiO_3$ nanoparticles. The coated layer of ca. 10-15 nm is observed on the nanoparticles. (Scale bar represents 100 nm)

The TEM image for the uncoated $BaTiO_3$ nanoparticles sample was also taken for highlighting the improvement due to the silica functionalisation of the nanoparticles. The agglomeration of the nanoparticles due to the dipole-dipole attraction amongst them is clearly observed in the following Figure 3.

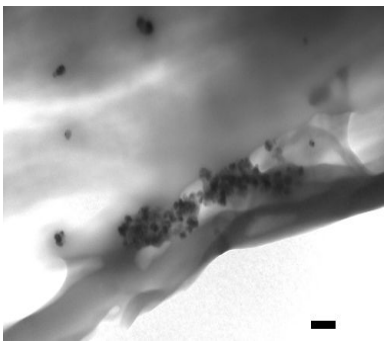

Figure 3. TEM image of uncoated $BaTiO_3$ nanoparticle sample. (Scale bar represents 500 nm)

The TEM images of all the polymer-nanoparticle composite samples prepared with the coated $BaTiO_3$ nanoparticles are shown as below in Figure 4. The dispersion state improvement is clear, when comparing the Figure 4 with Figure 3.

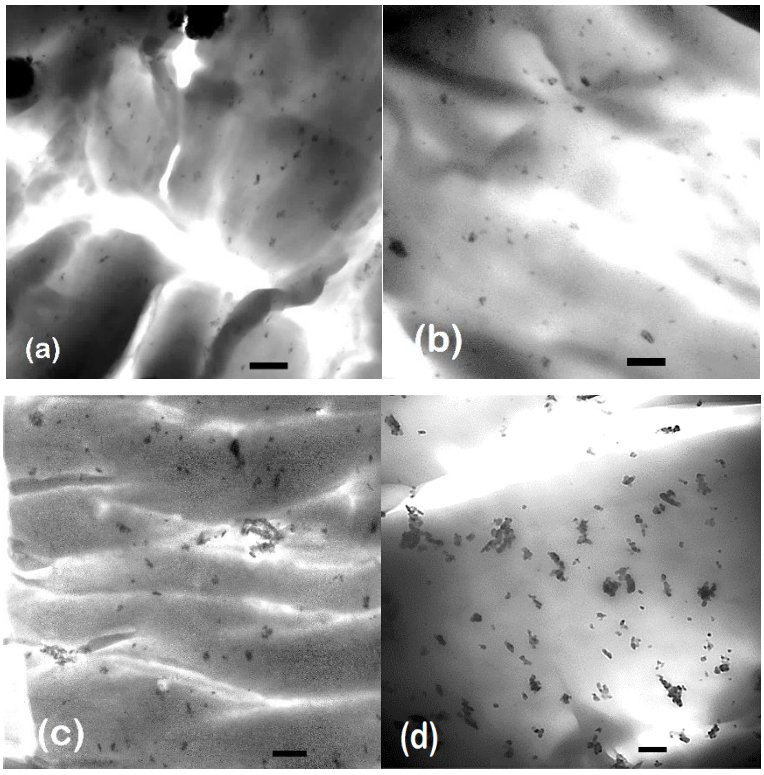

Figure 4. The TEM micrograph images for all the synthesised samples with varying wt.% of nanoparticles, wherein (a) 6% Sample, (b) 9% Sample, (c) 12% Sample, and (d) 15% Sample. (Scale bar represents 500 nm)

Section 2.

The enthalpy of all the samples were calculated using the Universal Analysis software that comes along with the DSC instrument control package. By quantifying the heat associated with the melting endotherm. This heat was then reported in terms of percent crystallinity by normalizing the observed heat of fusion with that of the 100% crystalline LDPE polymer. The area used for the enthalpy (crystallinity) calculation as identified using the "Integrate Peak" functionality of the TA Universal Analysis 2000 software [1] is recreated in the plots in Figure 6 (included in the main text). The same analysis also helped identify the "Melt Peak Temperature" of the endotherm peak, which was the melting point T_m of the samples and listed in the Table below. Adding to the discussion, the Glass transition temperature T_g was also identified using the "Glass/Step transition" functionality available in the same software.

The degree of crystallinity for all the samples was calculated from the following Equation 1 [1], using the standard reference value of LDPE as cited in the main text.

$$Sample\ Degree\ of\ Crystallinity = \frac{Sample\ Enthalpy\ from\ DSC\ plot}{PA6\ Enthalpy\ from\ Reference\ Text} \times 100\% \qquad \text{Eqn. 1}$$

The important observations from the DSC plot and the calculated degree of crystallinity are summarised in Table 1 below.

Table 1. Melting temperature (T_m) and degree of crystallinity from DSC results for Pure LDPE and the prepared 6%, 9%, 12% and 15% polymer-nanoparticle composite samples.

Sample	**T_m** (°C)	**Enthalpy** (J/g)	**Degree of Crystallinity** (%)
Pure LDPE	109 ± 1	110 ± 1	39 ± 1
6% Sample	111 ± 2	109 ± 2	38 ± 2
9% Sample	110 ±1	104 ± 1	36 ± 1
12% Sample	109 ± 1	99 ± 1	34 ± 1
15% Sample	108 ± 2	86 ± 3	30 ± 3

Section 3.

The TEM images were first processed using Photoshop® software; wherein they were rotated, cropped, and enlarged to remove edge distortion and any background distortion. Subsequently, these images were enhanced digitally using filters for background noise removal and their artefacts or improving the sharpness and definition of the image. Furthermore, the grayscale images were adjusted for their contrast and brightness to achieve correct tonalities of black and white shades. This helped in distinguishing the polymer matrix, as represented by white or grayscale region and the nanoparticles represented as pure black entities. Then the final processed image was saved as 8-bit TIFF format and loaded in ImageJ image processing software for estimating the nanoparticles/agglomerates sizes for all the processed TEM images of the sample variations.

Table 2. Calculated ferret diameters of NP/agglomerate regions as identified in TEM micrographs and calculated using ImageJ.

Sample	Biggest agglomerate size (nm)	Smallest nanoparticle/ agglomerate size (nm)
6% Sample	260 ± 10	30 ± 5
9% Sample	310 ± 25	30 ± 5
12% Sample	340 ± 20	40 ± 5
15% Sample	410 ± 20	35 ± 5

The values in Table 2 were then used as an input for the designed MATLAB® code to generate the simulated 3D model of the polymer nanocomposite with NP/agglomerates represented as spherical entities, as shown in Figure 4 here.

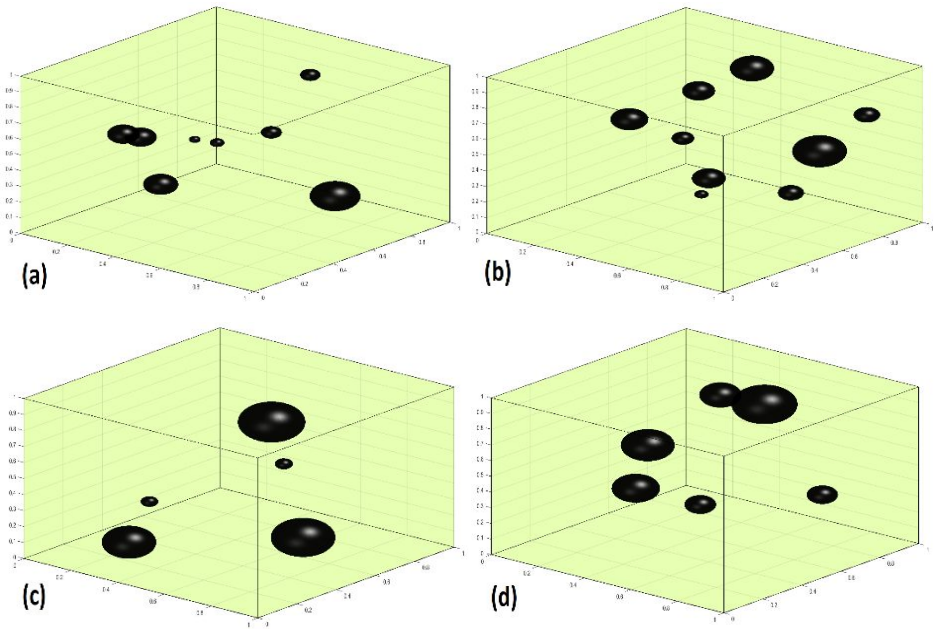

Figure 5. Simulated model representation of the individual nanoparticle/agglomerate present in the synthesised nanocomposite (1 cubic micron size) samples with varying wt% of nanoparticle loading, wherein (a) 6 wt% Sample, (b) 9 wt% Sample, (c) 12 wt% Sample and (d) 15 wt% Sample.

The interaction radius calculated by considering the positions of each nanoparticle/agglomerate in the simulated model is summarised in Table 3 as follows. This data is used for representing the interaction region or influencing region of each nanoparticle/agglomerate in the simulated model, as shown in Figure 9 of the manuscript.

Table 3. Interaction radius (IR) values as calculated by the MATLAB® code for the simulated model of each sample type.

Sample	Minimum Interaction Radius (nm)	Maximum Interaction Radius (nm)	Average Interaction Radius (nm)	Standard Deviation (nm)
6% Sample	143	521	275	120
9% Sample	174	515	290	90
12% Sample	260	450	310	70
15% Sample	255	440	300	100

References

1. Blaine RL. Determination of polymer crystallinity by DSC. TA Instruments, New Castle, DE. 2013.