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Supporting Information for

Experimental and Computational Conductivity Study of Multilayer Graphene in Polypropylene Nanocomposites

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EXPERIMENTAL SECTION AND SUPPLEMENTARY FIGURES.

1. Scanning electron microscopy (SEM). SEM images were acquired on a field emission scanning electron microscope (FESEM model Ultra 55, Zeiss) operating at 5 kV with X-ray spectroscopy (EDS). Electron micrographs were obtained using a Jeol JEM-1010 high-resolution microscope (JEOL, Japan). Dispersion analysis was carried out on samples with 5% MLG. Amount concentration higher than 5% the matrix was collapsed with the nanoparticles, and it is not possible to analyze the homogeneity and the particle size. Figures S1, S2, and S3, shows the SEM images for PP+5%MLG. From this figures, we can see that MLG flakes are aligned in the same direction, and there is no evidence of agglomeration. Figure S2b and S3b shows a detailed MLG flake forming the MLG particles into the matrix of PP. A close observation of the pictures using the appropriate software permit us to obtain the mean particle size and the agglomerate density.

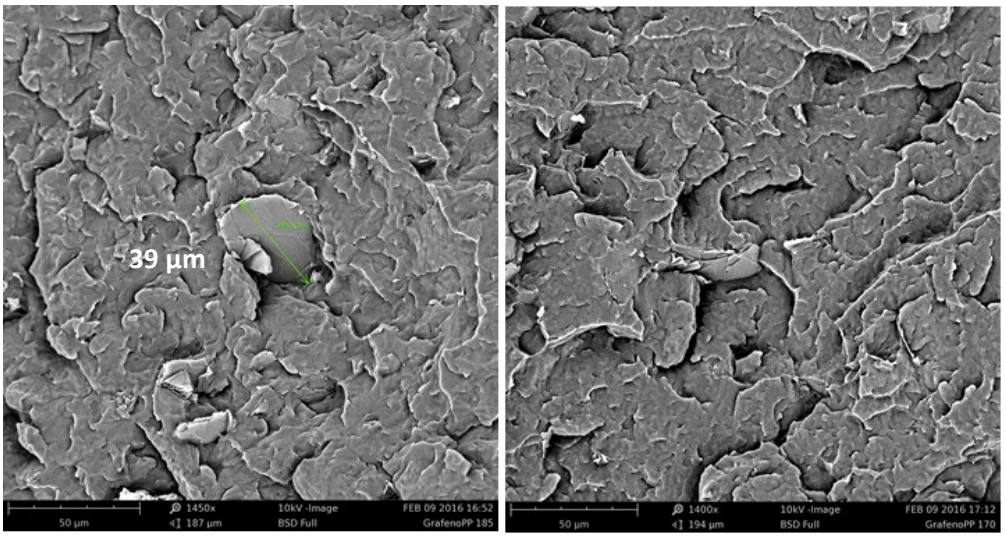

Figure S1. SEM Images of the simple PP+5%MLG at 1400x

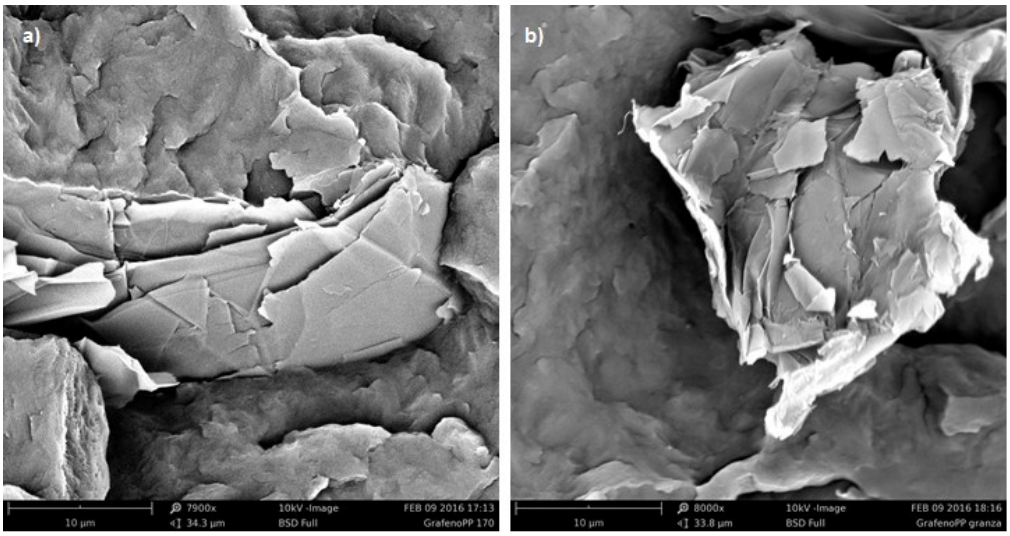

Figure S2. SEM Images of the simple PP+5%MLG, a) 7900x y b) 8000x

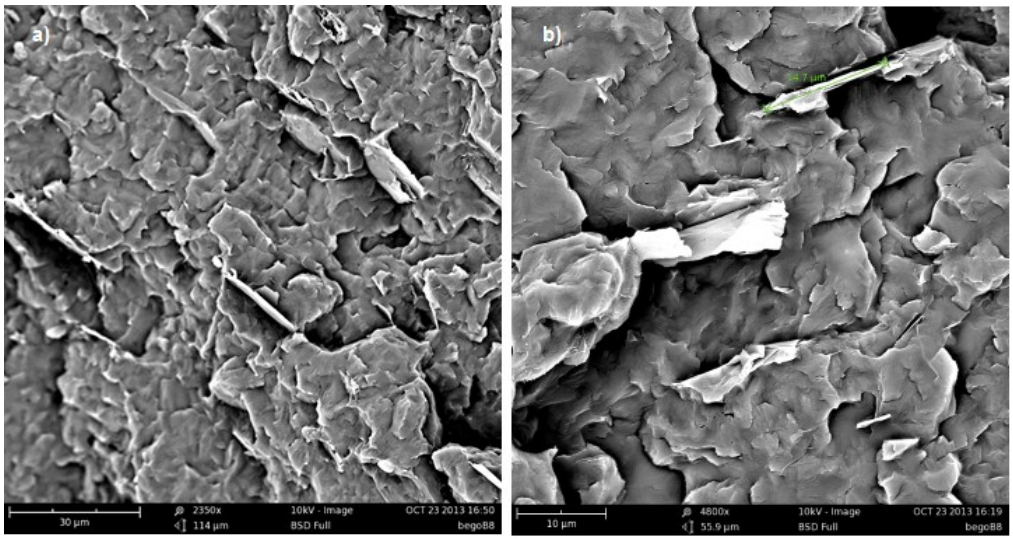

Figure S3. SEM images of the simple PP+ 5%MLG, a) 2350x, b) 4800x

The parameters measured in the samples were the mean particle size and agglomerates density. This last parameter gives as an estimation of the area of the sample, which is occupied by aggregates in relation with the total area of the sample. It is calculated by the expression[1]

$$\varphi = \frac{A_x}{A_0} x100$$

Where φ is the agglomerates density, A_x the area of the sample occupied by agglomerates and A_0 the total area of the sample. The obtained values of mean particle size were (12.5±1.6) µm and (5.6±0.5) % the agglomerates density.

2. CONDUCTIVITY FROM NYQUIST PLOTS.

The values of the conductivity obtained from the Nyquist plot, also permit us to calculate the conductivity from the intercept in OX-axes determine the real part of the impedance which using the expression R'= L/(A σ') we obtain the real part of the conductivity[2]. The Nyquist plots of the samples PP+10%MLG, PP+15%MLG at different temperatures and PP+20%MLG, PP+25%MLG and PP+30%MLGat 50ºC, are given in Figures S4, S5, and S6, respectively. Two well-defined regions are observed, high-frequency depressed semicircles followed by an accumulation of points when the imaginary part of the impedance tends to a zero value. The distribution of the relaxation times causes the depression of the semicircles. The typical equivalent circuit of a semicircle Nyquist plot consists of a capacitor in parallel with a resistor. When the semicircle is more depressed, the capacitor is replaced by a constant phase element (CPE).

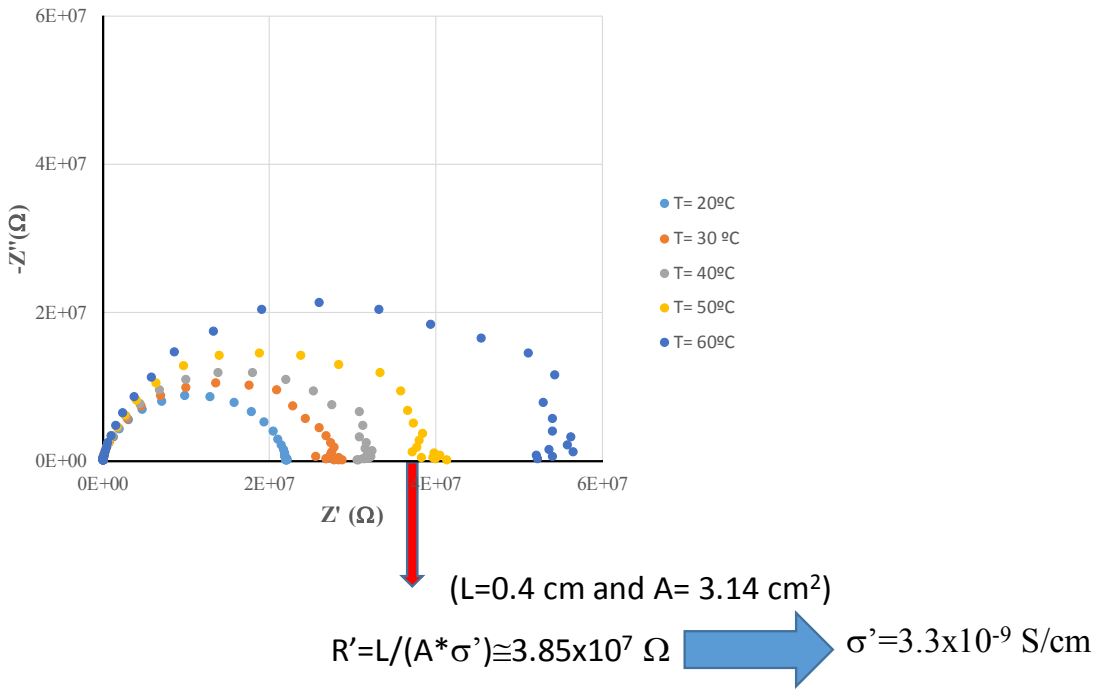

Figure S4. Nyquist plot for the sample PP+10%MLG for all temperatures.
We can see that the intercept we can calculate the conductivity. The value obtained is practically the same that the obtained following the Bode diagram.

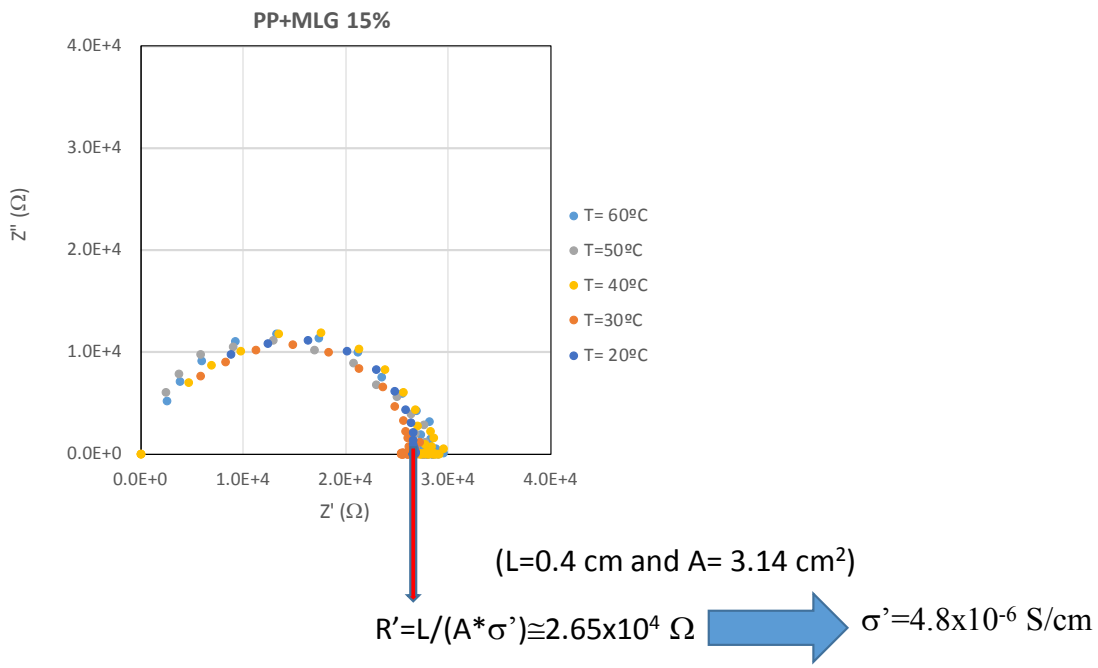

Figure S5. Nyquist plot for the sample PP+15%MLG for all temperatures.
We can see that the intercept at OX-axes we can estimate the real part of the impedance and then the conductivity from the equation: R'=L/(A*σ') . The value obtained is practically the same that the obtained following the Bode diagram.

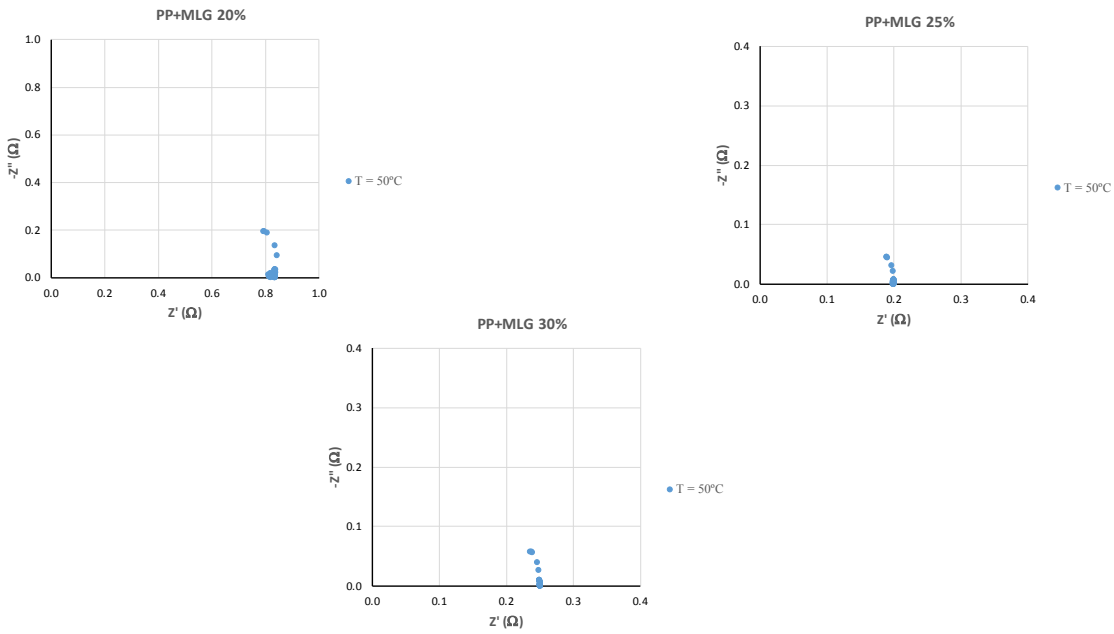

Figure S6. Nyquist plot for the samples PP+20%MLG, PP+25%MLG, and PP+30%MLG, respectively. We can estimate the real part of the impedance, Z', and then the conductivity from the equation: R'=L/(A*σ')

References

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2. Song J Y, Wang Y Y, Wan C C. Conductivity study of porous plasticized Polymer electrolytes base don Poly (vinylidene fluoride): a comparison with polypropylene separators. J. Electrochem. Soc. 2000, 147, 3219-25.