Study of the Crystallite Size of Chemically Synthesized Polyanilines using the Program FULLPROF

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Introduction

Among ICPs (Intrinsically Conductive Polymers), Polyaniline (PANI) is claimed to be one of the most versatile and to have one of the highest environmental stability[1-3]. Structural aspects in polymers are still a mystery and so continue to be an interesting researched topic. Understanding of the regular arrangement of polymer materials is essential for the prediction of processing methods and thus relates the material properties. Fullprof program[4] was successfully used to extract average microstructural properties from the analysis of broadened lines of constant wavelength diffraction patterns through a whole profile fitting approach. We report here a detailed systematic observation of crystalline phases in the doped and undoped polyaniline powder.

Results and Discussion

Figure 1 shows the X-ray diffraction patterns of the ES-PANI and EB-PANI. The ES-PANI powder exhibits broad peaks at 2θ angles around 6, 9, 11, 15, 21, 25, 27, 29, 33, 36 and 52°, which indicates some degree of crystallinity. When 3 hours of treatment with NH_4OH is used for the neutralization of ES-PANI, the diffraction peaks become progressively broader and the peaks located in 27, 29, 33, 36 e 52º 2θ gradually disappear. Thus, there is a decrease in the degree of crystallinity of EB-PANI in this process. A plot of the "average apparent shape" of crystallites was displayed using the GFourier program[5].The refined average crystallite size projections for ES-PANI and EB-PANI are shown in **Figure 2** and **3**.

Conclusions

The average crystallite size obtained from the refinement for ES-PANI is 34Å. For EB-PANI, the average crystallite size is 27Å. . The crystallite shape of ES-PANI can be described as a prolate ellipsoid while for EB-PANI we found smaller crystallites with a roughly spherical shape. The analysis of the crystallites size confirmed that EB-PANI presents a lower degree of crystallinity.

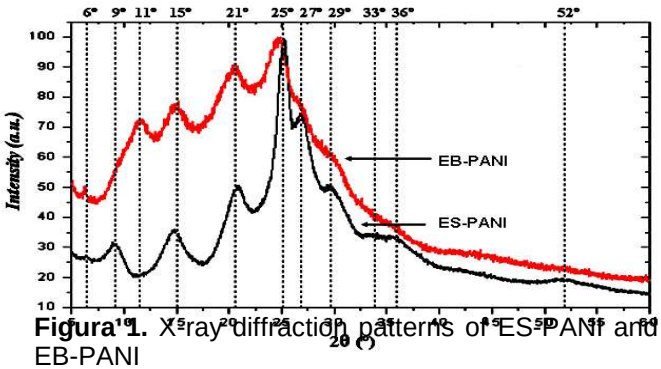

Figura 1. X-ray diffraction patterns of ES-PANI and EB-PANI

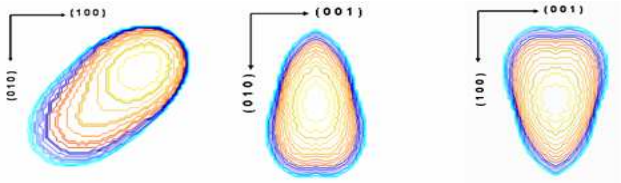

Figura 2. Visualization of the average crystallite shape in the directions [010], [001] and [100] for ES-PANI.

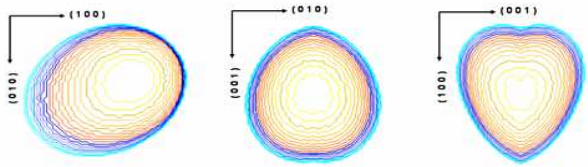

Figura 3. Visualization of the average crystallite shape in the directions [010], [001] and [100] for ES-PANI.

Agradecimentos

CAPES

[1] Cortés, M. T.; Sierra E. V. Polym Bull **2006**, 56, 37.
[2] MacDiarmid, A.G. Synth Met **1997**, 84, 27.
[3] Bhadra,S.; Singha,N.K.; Khastgir, D. J Appl Polym Sci **2007**, 104, 1900.
[4] Rodríguez-Carvajal, J. FullProf Program. Laboratoire Leon Brillouin (CEA-CNRS), version September **2007**.
[5] González-Platas, J.; Rodríguez-Carvajal, GFOURIER, Version 4.06, Universidad La Laguna, Tenerife, Spain, **2002**.