

Using Raman and FTIR spectroscopy for demonstrate fillers in polypropylene compound structure

N. Ramezani^{1*}, A. Rajabloo², P. Hemmati³

^{1,2,3}Department of Chemistry, Faculty of sciences, Ferdowsi University, Mashhad, Iran

*Ramezani@um.ac.ir

Abstract

Polypropylene (PP), a thermoplastic material is mostly used for its desired properties which respond to the techniques of processing materials. To detect specific chemical linkages, the chemical and physical full structure of polymers, description of qualitative and quantitative analysis of combinations, polymer compounds and spectroscopy are utilized. By the methods of infrared (FTIR) and Raman spectroscopy, this study, it is tried to achieve molecular microstructure and identify linkages that existed in both polypropylene compounds. FTIR and Raman spectrum are considered for both compounds in the areas of 400-4000cm⁻¹. Raman spectroscopy with three different wavelengths including 475nm, 532nm and 785nm was used through which the comparison of spectrum results obtained from three lasers, the presence of filler in both two compounds by relying on the final spectrum in $\lambda=785\text{nm}$ can be proved. Therefore, given the presence of filler was proved in the compounds, it is possible to replace this method with other methods of identifying filler and additives in mixing compounds such as TGA and ASH due to the non-destructive and inexpensive benefits, through Raman spectroscopy in this study.

Keywords: Compound, infrared spectroscopy, Raman spectroscopy, polypropylene.

Introduction

Polypropylene (PP), a thermoplastic material is mostly used for its desired properties which respond to the techniques of processing materials[1]. This polymer contains desired properties which are catalytically provided by Propene Olefin Monomer (propylene)[2]. To detect specific chemical linkages, the chemical and physical full structure of polymers, description of qualitative and quantitative analysis of combinations, polymer compounds and spectroscopy are utilized. Infrared spectroscopy was the first and the most common method used (FTIR) through which the chemical compound and interactions between functional groups in a polymer compound can be straightly gained. Using the recent scientific promotions, the Raman spectroscopy method has been replaced due to its easy utilization, low costs, and quick and non-destructive properties[3]. Accordingly, a study was conducted on the association with Raman chemical-spatial structure of polypropylene co polymer/1-octene in which the degree of crystallinity and structural order of macromolecules of the copolymer was investigated[4].

Using the methods to analyze devices such as Raman spectroscopy and FTIR, this study tried to compare these two compounds to achieve molecular structure and identify linkages that existed in two compounds of polypropylene. To increase the accuracy and correctness

of results, the two given methods were simultaneously used and their spectrum was compared, too.

Experimental

Materials:

In this study, granule particles i.e. two compounds of polypropylene which contain different thermal properties were used.

Methods:

FTIR spectroscopy: In this method, granule particles of two samples of polypropylene were eroded and using the KBr in the process of making a tablet, a tablet was gained with uniformity. The tablet gained was embedded in device FTIR made in Thermo Nicolet Company, model Avatar370FTIR with Resolution 4. And the desired spectrum was studied in the areas of 400-4000cm⁻¹. This experimentation was conducted on the space temperature and pressure.

Raman spectroscopy: In this approach, the specimen was put inside the laser without any process of preparation in the form of initial granules. Charge-coupled device (CCD) was used as a detector in this spectroscopy which contains at least -40°C. Both specimens of polypropylene were put within three lasers with 475nm, 532nm and 785nm wavelengths using Uni-



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crown spectroscopy made in northern Korea and the gained spectrum was studied.

Results and discussion

In the Raman spectrum, two compounds of PP (a) and PP (b) in the area of $400\text{-}4000\text{cm}^{-1}$ and the main peaks of two specimens in the area of $2800\text{-}3000\text{cm}^{-1}$ are observed which were seen using lasers such as 457nm , and 532nm . The strength peak in the areas of 2897cm^{-1} and 2899cm^{-1} which are observed in the spectrum can be assigned to the symmetrical linkages of methyl. The peaks are shown in the range of 1455cm^{-1} and 1333cm^{-1} for PP (a) and also those shown in the range of 1470cm^{-1} and 1348cm^{-1} are the indicators of final CH_2 and CH_3 groups. The peaks are shown in the areas of $500\text{-}1500\text{cm}^{-1}$ containing C-C stretching vibration in the polymer chain, CH_2 and CH_3 transformation. The severity in the CH Sp^3 peak of PP Aliphatic in laser 457nm is significantly more than its severity in laser 532nm . The severity of such peak was generally lost in laser 785nm but other peaks in the areas of $839\text{-}1470\text{cm}^{-1}$ were added to that. These signals related to filler materials used in both compounds of polypropylene in the areas of $394\text{-}1455\text{cm}^{-1}$ which has proved the presence of filler materials in both compounds.

Also, in the infrared spectrum for both PP specimens in the areas of $400\text{-}4000\text{cm}^{-1}$, the specimen PP (a) with enthalpy 100.64 J/g includes more peak area rather than the second specimen i.e. PP (b) with enthalpy 93.4 J/g . The strength peaks are shown in the areas of 2838cm^{-1} to 2960cm^{-1} and can be assigned to the asymmetrical stretching vibrations of methyl, symmetrical and asymmetrical stretch of CH_2 . The absorption peaks that are shown in the areas of 972cm^{-1} , 997cm^{-1} and 1165cm^{-1} , are also allocated to the rocking vibrations of CH_3 and the symmetrical bending vibration states of the CH_3 group are detected in 1375cm^{-1} . Also, another peak in the area of 1459cm^{-1} can be assigned to the symmetrical bending linkage of CH_2 . In this spectrum i.e. area of $808\text{-}997\text{cm}^{-1}$, the peaks related to filler have overlapped with peaks related to polypropylene in which based on the Raman spectrum, peaks related to filler can be separated and the presence of filler in specimens can be approved, too.

Conclusions

As seen before, Raman and FTIR spectrum adopted from two compounds of polypropylene have proved the presence of filler in mixing compounds, Raman spectroscopy as a filler method for FTIR spectroscopy has provided us with the subject, in better separation and accuracy, in $\lambda=785\text{nm}$ in comparison with 475nm and 532nm wavelengths without exhibiting signals related to polypropylene and/or only demonstrating signals related to the filler. The important result to be referred to in this study is that the presence of filler in compounds can be proved with high resolution, using Raman spectroscopy in $\lambda=785\text{nm}$. Accordingly, Raman spectroscopy can be replaced with other methods of identifying filler and additives in mixing compounds such as TGA and ASH, through non-destructive and low-cost benefits.

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