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材料化学工程与纳米技术

基于拉曼光谱的高密度聚乙烯质量检测

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摘要

密度和熔融指数是高密度聚乙烯（HDPE）产品最重要的质量指标。本文通过拉曼光谱，结合偏最小二乘法（PLS）分析，实现了对HDPE密度和熔融指数的同时检测。通过对2700～2970 cm^{-1}范围内HDPE的拉曼光谱进行PLS分析，发现了HDPE的密度与短支链数量的负相关，并建立了HDPE密度的PLS回归模型。模型所得密度预测值与真实值的相关系数（r）、平均相对误差（ARD）和预测标准误差（SEP）分别为0.950、0.09%和1.02，优于近红外光谱和基于凝聚态结构分析的拉曼光谱的检测结果。利用HDPE乙烯基含量与熔融指数的正相关，通过分析1288～1650 cm^{-1}范围内的拉曼光谱，建立了HDPE熔融指数的PLS回归模型，所得熔融指数的预测值与真实值的r、ARD和SEP分别为0.966、8.61%和0.99。与熔融指数的红外光谱检测结果相比，拉曼光谱的检测结果具有更高的精度。

关键词

高密度聚乙烯 熔融指数 密度 拉曼光谱 偏最小二乘法

分类号

扩展功能

本文信息

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Detection of HDPE properties by Raman spectrum based on partial least square

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Abstract

Density and melt index (MI) are the most important properties of high density polyethylene (HDPE) in industrial manufacturing.In this work, density and MI of commercial grade HDPE were detected by Raman spectrum, based on the partial least squares (PLS) method.The short-branch degree was found to be inversely proportional to the density, according to the PLS analysis of the characterization spectra in the range 2700—2970 cm^{-1}.A regression model between short-branch degree and density was built up.The correlation coefficient (r), average relative deviation (ARD) and standard error of the prediction (SEP) for density prediction were 0.950, 0.09% and 1.02, respectively.And the density regression model gave a better result than those obtained by near-infrared spectrum and Raman spectrum based on phase structure analysis.Furthermore, the vinyl content was found to be proportional to the MI value.A regression model between vinyl content and the MI of HDPE was established by analyzing the characterization spectra in the range from 1288 cm^{-1} to 1650 cm^{-1}.And the values of r, ARD and SEP for MI prediction were 0.966, 8.61% and 0.99, respectively.Comparing with the results measured by near-infrared spectrum, Raman spectrum showed higher precision for MI estimation.

Key words

high density polyethylene melt index density Raman spectrum partial least squares

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