

NEAR-INFRARED STUDIES ON STRUCTURE-PROPERTIES RELATIONSHIP IN HIGH DENSITY AND LOW DENSITY POLYETHYLENE

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Near-infrared (NIR) spectra have been measured for high-density (HDPE), linear low-density (LLDPE), and low-density (LDPE) polyethylene in pellet or thin films. The obtained spectra have been analyzed by conventional spectroscopic analysis methods and chemometrics. By using the second derivative, principal component analysis (PCA), and two-dimensional (2D) correlation analysis, we could separate many overlapped bands in the NIR. It was found that the intensities of some bands are sensitive to density and crystallinity of PE. This may be the first time that such bands in the NIR region have ever been discussed. Correlations of such marker bands among the NIR spectra have also been investigated. This sort of investigation is very important not only for further understanding of vibration spectra of various of PE but also for quality control of PE by vibrational spectroscopy.

Figure 1 (a) and (b) shows a NIR reflectance spectrum of one of the LLDPE samples and that of PE, respectively. Figure 2 shows a PC weight loadings plot of factor 1 for a score plot of PCA for the 16 kinds of LLDPE and PE based upon their 51 NIR spectra in the 1100-1900 nm region. The PC loadings plot separates the bands due to the CH₃ groups and those arising from the CH₂ groups, allowing one to make band assignments. The 2D correlation analysis is also powerful in band enhancement, and the band assignments based upon PCA are in good agreement with those by the 2D correlation analysis.

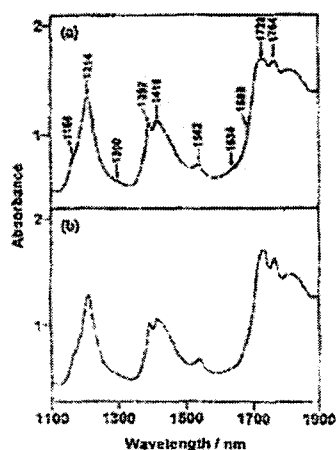


Figure 1 (a) and (b). A NIR reflectance spectrum of one of the LLDPE samples and that of PE, respectively.

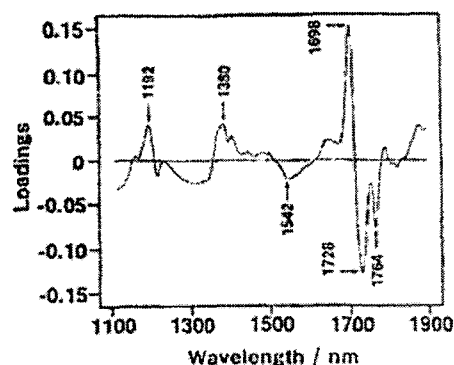


Figure 2. A PC weight loadings plot of factor 1 for a score plot of PCA for the 16 kinds of LLDPE and PE based upon their 51 NIR spectra in the 1100-1900 nm region.

We have made a calibration model, which predicts the density of LLDPE by use of partial least square (PLS) regression. From the loadings plot of regression coefficients for the model, we suggest that the band at 1542, 1728, and 1764 nm very sensitive to the changes in density and crystallinity.