Prediction of Monomer Concentrations in Copolymerization Reactions from Infrared (IR) Spectra

Swarit Jasial,[1,2] Araki Wakiuchi,[2,3] Shigehito Asano,[4] Ryo Hashizume,[4] Miho Hatanaka,[5] Yu-ya Ohnishi,[3] Takamitsu Matsubara,[1,2] Hiroharu Ajiro,[1,2] Tetsunori Sugawara,[4] Mikiya Fujii,[1,2] and Tomoyuki Miyao[1,2]

[1]Data Science Center, Nara Institute of Science and Technology, 8916-5 Takayama-cho, Ikoma, Nara 630-0192, Japan.
[2]Graduate School of Science and Technology, Nara Institute of Science and Technology, 8916-5 Takayama-cho, Ikoma, Nara 630-0192, Japan.
[3]Materials Informatics Initiative, RD technology and digital transformation center, JSR Corporation, 3-103-9 Tonomachi, Kawasaki-ku, Kawasaki, Kanagawa 210-0821, Japan.
[4]Fine Chemical Process Department, JSR Corporation, 100 Kawajiri-cho, Yokkaichi, Mie 510-8552, Japan.
[5]Department of Chemistry, Faculty of Science and Technology, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama, Kanagawa 223-8522, Japan.

Email: jasial@dsc.naist.jp

Fourier-transform infrared (FTIR) spectroscopy is generally used for the identification of functional groups and normal modes of vibration in a molecule. Since the absorbance of a solution at structure-specific wavenumbers are proportional to the concentration of the solution (Beer-Lambert law), one can estimate concentration of the reactants from the peaks of the spectra. However, quantitative analysis of FTIR spectra becomes difficult for copolymerization reactions where peaks of absorbance from different components, such as, comonomers and polymers, are usually overlapped. Hence, analyzing IR spectra for estimating residual concentration of monomers in copolymerization reactions forms a fundamental issue in the field of chemometrics. In this talk, two methods for the prediction of monomer concentration from IR spectra are discussed. The first approach uses wavelet transforms to decompose overlapped peaks of reaction data into features which are used as input for elastic net regression model for the prediction of reactant concentration. In the second approach, monomer mixture data of two reactant monomers is utilized as training set where second derivatives of spectra enhance the separation of overlapping peaks, thereby improving the resolution and prediction of monomer concentrations. These methods were used on five different monomer combinations in copolymerization reactions, showcasing their practical use.