Estimation of chemical resolution in Near Infrared Chemical Image (NIR-CI)

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Introduction

Near infrared chemical imaging (NIR-CI) is a new analytical technique. It combines NIR spectroscopy and image acquisition techniques, which allows the assembly of information about chemical composition and spatial distribution of sample components. Because diffuse reflectance is the normal acquisition mode in NIR-CI, final resolution of the image (which means ability to obtain pure spectra component without contamination of neighbouring pixels) depends on several factors, including depth of penetration of NIR radiation, and of scattering effects. As a result, optical and chemical resolutions may be different.

Materials and methods

An Image NIR Spectral Dimensions MatrixNIR instrument was used, working at a nominal optical resolution of 100 µm. NIR images of sieved powdered potassium hydrogen phtalate (KHP), and different chemical polymers, both in powdered and film forms, were recorded. The correlation coefficients were used to measure the spectra similarity.

Results and discussion

Chemical resolution has been found to be very dependent on the sample scattering properties, ranging from 0.5 mm to 3 mm. As an example of the results found, Figure 1 shows the correlation image of a sample composed by two polymer blocks, and Figure 2 shows the evolution of the correlation coefficient expressed in pixel units. Chemical resolution has been computed as the distance between pixels, with a correlation coefficient of 95% of the plateau value.

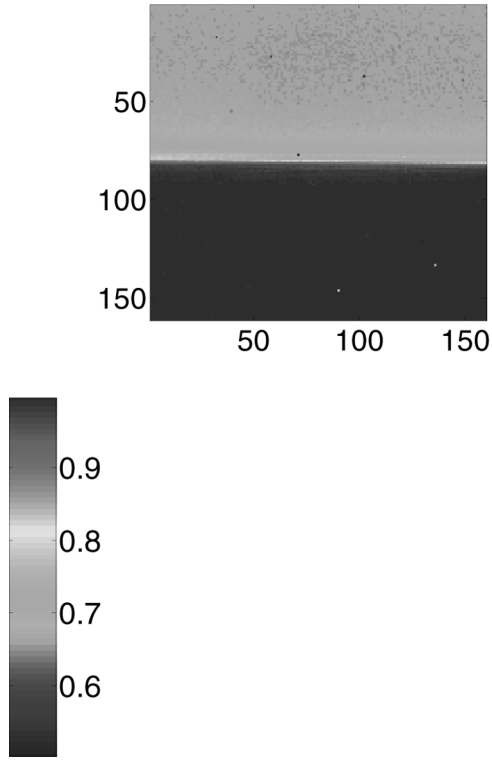

Figure 1. Correlation image of two polymers.

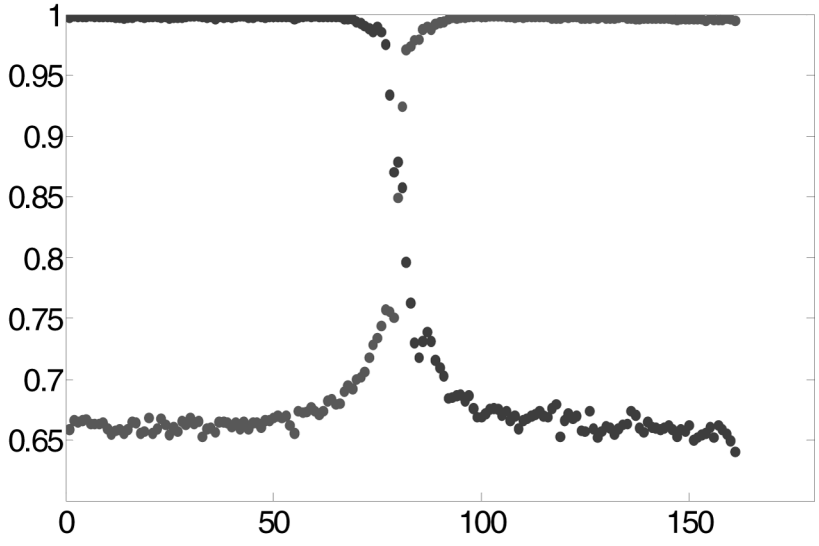

Figure 2. Plot of correlation coefficients vs pixel number.