

# Direct determination of diffusion coefficients in polymer solvent systems from Raman spectroscopic data

David Siebel, Philip Scharfer, Wilhelm Schabel

*Institute of Thermal Process Engineering, Thin Film Technology (TFT), Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe, Germany*

*Corresponding author: david.siebel@kit.edu*

(Please underline speaker. An optional short paragraph containing any additional information about the authors may be added here.)

**Keywords:** diffusion, spectroscopy, polymer solutions

Diffusion coefficients in polymer solvent systems are strongly dependent on the concentration of the solvent. Especially at low solvent concentrations the diffusion coefficients change by several orders of magnitude. Exact knowledge of the transport parameters is of crucial importance for the process design. In literature different measurement techniques have been discussed. All of them have specific advantages and disadvantages. Nevertheless, the availability of diffusion data in polymer solvent systems is very low due to time consuming measurements and a very high number of material systems of interest. Predictive methods on the other hand have not yet shown satisfactory results.

In this work, a new concept for a fast and reliable determination of concentration-dependent diffusion coefficients in polymer solvent systems is discussed. The diffusion coefficients are calculated directly from spectroscopic data, which renders a quantitative description of the phase equilibrium and mass transport in the gas phase unnecessary. Measurement data is provided by means of inverse micro raman spectroscopy (IMRS). For the calculation of diffusion coefficients, measurement data has to be processed by a suitable method of smoothing. Furthermore, an approximation of the local mass flux, which cannot be measured directly, has to be found. Different approaches to these challenges and initial results are shown.

Please consider this topic for poster presentation.