DIFFUSION IN SOLUTION PROCESSED ORGANIC MULTILAYERS

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Presented at the 16th International Coating Science and Technology Symposium,
September 9-12, 2012, Midtown Atlanta, GA[1]

Introduction

The dissolution between organic layers caused by diffusion in solution-processed multilayer stacks, found in organic semiconducting devices like organic light emitting diodes, has a huge impact on the device performance. To improve the device quality, it is important to control the intermixing of the single layers by choosing optimal production process parameters. To this, a detailed understanding of phase equilibrium and mass transport properties is crucial. In the scope of this work, the intermixing of two single layers coated on top of each other is investigated by means Inverse-Micro-Raman-Spectroscopy (IMRS). Data for different material classes are used to generate a simulation for prediction of diffusion and mass transfer between organic layers under different process conditions.

Experimental Methods

The local concentration profiles of multiple species within an organic multi-layer model structure are measured under well-defined boundary conditions during the drying process or with a constant solvent activity in the gas phase by Inverse-Micro-Raman-Spectroscopy (IMRS). Figure 1 shows a schematic drawing of the IMRS measurement technique. Through the thin glass slide, the non-invasive measuring technique is able to detect the local chemical composition within polymeric films with a spatial resolution of 2 µm and an integration time of 1 second per measured data point. The accuracy of the measurement technique is about 1 % content. Diffusion coefficients are determined by fitting simulation results to the measured data [1]. In the drying channel, the polymeric film is dried under defined isothermal drying conditions.

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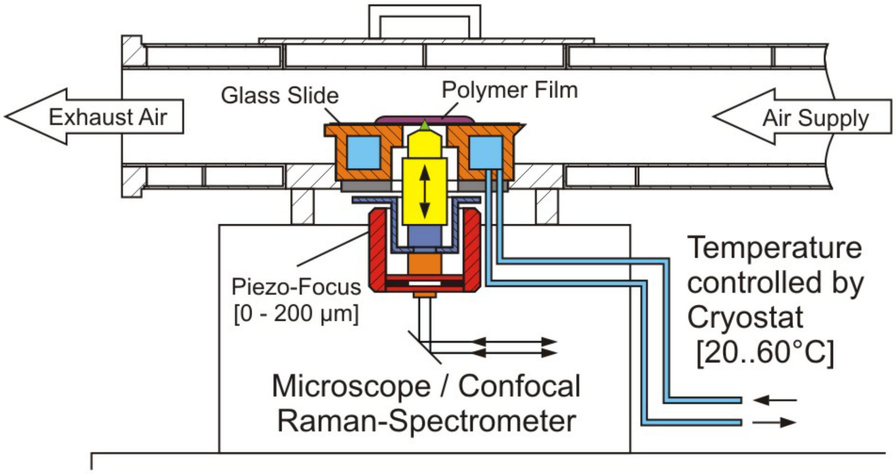

Fig. 1: Drying channel with coupled measuring technique (IMRS).

In order to measure the intermixing process at constant temperature and solvent concentration in the film, a stable environment has to be assured. An existing sorption cell for measurements of water sorption in polymer films [2] was modified for the use of solvent vapour (see figure 2). The gas phase activity of the solvent is controlled by filling the reservoir with a polymer solution with known vapour liquid equilibrium and defined composition.

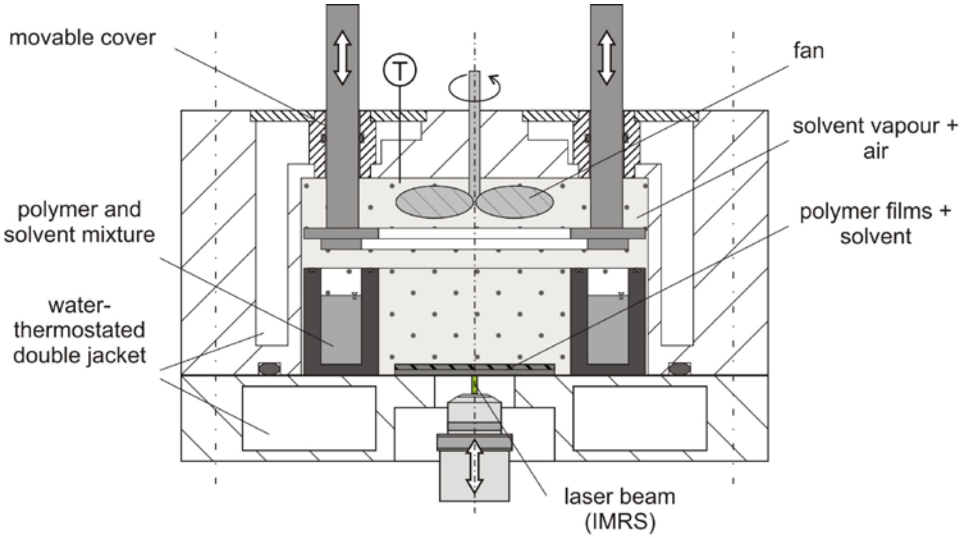

Fig. 2: Experimental setup for the in situ characterisation at variable vapour phase solvent activity.

As mentioned above, the experimental investigations are performed with model systems. The molecular mass of one of the layers is varied in order to understand the influence of molecular size on the intermixing process. The mobility of the molecules is increased by the presence of a solvent. In case of the drying experiments, the solvent is applied with the second layer, while in case of sorption cell experiments the solvent is absorbed from the gas phase.

Simulation

To simulate the dissolution and drying process of the organic multilayer, the mass transport in the gas phase, the sorption equilibrium at the phase interface and the diffusive mass transport in the film have to be taken into account. Based on a VISUAL BASIC program using FORTRAN routines and numerical libraries from NAG (Numerical Algorithms Group) [1] a new simulation was developed to solve the equations.

References

[1] W. Schabel, Trocknung von Polymerfilmen – Messung von Konzentrationsprofilen mit der Inversen-Mikro-Raman-Spektroskopie, PhD Thesis, University of Karlsruhe (TH), Karlsruhe, 2004

[2] S. Jeck et al., Water sorption in semicrystalline poly(vinyl alcohol) membranes: In situ characterisation of solvent-induced structural rearrangements, Journal of Membrane Science, 389, 162– 172, 2012