Report on PIRSES visits for J.Ilnytskyi, Institute for Condensed Matter Physics, NANU.
15 January-14 February 2012, visit to: UMCS Lublin, Prof. S.Sokolowski.
Scope of work: Development of simulation tools for Poiseuille flows, study of microphase separation of a binary mixture in patterned pore.

The dissipative particle dynamics code was developed which enables the study of Poiseuille flows in microchannels. To this end the code includes the bulk forces imposed on selected flow particles and special attention is paid to preserve the total momentum in the system, as an important feature of the method. To this end the simulation box is enlarged twice in Z direction (at both pore boundaries) and contra-flows are introduced at both extended slabs. This ensures that the total momentun is preserved. We performed a set of simulations with various boundary conditions at the mid-walls separating main flow from the contra-flow. The cases included: completely transparent and non-transparent reflective mid-walls. The first case was found prone to the artefacts in a way of influencing the microphase separation inside the internal flow channel. The non-transparent walls are found to have minimal effect on micro-phase separation but can also switch from pillar to lamellar phase at zero bulk force close to the transition region between the two. The applicability of the method is tested via monitoring transverse temperature and the histograms for bond lengths for the brush grafted to mid-walls when the mixture of solvents is driveb through the channel by means of a bulk force. We found that if the zero-flow case has a symmetry of a pillar phase, then the floowing sequence of phases appear with the increase of a bulk force: pillar, bended pillar, distorted disconnected droplets on each wall, modulated lamellar phase, planar lamellar phase. The last two phases takes place at the bulk force at which unphysical bond stretch and essential increase of the transcerse temperature are detected. The work was done in close cooperation with Dr. P.Bryk from UMCS.

During the visit we also extend our previous study [J. Chem. Phys. 134, 204903 (2011)] on self-assembly of a binary mixture of components A and B confined in a slit-like pore with the walls modified by the stripes of tethered brushes made of beads of a sort A. The emphasis of the research was put on solvent mediated transitions between morphologies when the composition of the mixture varies. For certain limiting cases of the pore geometry we found reduction of an effective dimensionality including cases of a quasi one- and two-dimensional demixing. The change of the environment for the chains upon changing the composition of the mixture from polymer melt to a good solution provides explanation for the mechanism of development of several solvent mediated morphologies and, in some cases, for switching between them. We found solvent mediated lamellar, meander and inlined cylinder phases. Quantitative analysis of morphology structure is performed considering brush overlap integrals and gyration tensor components.

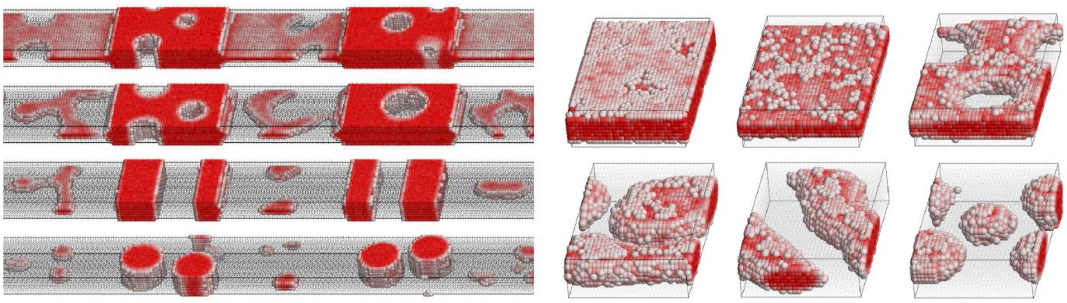

Fig.1. Morphologies at wide stripes showing periodic pattern of bulk 3D regions and quasi 2D slabs (left) and quasi-2D microphase separation in slabs filled by the mixture of solvents (right). Only bad solvent (in red) is shown.

The overlap integrals are introduced for brushed overlap along and across the pore walls and the case of a mixture of solvents is compared with the case of a one-component solvent of comparable quality. We demostrate the anomalies in behaviour of overlap integral and the components of gyration tensor for polymer brush for the case of the mixture (and not existing for the one-component solvent), which is the result of the microphase separation effects.

The solvent-mediated transitions are studied for various pore geometries, especially at closely separated brush stripes (Fig.2).

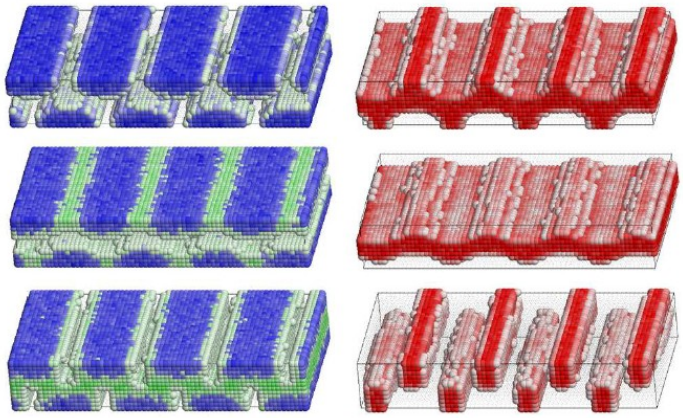

Fig.2. Sequence of morphologies obtained with the increase of the amount for good solvent (in green) in the mixture of good and bad (in red) solvent that fills the interior of the pore formed by weakly separated stripes of brushes (in blue).

Based on the study the paper: “Dissipative particle dynamics study of solvent mediated transitions in pores decorated with tethered polymer brushes in the form of stripes” J.Ilnytskyi, T.Patsahan S.Sokolowski is prepared and is submitted to Condensed Matter Physics journal.