CPP 50: Nanostructures, Nanostructuring and Nanosized Soft Matter

Time: Friday 12:30–13:00 Location: H38

CPP 50.1 Fri 12:30 H38

The effect of solvent vapor annealing on diblock copolymer templated mesoporous Si/Ge/C thin films — •Christian L. Weindl[1], Christian E. Fajman[2], Michael A. Giebel[2], Kerstin S. Wienhold[1], Shanshan Yin[1], Ting Tian[1], Christina Geiger[1], Lucas P. Kreuzer[5], Matthias Schwartzkopf[3], Stephan V. Roth[3,4], Thomas F. Fässler[2], and Peter Müller-Buschbaum[1,5] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]TU München, LS Anorganische Chemie mit Schwerpunkt Neue Materialien, Chemie-Department, 85748 Garching — [3]DESY, 22607 Hamburg — [4]Royal Institute of Technology KTH, 100 44 Stockholm — [5]MLZ, TU München, 85748 Garching

The latest research has revealed promising results for silicon (Si) and germanium (Ge) as anode materials for lithium-ion batteries. These two group 14 semiconductors are considered auspicious additives in graphite anodes due to their high specific capacity (Si) and electron mobility (Ge). This study aims to synthesize a mesoporous Si/Ge/C structure by using a wet chemical sol-gel approach with the structure-directing amphiphilic diblock copolymer PS-b-PEO and the Zintl cluster $K_{12}Si_xGe_{17-x}$. Furthermore, we investigate the structural changes on the spin-coated thin films upon exposure to a saturated toluene/butanol atmosphere. For morphlolgical analysis, scanning electron microscopy will be combined with grazing-incidence small-angle x-ray scattering (GISAXS). Moreover, energy-dispersive X-ray spectroscopy, Raman spectroscopy and powder X-ray diffraction are used for further elemental and crystalline phase analysis.

CPP 50.2 Fri 12:45 H38

The kinetics and free-energy landscape of grain-boundary motion incylinder-forming copolymers — •Niklas Blagojevic and Marcus Müller — Universität Göttingen, Institut für Theoretische Physik

Block copolymers which self-assemble into a dense array of hexagonally-packed cylinders are promising canditates for filtering membranes with pore sizes in the nanometer range used to extract or to purify a substance. The cylinders act as selective transport channels and it is important to align the cylinders along the desired flux direction. A fundamental understanding on how to control the cylinder orientation in the processing of the membrane, however, is incomplete and successful applications have often relied on trial-and-error searches in the high-dimensional space of process parameters.

To gain fundamental understanding about orientation mechanisms of cylindrical copolymer phases, we employ large-scale computer simulations of a particle based model in a highly efficient GPU-parallel implementation with sophisticated free-energy techniques. With this, we study the kinetics of grain-boundary motion of cylindrical copolymer domains – resembling the (re-)orientation mechanisms – and the Minimum Free-Energy Path of the associated changes of the domain topology. The simulation study has provided direct insights into the kinetics and the free-energy landscapes of orientation mechanisms and ordering in the early and late stages.