CPP 39: French-German Session: Nanomaterials, Composites and Hybrids I

Time: Wednesday 15:00–16:45 Location: ZEU/0260

Invited Talk CPP 39.1 Wed 15:00 ZEU/0260

A polarizable model for atomistic simulations of metals and graphitic material/ liquid interfaces — Krishan Kanhaiya[1], Hendrik Heinz[2], and •Marialore Sulpizi[1] — [1]Department of Physics and Astronomy, Ruhr-University Bochum, Universitätsstraße 150, 44801 Bochum, Germany — [2]Department of Chemical and Biological Engineering, University of Colorado at Boulder, Boulder, CO 80301

Polarization significantly affects the interaction and adsorption energy of molecules on metal surfaces. The ability to describe at a metal surface the classical "image charge" potential is a direct result of its polarizability, which needs to be modelled correctly to accurately simulate interfacial phenomena e.g. in electrochemistry or catalysis. Recently, we have introduced a polarizable model for metals which permits to describe also electrified interfaces. Here we extend the idea to graphitic material introducing flexible dummy electrons to represent the polarizable π-electron cloud. The model accurately predicts surface and hydration energy, water contact angle as well as experimental and DFT data on molecular adsorption on surfaces. A considerable improvement is obtained in the prediction of water-graphite interfacial friction, which is obtained at the level of electronic structure calculations.

CPP 39.2 Wed 15:30 ZEU/0260

Lamellar Domain Spacing of Copolymers with Nonlinear Block Architectures — Andrzej Grzyb[1], Jarosław S. Kłos[2], Aykut Erbaş[3], Michael Lang[4], and •Jarosław Paturej[1] — [1]Institute of Physics, University of Silesia, Katowice, Poland — [2]Faculty of Physics, A. Mickiewicz University, Poznań, Poland — [3]UNAM, Bilkent University, Ankara, Turkey — [4]Leibniz-Institut für Polymerforschung Dresden e.V., Germany

Topological modification of block copolymer (BCP) conformations offers a promising approach for developing self-assembled periodic nanostructured materials with smaller domain sizes, which are essential for a range of technological applications. Cyclic polymers, with their inherently more compact conformations, present an effective strategy for achieving this miniaturization. In this work, through a combination of analytical theory and coarse-grained molecular dynamics simulations, we establish a relationship between different nonlinear topologies and the corresponding domain size of lamella-forming BCPs. Our investigations includes BCP architectures with one or two cyclic segments such as tadpoles, diblock and triblock 8-shaped polymers, and diblock nonconcatenated and concatenated rings. We demonstrate that the primary reduction in lamellar domain size is driven by the more compact arrangement of monomers in the cyclic architectures, with an additional contribution from the nonconcatenation of cyclic segments. This is corroborated by theoretical predictions for both domain size reduction and BCP conformations across different architectures.

CPP 39.3 Wed 15:45 ZEU/0260

Self-Healing Composite Structures for Aerospace Applications — •Merve Ozkutlu Demirel[1], Eray Kostur[1,2], Yigitalp Okumus[1], Bilal Altin[1], Melih Seckin[1], and Yahya Oz[1] — [1]Turkish Aerospace, R&D and Advanced Technologies Directorate, 06980 Ankara, Turkiye — [2]Cukurova University, Department of Mechanical Engineering, 01330 Adana, Turkiye

Self-healing composite structures offer a promising solution for enhancing durability and reducing maintenance costs in aerospace platforms. In this study, a self-healing mechanism based on a microvascular channel network was developed. Composite laminates were fabricated using carbon fabric and epoxy resin. Polyamide monofilaments with a diameter of 450 um were integrated into a hand lay-up process by placing them between composite layers. After curing, these fibers were removed to create hollow channels. Various channel configurations were manufactured and evaluated through bending tests. 5-Ethylidene-2-norbornene was selected as healing agent because its operating temperature range is similar to flight temperature conditions. The healing agent was injected into the channels, while the Grubbs catalyst that would start the polymerization reaction was uniformly dispersed within the polymer matrix. Upon crack formation, the healing agent is expected to flow into the damaged region and polymerize upon contact with the catalyst, thereby filling the crack. Compact tension tests were performed to analyse the healing performance. The results demonstrated that the microvascular channel approach exhibits strong potential for aerospace applications.

CPP 39.4 Wed 16:00 ZEU/0260

Increasing the Mechanical Stability of Carbon Nanomembranes Using a Holey Carbon Interlayer — •Luzie Lina Heinrichs, Zhen Yao, Yang Yang, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Carbon nanomembranes (CNMs) are atomically thin, with subnanometre pores that enable strong gas selectivity and fast, efficient water transport. However, their limited mechanical robustness has constrained their integration into practical filtration technologies.

In this study, we introduce a reinforced CNM architecture that incorporates an intermediate holey support layer. We fabricate and compare single-layer, double-layer, and holey film reinforced composite CNMs. Water permeation measurements using a cup test, combined with nanoindentation characterisation, show that the reinforced architecture preserves high water permeability while markedly improving mechanical stability. The effective Young's modulus reaches ˜25 GPa, approximately five times higher than that of an unreinforced double layer.

By combining mechanical robustness with efficient single-file water transport and precise selectivity, the holey-layer-reinforced CNMs provide a promising route toward real-world applications, especially in seawater desalination.

CPP 39.5 Wed 16:15 ZEU/0260

Particle distribution and thermoresponsive properties of PNIPAM brush/gold nanoparticle composite films — •Elias Hallenbach, Marvin Glock, Hayden Robertson, and Regine von Klitzing — TU Darmstadt, Institute for Condensed Matter Physics, 64289 Darmstadt, Germany

Metal/polymer nanocomposites are versatile hybrid materials and find use in many fields such as photonics, biomedical engineering and catalysis. A promising realization of this type of hybrid material is the controlled self-assembly of gold nanoparticles (AuNPs) inside a polymer brush, which induces color changes upon exposure to environmental changes, enabling sensor applications.
Polymer brushes can serve as a matrix for the immobilization of AuNPs. Particle uptake into the brush matrix is affected by parameters such as thickness, particle size and grafting density [1]. Nanoparticle uptake has proven to be highest at intermediate grafting densities [2]. In the present study thermoresponsive Poly(*N*-Isopropylacrylamide) brushes with varying grafting densities were synthesized directly from a silicon substrate. Nanocomposite materials were fabricated by dip-coating of polymer brushes into an AuNP suspension. Characterization of nanocomposites was performed by (in situ) spectroscopic ellipsometry, atomic force microscopy and (in situ) X-ray reflectometry. The relation between particle distribution and temperature-induced structural changes will be discussed.
[1] S. Christau et al., *Polymers* **2014**, *6*, 1877-1896.
[2] R.R. Bhat, J. Genzer, *Appl. Surf. Sci.* **2006**, *252*, 2549-2554.

CPP 39.6 Wed 16:30 ZEU/0260

Morphology-controlled electrical and thermal conductivity of filled diblock copolymers: effect of filler shape. — •Alexander Chervanyov — University of Münster, Münster, Germany

We investigate the electrical and thermal conductivity of an electrically insulating diblock copolymer (DBC) matrix filled with conductive cylindrical and spherical nanofillers modeling carbon nanotubes (CNTs) and carbon black (CB), respectively. The composite transport properties are examined as functions of the underlying DBC morphology, the selective affinities of CNTs and CB for the dissimilar DBC blocks, and inter-filler interactions that determine the positional and, for CNTs, orientational correlations. Using a combined phase-field description of the DBC host and Monte Carlo simulations of anisotropic CNT fillers, we show that the localization and alignment of CNTs within the microphase-separated domains are highly sensitive to the above parameters. The simulated CNT and CB network structures are used to compute the electrical and thermal response of the composite. We quantitatively elucidate how the morphological transitions in

the DBC correlate with structural rearrangements of the filler networks. Furthermore, we demonstrate that both the order-disorder transition and the order-order transitions between distinct DBC morphologies lead to pronounced changes in composite conductivity, driven by morphology-induced restructuring and alignment of the conductive pathways formed by CNT and CB.

Financial support of Deutsche Forschungsgemeinschaft (DFG) through Grant No. CH 845/2-3, is gratefully acknowledged.