SUBPROJECT 5: Evidence-based design of new I-FRCs using bottom-up methods

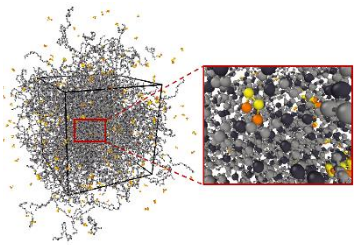
C. Breitkopf in cooperation with S. Wießner;
external advisor: V. Vinš (Czech Academy of Sciences/ CZ)

Motivation

The aim is the multi-scale prediction of the thermo-mechanical behaviour of fibre rubber composites and the description of the interaction of individual I-FRC components at the molecular scale by means of theoretical simulations and accompanying validating experimental investigations in order to generate data for modelling at the meso and macro levels so that evidence-based models for new materials can be derived.

State of the art and previous research

In the previous project phases, thermal conductivities for various uncrosslinked or crosslinked polymers/ elastomers were calculated with the help of molecular dynamics (MD) simulations using the Green-Kubo method. Furthermore, heat capacities, glass transition temperatures and crosslinking types and degrees [1–8] were simulated and validated through, for example, calorimetric investigations and measurements using the heat flow method. In addition, mechanical properties of various model substances such as the stress-strain behaviour as well as the Young's modulus were simulated by MD.


Scientific questions and project objectives

On the basis of experimentally obtained and simulated data from cohorts I and II, a screening of possible substances (e.g., polymers/elastomers for matrices) is to be carried out using an AI algorithm and a prediction of substance properties is to be made. Existing AI algorithms are to be expanded and improved for this purpose.

Another focus is the investigation of temperature stability and mass transfer within the new materials (e.g., gas diffusion stability) in order to assess potential applications so that, for example, predictions can be made about material ageing, thermal and mechanical stability under continuous load.

The simulations within the sub-project are to be carried out both at the molecular level (e.g., ab initio MD) and using FEM, which should ultimately provide realistic material data models, for example for polymer/elastomer networks.

The work in this subproject interacts primarily with SP 2 (thermal and mechanical properties of the fibers), SP3 (thermal and mechanical properties of the polymer matrix) and SP 6 (transfer of material data for meso- and macroscopic models).

References

[1] Vasilev, A.; Lorenz, T; Breitkopf, C.: Thermal Conductivity of Polyisoprene and Polybutadiene from Molecular Dynamics Simulations and Transient Measurements. Polymers 2020, 12(5): 1081, https://doi.org/10.3390/polym12051081.

[2] Vasilev, A.; Lorenz, T; Breitkopf, C.: Thermal Conductivities of Crosslinked Polyisoprene and Polybutadiene from Molecular Dynamics Simulations. Polymers 2021, 13(3): 315, https://doi.org/10.3390/polym13030315.

[3] Vasilev, A.; Lorenz, T; Kamble, V.K.; Wiessner, S.; Breitkopf, C.: Thermal Conductivity of Polybutadiene Rubber from Molecular Dynamics Simulations and Measurements by the Heat Flow Meter Method. Materials, 2021, 14 24): 7737, https://doi.org/10.3390/ma14247737.

[4] Kanan; A.; Vasilev, A.; Breitkopf, C.; Kaliske, M.: Thermo-Electro-Mechanical Simulation of Electro-Active Composites. Materials, 2022, 15(3): 783, DOI: 10.3390/ma15030783.

[5] Vasilev, A.; Lorenz, T; Breitkopf, C.: Prediction of Thermal Conductivities of Rubbers by MD Simulations - New Insights. Polymers, 2022, 14(10): 2046, https://doi.org/10.3390/polym14102046.

[6] Alamfard, T.; Lorenz, T; Breitkopf, C.: Thermal Conductivities of Uniform and Random Sulfur Crosslinking in Polybutadiene by Molecular Dynamic Simulation. Polymers 2023, 15(9): 2058, https://doi.org/10.3390/polym15092058.

[7] Alamfard, T.; Lorenz, T; Breitkopf, C.: Glass Transition Temperatures and Thermal Conductivities of Polybutadiene Crosslinked with Randomly Distributed Sulfur Chains Using Molecular Dynamic Simulation. Polymers, 2024, 16(3): 384, https://doi.org/10.3390/polym16030384.

[8] Breitkopf, C.: Theoretical Characterization of Thermal Conductivities for Polymers - A Review. Thermo, 2024, 4(1): 31-47, https://doi.org/10.3390/thermo4010004.