Study, seminar or master's thesis

on the subject

Molecular dynamic simulations of nano-modified composites

Motivation

Environmental influences such as moisture play an important role in the application of Fiber-composite. Polymers are known for the absorption of water, which leads to the reduction of the specific properties. Among other things, water molecules in the polymer leads to plasticization of the polymers and have an immense influence on the mechanical properties of the matrix. Swelling is another problem that affects mechanical properties such as viscosity and leads to hydrostatic stresses. The effects associated with moisture cannot always be explored experimentally. One way to quantify these effects is numerical simulations at the nano level. Molecular dynamic simulations are used for the simulations at the nano level used to capture the influence of water. This allows to calculate parameters such as diffusion coefficient, elastic modulus, glass transition temperature etc. and ensures a reduction of experiments.

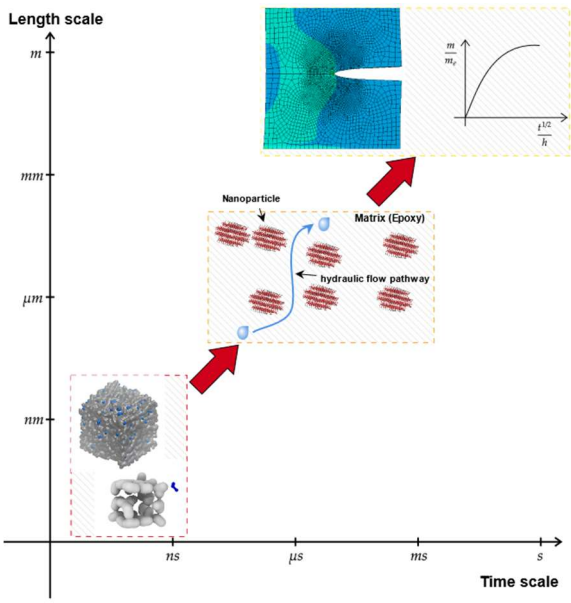
What properties of the polymer are to be studied in the work will be discussed with the student. This will involve the student in creating the task.

Goal

The aim of the work is to investigate and describe the influence of water molecules on properties such as glass transition temperature, elastic modulus, viscosity and other properties. The reactive force field (ReaxFF) is used for the simulations, which allows us to accurately describe the polymer. Scaling on the micro level can be done using the finite element method so that the effect of the nanoparticles and fibers can also be taken into account.

Structure

- Literature research on the subject of molecular dynamic simulations with reactive force fields (ReaxFF)
- Development of simulation models on the nano level for molecular dynamic simulations
- Investigation of the material parameters and the influence of moisture on them
- Interpretation of results and validation
- Effect of the nanoparticles on the material parameters (if necessary, investigation using the finite element method)



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