Inorganic-Organic Hybrid Polymers: A Force Field Modeling Approach

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Inorganic-Organic Hybrid Polymers like ORMOCER®s offer a wide range of tunable properties. This makes them suitable for many applications, from simple coatings to complex optical or biomedical demands. [1] ORMOCER®s are synthesized in a two-step synthesis (Fig. 1), the first step being a (poly)condensation of silanols or alkoxysilanes – the precursors – resulting in the so-called resin, an organically modified inorganic-organic network with a cross-linked $[Si\text{-}O]_n$ backbone. The resin may already contain a large number of different species, leading to a rather complex system. In the second step, a polymerization is initiated either thermally or photochemically via UV irradiation or two-photon absorption.

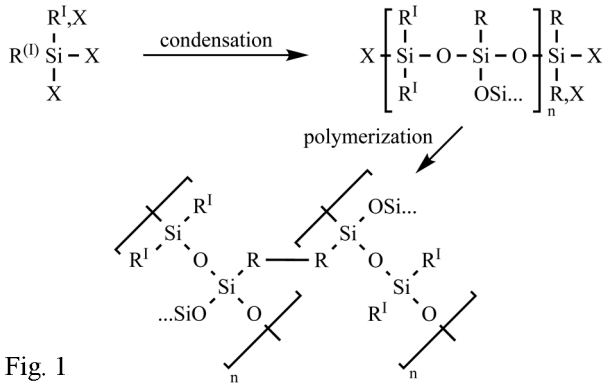

Fig. 1

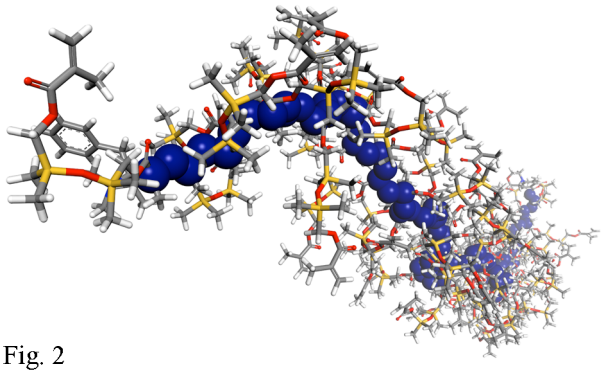

Fig. 2

The macroscopic properties of these materials have been determined in detail, nevertheless the structure of these materials on an atomistic scale is still unknown. Therefore, the application of modeling techniques to gain more insight into the molecular structures seems a suitable approach. Due to the complexity of the investigated materials, only force field methods are resonable for this modeling study. The COMPASS force field was chosen because its applicability for ORMOCER®s was already proven in previous studies. [2]

Here, we present the model system ORMOCER®-DIM01 that forms only two different species in the resin. The ratio of these species was determined by ^{29}Si-NMR spectroscopy. The degree of conversion after the polymerization reaction was obtained by RAMAN spectroscopy. Our models represent all three stages of the material, namely the precursor, the resin and the polymer.

Precursor and resin models are used for validation purposes, mainly to define the appropriate size of the models and the parameters for Molecular Dynamics. These simulations are performed to describe macroscopic properties at room temperature, e.g. the density as a first benchmark for the practicability of our models.

The polymer models consist of organic polymer chains (Fig. 2, backbone shown as balls) with a length of 10 – 100 repeat units, giving simulation cells with up to 4600 atoms. They contain either individual or cross-linked chains, depending on thermoplastic or thermosetting behavior, respectively. The structure of all models is entirely amorphous, which is in agreement with X-ray diffraction data.

[1] F. Burmeister, S. Steenhusen, R. Houbertz, U. D. Zeitner, S. Nolte, A. Tünnermann, *J. Laser Appl.*, **2012**, *24*, 042014.

[2] S. Fessel, A. M. Schneider, S. Steenhusen, R. Houbertz, P. Behrens, *J. Sol-Gel. Sci. Technol.*, **2012**, *63*, 356-365.