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Multiscale simulations of structure and thermomechanical properties of phthalonitrile heat-resistance resins

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Abstract content
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Phthalonitrile-based matrixes are thermostable resins used for durable reinforcement materials. The resins are typically produced by two-stage curing of phthalonitrile monomers in presence of initiator. During the first low temperature stage (~200deg;C), nitrile groups transform into inter-monomer bonds between isoindoline groups, which is the typical polymerization path. The second curing stage is aimed to reach higher conversion rate and produced at elevated temperatures (300 – 350deg;C), at which triazine can be formed by three monomers. Effectively, triazine is a triple link between monomers, making the topology of the polymer network even more complex. The effect of triazine crosslinks in the structure and physical properties of the material is important but unclear up to now.

We have developed a multiscale simulations scheme of phthalonitrile thermosetting resins. The scheme contains a set of consecutive phases from dissipative particle dynamics (DPD) level to molecular dynamics. On the first step, we simulate two-stage curing process with DPD technique. The length of low-temperature and high-temperature stages is controlled by the aim conversion rates known from experimental study. On the next step, a reverse mapping procedure is used to convert coarse-grained structures onto atomistic ones. The obtained atomistic structures are then refined by a Monte Carlo procedure with soft repulsive potentials to avoid insufficient structural motifs such as the short cycle spearing. Then we run short relaxation within molecular dynamics (MD). The prepared material samples are used for the following MD simulations to estimate thermophysical and mechanical properties of the material.

In this report, we present and discuss thermophysical and mechanical properties for the phthalonitrile matrixes obtained with using different comonomers and polymerization protocols.

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