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Modeling of acoustic waves propagation in branched polymers using metric graphs approach

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Branched polymers occur when groups of units branch off from the long polymer chain. These branches are known as side chains and can also be very long groups of repeating structures. Branching polymers can be further categorized by how they branch off from the main chain. Polymers with many branches are known as dendrimers, and these molecules can form a webbing when cooled. This can make the polymer strong in the ideal temperature range. Such branched polymer chains can be modeled in terms of so-called metric graphs, which are the set of bonds connected at the vertices. The connection rule is called the topology of a graph. Modeling of wave dynamics in branched polymers require developing of effective methods allowing to take into account the transition of the waves from one to another branch via the branching points. One of such approaches is based on the use of metric graphs as the models of the branched polymers. Within such approach, the wave dynamics in branched systems can be modeled in terms of the wave equations on metric graphs. In this work, we use linear and nonlinear acoustic equations for modeling of elastic waves in branched polymers. In particular, we consider star (Y-junction) and tree-shaped polymers. The boundary conditions are imposed as continuity of the wave function at the branched point. Also, energy conservation is used to derive the second set of the vertex boundary condition. Speed and profile of the acoustic waves are explored on different polymer branches.

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