

## **Mesoscopic dynamic simulation of diblock copolymers for the automotive industry**

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The particular chemical structure of block copolymer materials is reflected in the most fundamental and interesting way by incompatibility effects. These effects give block copolymers a number of specific, new morphologies and original physical and mechanical properties, which have led to valuable technological applications.

Diblock copolymers are polymers consisting of two linear blocks (A and B) of mutually insoluble polymers, chemically connected end-to-end. When a melt of these polymers is quenched, the A-blocks and the B-blocks tend to form separate phases, but because of the chemical connectivity, macroscopic phase separation is prevented. Instead, the melt forms a microphase separated structure, the shape of which depends on the length ratio of the two blocks.

To predict the phase structure of diblock copolymers by direct simulation, a number of methods are possible in principle. In recent years, however, a relatively new method, known as dissipative particle dynamics (DPD), has been proposed to simulate polymers off-lattice in a coarse-grained fashion.

Accordingly, we have used the DPD simulation method to study the microstructure of mesophase formation of linear ( $A_mB_n$ ) methacrylate diblock copolymer melts of special interest in the automotive industry. The underlying idea is that, in principle, the particular chemical structures of block methacrylate copolymer materials may be reflected in the most fundamental and interesting way by incompatibility effects. These, in turn, give these materials a number of specific, new morphologies and original physical and mechanical properties, which may lead to valuable technological applications.

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