Innovative procedures based on advanced mesoscale simulation techniques for functional polymers in 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 nanoscopic morphologies and original physical and mechanical properties, which have led to valuable technological applications.
In this work we have applied the mesoscale simulation approach to study the equilibrium morphology of linear (AmBn) 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. In particular, starting from atomistic-based simulations we derived a procedure to:

1. Describe in appropriate fashion the polymer chains in terms of the relevant Gaussian models;
2. Determine the appropriate Flory-Huggins interaction parameters;
3. Determine the bead self-diffusion coefficients, necessary to convert the mesoscopic dimensionless time step to an effective time scale.