Upgrading polymeric materials from post industrial rejects: a multiscale simulation approach

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Industrial scraps cannot be reused in an advantageous way, mainly because of their degradation. When possible, rejects are added to the virgin material for new molding, although the amount of recycled polymer cannot exceed 15% of moldable material to obtain good final performances. The remaining amount of scraps then follows two different routes: i) employment in very poor applications, and ii) land filling. For this reason, post industrial rejects constitute a major problem both from the standpoint of the European legislation and policy, and from the economic side where enterprises are concerned.
In this work we have applied a multiscale simulation approach to study the equilibrium morphology of blends consisting of both virgin and recycled polymers of special interest in the automotive industry. The main goal was the definition of the possible causes leading to incompatibility between virgin and non-virgin materials. 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.
The results from the multiscale modeling will be discussed in details.