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Structure and properties of isotactic polypropylene modified with siloxane-silsesquioxane resin and sorbitol derivatives

Abstract

This study details new polypropylene-based materials containing a siloxane-silsesquioxane resin functionalized with phenyl groups and two types of sorbitol derivatives, namely 1,3:2,4-bis(3,4-dimethylbenzylidene)sorbitol, Millad 3988 (DMDBS) and 1,2,3-tridesoxy-4,6:5,7-bis-O-[(4-propylphenyl)methylene]nonitol sorbitol, Millad NX8000 (NX8000). The aim is to investigate the influence of such additives on the crystallization behavior and morphology, as well as on thermal and mechanical properties of isotactic polypropylene nucleated with the modified sorbitols, as a function of the molecular characteristics of both the sorbitol derivative and phenyl siloxane-silsesquioxane resin. The goal is to develop an iPP-based formulation whose crystallization kinetics is tailored for extrusion processing, in order to optimize material properties without enhancement of production costs.

Composites based on isotactic polypropylene (iPP) modified with a sorbitol derivative (NX8000) and siloxane-silsesquioxane resin containing reactive phenyl groups (SiOPh) were prepared by melt extrusion. The addition of sorbitol fastens crystallization kinetics of iPP and leads to higher transparency of iPP films. Upon the incorporation of siloxane-silsesquioxane resin, no further effect on iPP crystallization kinetics is evidenced by calorimetry, optical microscopy, and X-ray diffraction analysis. Transparency of iPP-based composites is improved upon the addition of sorbitol, but decreased when SiOPh is added to the formulation. The composites are also stiffer, compared to neat polypropylene with a decreased elongation at break and increased Young's modulus values, with increasing amounts of fillers. The effect of the siloxane-silsesquioxane resin on properties of iPP/NX8000/SiOPh composites was explained taking into account compatibility of the components and morphology of the composites. Compared to NX8000, DMDSB has varied functionalization of the hydroxyl rings, which may affect interaction with SiOPh.

Molecular adducts originating from the synergistic interactions of siloxane-silsesquioxane resin (SiOPh) and Millad 3988 (DMDBS), influence crystallization kinetics of isotactic polypropylene (iPP), as well as its spherulitic morphology, transparency and mechanical properties. DMDBS is a commonly used clarifying agent for a variety of iPP grades. However, its disadvantage is that when added into iPP during extrusion, it allows only low draw ratios, because it increases crystallization temperature of iPP. Addition of SiOPh allows for control of the nucleation efficiency of the sorbitol derivative and adjust crystallization rate of iPP, to attain transparent formulations suitable for extrusion processes.

All presented iPP-based compounds were produced by co-rotating twin screw extrusion and further analyzed by differential scanning calorimetry, wide-angle X-ray diffraction, scanning electron microscopy and Fourier transform infrared spectroscopy. Moreover, rheological, haze and static tensile measurements were conducted to determine the influence of composition on material properties. It was found that the best combination of properties is achieved when 1 wt% of SiOPh and 0.25 wt% DMDBS are added to iPP. This formulation can significantly change the crystallization behavior of iPP to be tailored for production of highly oriented and transparent products.

Moreover, iPP composites modified with NX8000 sorbitol derivative and siloxane-silsesquioxane resin (SiOPh) containing maleated polypropylene (MAPP) as compatibilizer were prepared in order to favor interaction between fillers. Calorimetric investigations revealed no influence of SiOPh and a slight effect of MAPP addition on the crystallization kinetics of polypropylene. Additionally, the introduction of MAPP into the iPP+NX8000+SiOPh composites increased plastic properties of the samples. All the above was attributed to the compatibilizing effect of MAPP which improved interfacial adhesion between iPP, NX8000 and SiOPh. This phenomenon was also confirmed by the SEM images illustrating more homogenous distribution of the filler in the compatibilized samples.

Based on previous research it was proposed to produce iPP-based composites containing the sorbitol derivative and compatibilizer only as its functional groups may in principle suppress fibrillation of sorbitol derivative upon cooling of polypropylene and result in a control of crystallization kinetics in iPP-based composites during production. Moreover, polypropylene-*graft*-maleic anhydride (MAPP) is commercially available and relatively cheap in use. The addition of MAPP strongly influences crystallization of isotactic polypropylene (iPP) as evidenced via differential scanning calorimetry measurements. Changes in rheological properties and transparency were also examined and turned out to be improved by the proposed modification.