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Ton That, Minh Tan; Li, Jianming

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The Role of Interface and Crystallization in Fabrication of Clay-Polyolefin (PO) Nanocomposites: Computation and Reality

Minh-Tan TON-THAT and Jianming LI
National Research Council Canada

The effect of interfacial interaction between the nano-particles and the polymer matrix plays a determined role in the fabrication of polymer nanocomposites. For layered structure nano-particles like nanoclays, depending on the level of such interaction, the dispersion of the nanoclays can vary from micro-size (micro-composite) to nano-size (nano-composite, both intercalated and exfoliated structure). In addition, in the absence of good interface in semi-crystalline polymer as in POs, crystallization makes the dispersion process becomes more complicated because the polymer crystals have a tendency to reject the nanoparticles to enter to their structure.

This article focuses on the effect of the interaction between the nanoclay and polypropylene matrix on the dispersion, the crystallization and thus the performance of the obtained nanocomposites. Both computation (molecular modeling) and experiments have been conducted on various systems (with different modifications of clay surface and polymer matrix) in order to get a better understanding about this complex issue. The results have provided different useful highlights for the fabrication of polyolefin nanocomposites.