ABSTRACT

Model Prediction and Morphological Investigation in Polymer Clay Nanocomposites

Name: Debashis Sikdar, Dr. Dinesh R. Katti, Dr. Kalpana Katti

Department of Civil Engineering

North Dakota State University

1410 North 14th Avenue

Fargo, North Dakota-58105. USA

E-mail: Dinesh.Katti@ndsu.edu

Phone: 701-231-7245; Fax: 701-231-6185

Polymer-clay nanocomposites (PCN) show enhanced mechanical, thermal and other physical properties in comparison to pure polymer. However, the mechanism behind the property-augmentation in PCN over the pristine polymer is not well understood. Nanostructure and interactions among different constituents of PCN may be key reason for the improvement of physical properties in PCNs. Molecular dynamics (MD) is an excellent tool to study the structure, dynamics and interactions for composite materials at the nanometer length scale. However the accuracy of results obtained from MD depends largely on the accuracy of the model used in simulation. In this study, the model of the intercalated PCN structure have been constructed based on the result of the combination of experimental observation (X-ray diffraction) and conventional molecular modeling to obtain a more representative model of intercalated PCN. The interactions among different constituents of PCN and morphological aspects (orientation of organic modifiers, proportion of polymer-organic modifier mixing etc) are also discussed.