Contribution ID: **198** Type: **Poster**

A Molecular Dynamics Study of the Interfacial Regions Between Polymer and Carbon-Based Nanoparticle Fillers

Thursday, 25 May 2017 17:45 (15 minutes)

A novel polymer composite material with high stiffness and thermal endurance can be designed by optimizing the filler content. We investigated the microscopic properties of the interfacial regions between cis-polyisoprene (natural rubber) and carbon-based fillers, e.g. fullerenes by using classical molecular dynamics (MD) simulations. The microscopic analysis shows that increasing filler concentration results in the growing of the regions containing ordered cis-PI chain at the interfacial areas. In this work, we analysed the order parameter, e.g. local density and orientation at the interfacial and confined regions which correspond to changes in mechanical and thermal properties. These results could provide the information for the parameterisation of the coarse-grained or the continuum models.

Primary authors: Dr KHUNTAWEE, Wasinee (Computational Biomodelling Laboratory for Agricultural Science and Technology (CBLAST), Department of Physics, Kasetsart University.); Dr SUTTHIBUTPONG, Thana (Theoretical and Computational Science (TaCS) Center); Dr WONG-EKKABUT, Jirasak

Co-authors: Prof. KARTTUNEN, Mikko (Department of Mathematics and Computer Science & Institute for Complex Molecular Systems, Eindhoven University of Technology, MetaForum, 5600 MB Eindhoven, The Netherlands); Mr KERDKAEN, Nathanon (Theoretical and Computational Physics (TCP) Group, Department of Physics, KMUTT)

Presenter: Dr SUTTHIBUTPONG, Thana (Theoretical and Computational Science (TaCS) Center)

Session Classification: Poster Presentation II

Track Classification: Material Physics and Functional Materials