Study of physical properties of thermoplastic elastomer in molecular scale

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Abstract

Thermoplastic elastomer SIS(poly**S**tyrene-poly**I**soprene-poly**S**tyrene:triblock copolymer) is known as adhesive materials, where S works as physical cross link point due to the glass state of polymer, and I is rubber polymer in normal temperature. Recently, SIS has been modified as a polymer alloy which is the blend of symmetric SIS and asymmetric SIS' (Chain length of S < that of S') and a special SIS has been developed. The special SIS earns good biocompatible properties for film material and the use as elastic films for disposable diapers is started. The market expansion of the special SIS as high-performance film materials is expected. However, the special SIS has complicated morphology caused by the phase separation between S and I in nano-scale level. It has not been cleared the relation between such complicated morphology and physical properties. Thus, we investigated the nano-structure change of the special SIS in extension mode by using the coarse-grained large scale molecular dynamics simulation on the Earth Simulator (ES) and found characteristic polymer chains anchored at large S domains and extended through I domains. We estimated that such chain extensions cause high strain in extension mode and play a good role for the physical properties of film. In addition, we prepared the initial phase separated structure by the SCF method of polymer and this study becomes the proof example of the large and multi-scale simulation of polymer material with phase separated structure.

Keywords: large-scale simulation, SCF method of polymer, self-organization, coarse-grained molecular dynamics, elastomer materials