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Strasbourg, France

GRANT BASED PHD PROJECT

(position to be opened in 2007)

Field of research: molecular modeling, physicochemistry of polymers
Title : MOLECULAR MODELING OF THE DIFFUSION OF MOLECULES WITH INTERMEDIATE MOLECULAR WEIGHT IN POLYOLEFINS.

Context

Because the diffusion modifies the reactivity of the additives (e.g. antioxidant) and their desorption ability, the understanding and the control of the molecular processes of diffusion are particularly significant for the optimization of the lifetime and the functions of use of plastic materials. Nowadays, there is no general model to predict the diffusion coefficients of native or degraded molecules of additive-type (i.e. with molar weights ranged between 100 and 1000 $g \cdot mol^{-1}$) in entangled polymers. The project aims at studying, at a molecular scale, the cooperative motions of the polymer-additive system, which are responsible for the translation and consequently from the random walk of the additive within the matrix.
This work is part of a collaborative and interdisciplinary research program of CNRS named "Composite Polymer Ageing" (acronym COPOLA), to which participate 14 research units of CNRS, CEA and INRA and of significant companies (EDF, Nexans, Laborelec). The subject suggested is based on collaboration between a team of the Institute Charles Sadron specialized in the theory and the simulation of polymers and a team of the National Institute for Agronomic Research attached to the control of the risk of contamination of food by packaging material substances.

Description

With the difference of the diffusion of gases, the translation or the reorientation of medium-sized molecules such as additives requires a succession of cooperative motions of the polymer segments. The amplitude of the fluctuations necessary for their translation strongly depends on the size, the rigidity and the shape of the diffusing probe. Molecular dynamics confirmed the very significant effects of the confinement and trapping of these molecules. These entropic effects are particularly significant for the molecules presenting many symmetry planes. They lead to many changes of conformations or reorientations, which are not accompanied by a translation by the center of mass on the long term. In order to assess these effects on more significant time scales (beyond a hundred of nanoseconds), coarse-grained models of additive prototypes and polymers will be set up and studied. Some identified results (motion type, activation energy) will be compared with experimental results derived from Electron Spin Resonance (ESR) and confocal microscopy experiments performed on paramagnetic probes and fluorescent probes respectively.

Methods: semi empirical molecular dynamics, statistical physics, knowledge in programming will be appreciated.

Applicants should ideally have a MS degree related to the following disciplines: Condensed matter physics, *Chemistry and Physicochemistry of matter/polymers/macromolecules, Theoretical and/or computational Chemistry, Polymers, Spectroscopy and Structural Physicochemistry.*

The application form is available at:
http://www.sg.cnrs.fr/drh/emploi-nonperm/pdf/dossier-bdi-06.pdf

Project supervisor: Dr Hendrik Meyer (hmeyer@ics.u-strasbg.fr)
Most of the work will be carried out at the Charles Sadron Institute (Strasbourg, France).

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