Studying the Structural Properties of Cellulose Acetate by Molecular Simulation

Anthony Bocahut*[1] and Karim Mazeau[2]

[1]Solvay – Solvay (France) – France
[2]CERMAV – CNRS : UPR5301 – France

Résumé

Cellulose acetate (CA) is a common derivative of cellulose with many applications. Most of the industrially relevant CA possess a complex chemical structure, are highly heterogeneous and have a dominant amorphous organization. This polymer is particularly difficult to characterize by experiments.
In this work we study the structure and thermal properties of amorphous CA using molecular modeling. We consider five degrees of substitution (DS) of the chains: 0; 1.5; 2; 2.5; 3, the distribution of the acetate moieties is implemented according to experimental data. The equilibration of the periodic models is performed using molecular dynamics with the OPLS-AA force field. In order to provide an estimate of the first order phase transition temperature, assimilated to the glass transition temperature, we carry out a simulated annealing protocol mimicking calorimetric experiment. The DS dependence of the transition temperature is similar to the one described experimentally.

Analyzing some structural characteristics of the polymer like the number of hydrogen bonds, the average distance between chains, or the Φ/Ψ torsional space explored by the glycosidic bonds, gives evidence that a delicate balance between hydrogen bonding and acetate dipole interactions governs the thermo-mechanical behavior of the material.

Mots-Clés: Molecular Dynamics, Cellulose Acetate

*Intervenant