Supplementary Information

"Development of force field parameters for molecular simulation of polylactide"

by J.H. McAliley and D.A. Bruce

Introduction

The following is a list of files included in the .zip archive of supplementary information to the manuscript referenced above. Files are either plain (ASCII) text files, or in Adobe .pdf format. For more information on files that are specific to the GROMACS simulation program, please see the GROMACS user manual which can be downloaded at www.gromacs.org .

PDF Documents

BondedParameters.pdf: Document describing details of adjusting bond stretching and angle bending parameters in PLAFF2 and PLAFF3.

PLAFF3Parameters.pdf: Document listing the PLAFF3 potential and parameter set.

GROMACS Files

Force Field Parameters File

PLAFF3.itp: GROMACS include file for PLAFF3. This file is referenced in the GROMACS topology files and contains the force field parameters.

Topology Files for Amorphous PLA

3x500LA_2xLactide.top: Example of a GROMACS topology file using PLAFF3. The system box contains three PLA 500mers and two lactide molecules.

500LA.itp: The GROMACS topology include file defining a PLA 500mer.

Lactide.itp: The GROMACS topology include file defining a lactide molecule.

Equilibrated Conformations for Amorphous PLA

3x500LA_2xLactide_conf1.gro: Sample GROMACS conformation file for amorphous PLA, equilibrated using NPT-REMD as described in the manuscript.

3x500LA_2xLactide_conf2.gro: Sample GROMACS conformation file for amorphous PLA, equilibrated using NPT-REMD as described in the manuscript.

3x500LA_2xLactide_conf3.gro: Sample GROMACS conformation file for amorphous PLA, equilibrated using NPT-REMD as described in the manuscript.

3x500LA_2xLactide_conf4.gro: Sample GROMACS conformation file for amorphous PLA, equilibrated using NPT-REMD as described in the manuscript.

Topology Files for Crystalline PLA

32x50LA_crystal.top: Example topology file for simulating the α-form of the PLA crystal. The system is made up of chains that are 50 repeat units long, and extend infinitely in the z-direction (the GROMACS option 'pbc = full' must be specified in the .mdp file).

50LA_crystal.itp: The GROMACS topology include file for a PLA 50mer, with end repeat units bonded together as appropriate for fully periodic boundary conditions.

Conformation of Crystalline PLA

32x50LA_crystal.gro: Conformation of crystalline PLA as described by Sasaki and Asakura (*Macromolecules* **2003**, *36* (22), 8385-8390.)