Coarse-graining polymers with the MARTINI force-field: polystyrene as a benchmark case

Electronic Supplementary Information

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Equilibration of PS melts

The equilibration of PS melts has been performed by letting the system evolve at constant temperature (500 K) and pressure (1 atm) till the chains diffused over a distance comparable to their radius of gyration. As shown in Fig.1, the time required for this condition to be satisfied is $<$ 100 ns for PS10, 100 ns for PS30, 1 μs for PS60 and 3 μs for PS100.

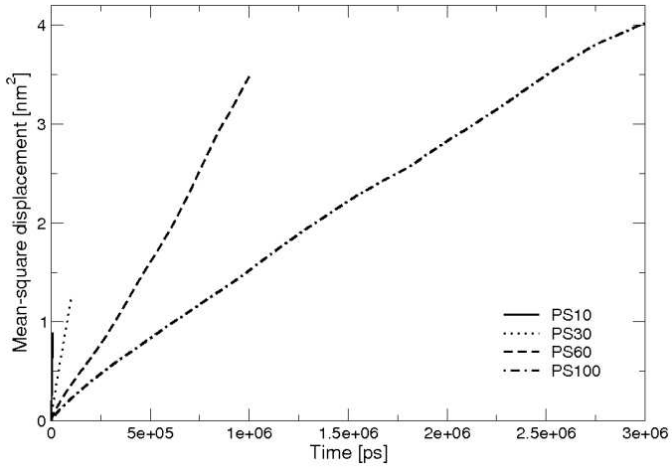

Figure 1 Mean-square displacements (msd) of the center of mass of the chains during the equilibration of PS10, PS30, PS60 and PS100 melts (data refer to A-mapping, which has a lower diffusion constant than B-mapping). In all cases, the total duration of the simulation allowed for a reliable sampling of the msd in the time window shown here.

Mapping of bonded interactions - atomistic bond and angles distributions

Figure 2 shows the distributions of bond and angle degrees of freedom included in A- and B- mapping. The original atomistic trajectory has been converted into the trajectory of the center of mass of the groups of atoms that, in the CG model, are described by a single bead. From the center of mass trajectory, the distributions shown in Figure 2 (thick lines) have been obtained. CG parameters (equilibrium values and force constants of harmonic bonds and angles) were adjusted in order to get the best overlapping between CG and atomistic distributions.

Radial distribution functions

Figure 3 shows the RDFs obtained from the atomistic simulations of a melt of PS30 and those obtained by the CG simulation of a melt of PS30 (A-mapping). Atomistic RDFs have been obtained from the trajectory of the center of mass of the atoms representing the A-mapping beads.

References

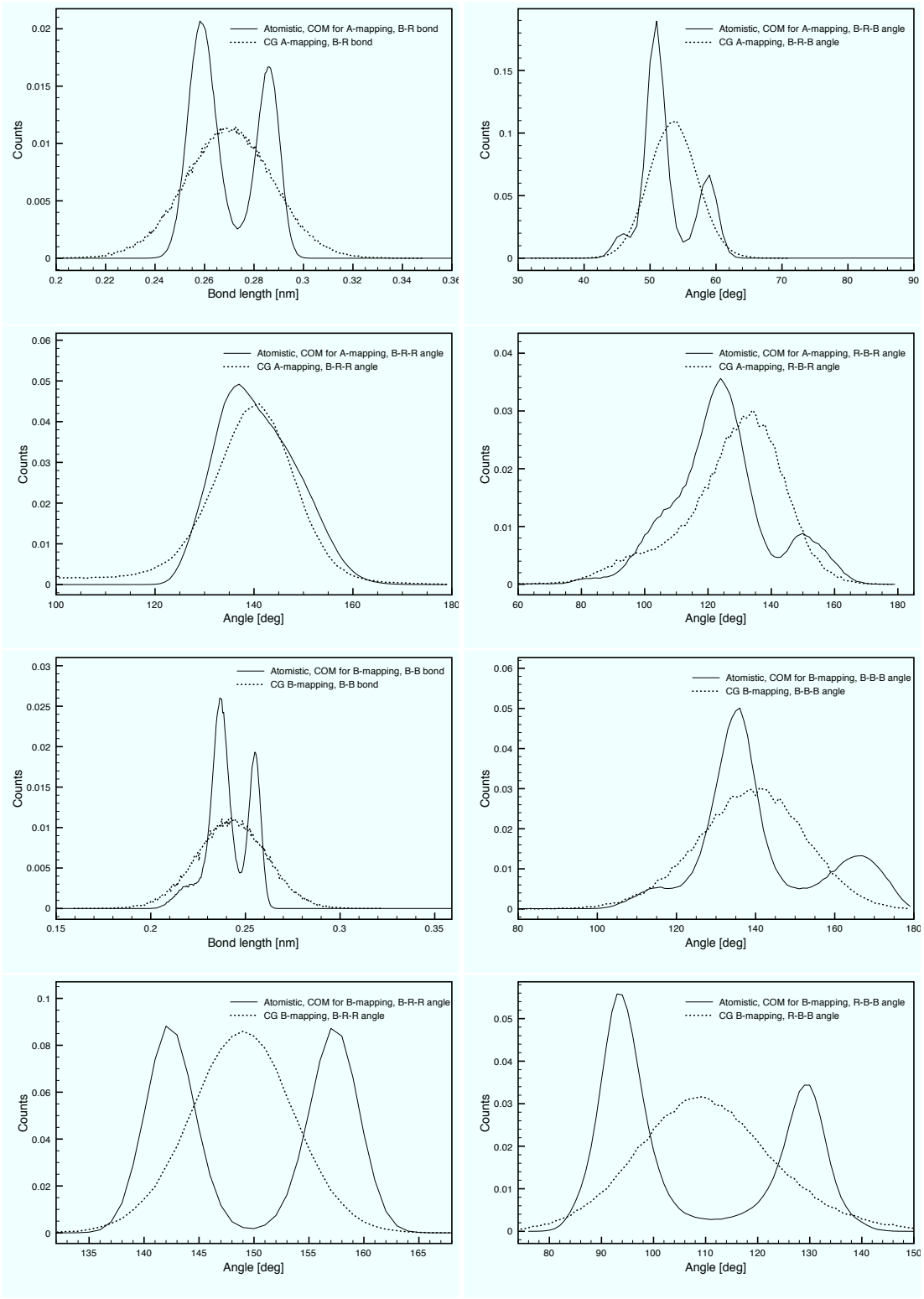

Figure 2 Distributions of the bonded degrees of freedom included in A- and B-mappings, as obtained from atomistic simulations and from the optimized sets of CG parameters.

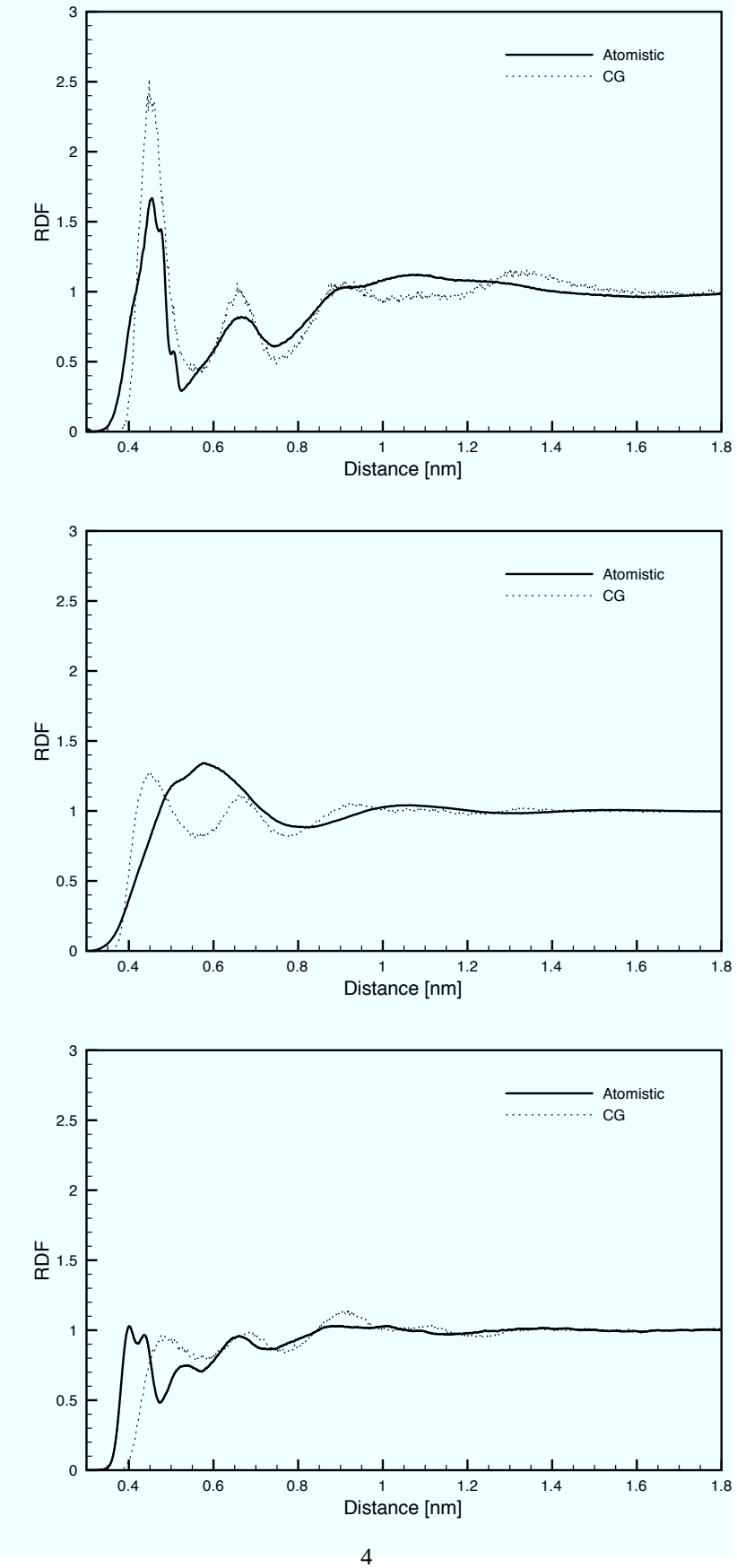

Figure 3 From top to bottom: atomistic and CG (A-mapping) RDFs for B-B, R-R and B-R beads, respectively.