

Coarse grain modeling of carbohydrates

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Carbohydrates are principal components of many natural products, and form structures ranging from monosaccharides (24 atoms, molecular weight 180) to complex polysaccharides composed of thousands of these units. In many relevant cases –as glycogen, cellulose and their hydrolysis products- the polymers are composed of only one subunit (monosaccharide) type, the complexity of the natural product coming from the length, connectivity and branching of these chains. Fig. 1 shows some molecules formed by only α -glucose units.

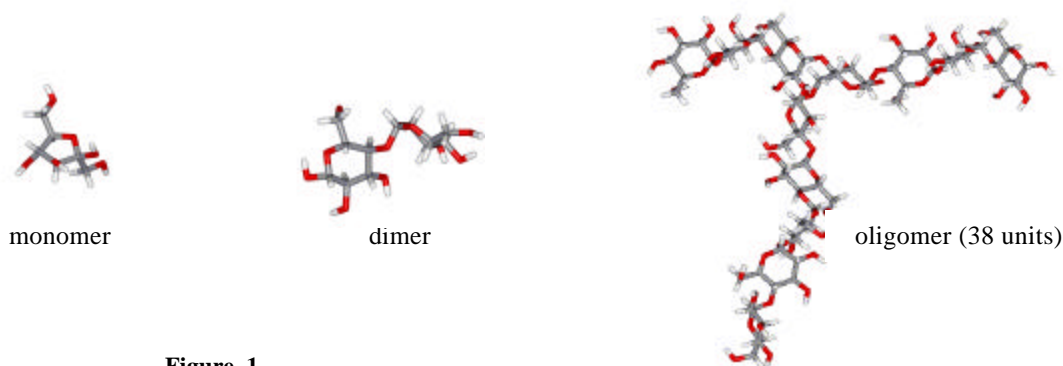


Figure 1.

The simulation of mixtures of saccharides with different degrees of polymerization is a challenge. Not only the simulation of large numbers of atoms must be considered but also very different time scales. For example, the vibrational modes of any unit are much faster than the librations of long chains. A fully atomistic simulation –considering all the internal degrees of freedom of the molecules- of such a system, will require more than a month to perform a 200 ps simulation of 2500 atoms in Cerius2 with an SGI R10000 processor.

These limitations can be lifted if one adopts simplified models that speed up the calculations yet maintain the essential features of the atomistic representation. The most simplified model corresponds to the replacement of any monosaccharide unit by one particle, a *bead*. Bead-bead interactions were modeled via a Morse potential and their three parameters optimized through simulated annealing. The training set was obtained from fully atomistic simulations of crystalline structures with different symmetries in a wide compression range.

Considering the significant departure from sphericity of a typical monosaccharide, as the α -glucose molecule, we also considered a two-bead model for each monosaccharide. Figure 2 depicts a “front” and “side” view of the α -glucose and some schematic representation of the one and two bead model.

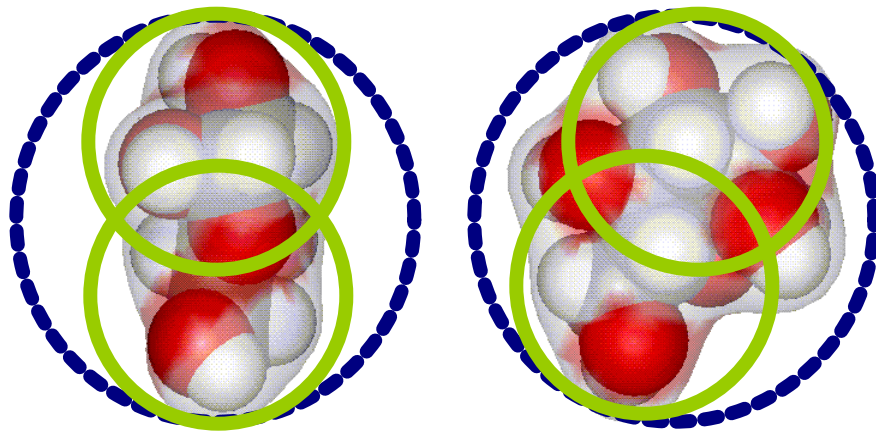


Figure 2.

We obtained van der Waals parameters for the beads representing the α -glucose molecules. The calculated stresses and cohesive energies, and relaxed structural parameters for the different α -glucose crystals as well as the amorphous phase are compared with the results obtained from the atomistic force field.