Measurements of forces between cellulose fibril surfaces – A molecular dynamics study

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Molecular models of non ionic Iβ cellulose fibril surfaces (CFS) were developed to study the modes of interaction and force needed to pull out surfaces in the pristine state or with non-covalently surface modification with two types of polyelectrolyte derivatives, sodium carboxymethyl cellulose (CMC-ONa) and a cationic polyacrylamide (CPAM). All calculations were performed using the LAMMPS simulation code [1].

The pair correlation distribution function g(r) or RDF was studied to establish the modes of interaction of the polyelectrolyte molecules towards the non ionic CFS. Electrostatic interactions coupled with hydrogen bonding were developed in the adsorption of either CMC-ONa or CPAM. Experimental studies found similar adsorption interactions in other hydroxyl containing substrates [2].

The fibril bond strength was calculated from pull out simulations using steered molecular dynamics (SMD). The neat cellulose fibrils exhibited a value of around 130 MPa in bond strength, in the order of similar studies found in literature [3], and this result was compared to those of modified CFS models to analyze the effect of surface modification with polyelectrolytes. The measured bond strength between fibrils was directly proportional to the product of the relative bonded area (RBA) and the specific number of total interactions, here defined as the strength factor. The studied derivative of CMC-ONa exhibited higher strength of adhesion towards cellulose fibrils than the CPAM molecules, although the modification of fibrils with CPAM produced higher increments of RBA that finally produced higher increments of the bond strength between fibrils for a given surfactant concentration.

REFERENCES

[1] S. Plimpton, «Fast Parallel Algorithms for Short-Range Molecular Dynamics», J. Comput. Phys., vol. 117, n.o 1, pp. 1-19, mar. 1995.
[2] J. Wang y P. Somasundaran, «Adsorption and conformation of carboxymethyl cellulose at solid–liquid interfaces using spectroscopic, AFM and allied techniques», J. Colloid Interface Sci., vol. 291, n.o 1, pp. 75-83, nov. 2005.
[3] Z. Zhao, V. H. Crespi, J. D. Kubicki, D. J. Cosgrove, y L. Zhong, «Molecular dynamics simulation study of xyloglucan adsorption on cellulose surfaces: effects of surface hydrophobicity and side-chain variation», Cellulose, vol. 21, n.o 2, pp. 1025-1039, abr. 2014.