Computer Simulations of Structural and Mechanical Properties of Cellulose Allomorphs

By

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Declaration

I declare that the dissertation hereby submitted to the University of Limpopo for the degree of Master of Science has not been previously submitted by me for a degree at this or any other University, and that the work herein is originally my own.

Mashapa Matete Gilbert

Signed 

Acknowledgements

All praise and thanks is due to GOD, the one, the only, and the indivisible creator and the sustainer of the world. To HIM we belong and to HIM we shall return. I wish to thank HIM for all that HE has gifted me with, although, HE can never be praised or thanked enough.

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Dedication

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Abstract

Cellulose is regarded as the most abundant polymer in nature and the first on which X-ray investigations had been performed, a year after the discovery of diffraction of X-rays on crystalline materials in 1912. It is one of the most abundant and important polymers on the planet. It comprises of four allomorphs, cellulose Iβ, II, III and IV_1 and IV_2 of which Iβ and II are the most stable and industrially important. Cellulose I is the native form of cellulose.

Molecular dynamics (MD) simulations have been carried out to study the structural and mechanical properties of cellulose, cellulose Iβ, II, III and IV_1 and IV_2 bulk systems. Simulations were carried out using Polymer Consistence Force Field (PCFF) and Compass force field in conjunction with the Discover simulation program at various temperatures. We used molecular dynamics simulation to obtain a better insight about temperature dependence of cellulose. Further investigations on mechanical properties of this material at various temperatures were carried out.

Using pair correlation functions g(r) or radial distribution functions (rdf's) we were able to investigate phase transitions wherein as the temperature was increased we observed peak broadening. These enabled us to study the similarities between the structures investigated. Also studied was water uptake in celluloses by way of introducing water at different concentrations. Analysis of lattice parameters compared reasonably well with the experimental. Lattice parameters were calculated using PCFF and they compared well with results found using Compass force field. Calculation of temperature and pressure dependence on bulk systems has

been done and it was noted that as the pressure increases the lattice parameters decrease.