Interactions between cellulose chains and waters

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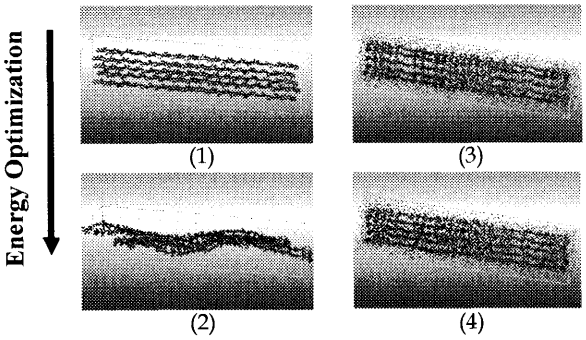
Most of the structural studies of cellulose have been based on the crystallographic data obtained by diffraction measurements under the waterfree dried environment. So the highly crystalline state of cellulose has been obtained from the measurements. Then, the cellulosics were interpreted to be stiff and rigid materials. However, cellulose molecules originally exist with waters in biosystem. The dried state cellulose must be a kind of artificial material. Is the conventional argument for cellulose until now adequate to discuss the physical properties of cellulosic material? Then, we investigated the characteristics of cellulose in aqueous conditions by molecular simulation technique.

The threedimensional features of cellulosic aggregates in aqueous conditions were simulated as a model of cellulose in biosystem ((3) and (4) in the Figure) compared with those in nonaqueous state ((1) and (2) in the Figure). Cellulose chains in aqueous environment were found to have no direct hydrogen bondings between the chains. Most of hydrogen bondings in the cellulosic aggregates were formed through waters in aqueous state. This situation was not changed after the optimization process. The new hydrogen bonding between cellulose chains directly was not formed in aqueous conditions even after the optimization process. This meant that waters were preventing to form hydrogen bondings directly between cellulose chains. This feature showed the low crystallinity of cellulose in green conditions. The low crystallinity of cellulose was observed in fact from the plant specimens in green conditions. On the other hand, the cellulose chains in nonaqueous environment approached each other very quickly and formed the hydrogen bondings directly between them. This was a tight aggregate like a crystal.



Interactions between cellulose chains and waters. (1) and (2) showed in non-aqueous state. (3) and (4) showed in aqueous state. (1) and (3) showed pre-optimization state. (2) and (4) showed after-optimization state.

The highly crystalline materials are stiff and strong, but a little bit brittle. On the contrary, low crystalline materials are a little bit flexible. Above is the reason why the green tree is more resilient than the dried wood.

REFERENCES

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