Materials Science

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Molecular aggregation of xyloglucan and iodine and/or iodide ions

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Introduction

Xyloglucan exists in plant cell walls and plays a role of binding plant cells by the physical association with cellulose microfibriles on the walls. It also exists in some seeds of trees growing in the tropical zone. Tamarind seed xyloglucan, which is stored in seeds of *Tamarindus indica*, is used as food additives such as a gelling agent, a stabilizer, a starch modifier, etc, in Japan. Xyloglucan has a cellulose backbone with branched (1→6)-α-xylose or (1→2)-β-galactoxylose as a side chain. Although cellulose is insoluble in water because the chains are crystallized with cooperative hydrogen bonds, but xyloglucan is a water-soluble by suppressing the cellulose-like chain aggregation due to steric hindrance of the side chains. The addition of iodine to xyloglucan in aqueous solution causes color formation. We investigated a novel thermo-reversible gelation system by mixing xyloglucan with an iodine solution. In this study the aggregation of xyloglucan chains with iodine was observed by means of small angle X-ray scattering (SAXS).

Experimental

A xylogluncan sample was provided by Dainippon Pharmaceutical Co., Ltd. It was purified with an alcohol precipitation method before preparation of samples for measurement. SAXS experiments were carried out with SAXES optics installed at BL-10C in Photon Factory.

Results and Discussion

Xyloglucan is colorless and transparent in aqueous solutions. However a xyloglucan solution developed a blue color and took place gelation upon addition of an iodine solution prepared with I_2 and KI. Figure 1 shows the cross-sectional Gunier plots for SAXS [*ln(qI(q))* vs q^2, *I(q)* is scattering intensity and *q* is the magnitude of scattering angle) from xyloglucan solution and the colored gel with iodine. Linear profiles were obtained for the xyloglucan sol and gel, suggesting that chain the conformation at each states were rod-like. The size of cross-section at gel state corresponds to the two xyloglucan chains associate in parallel and we can speculate that they incorporate iodine/iodide ions. As shows in Figure 2, molecular modelling and dynamics simulation was performed to examine the proposed complex model.

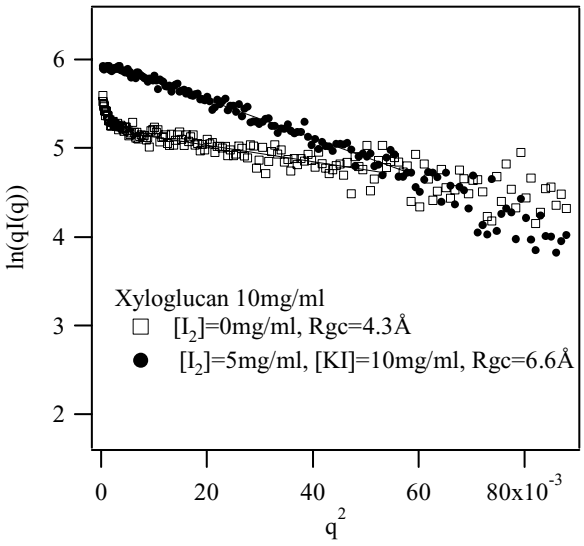

Figure 1. Cross-sectional Guinier plots for SAXS from xyloglucan aqueous solution without and with iodine solution.

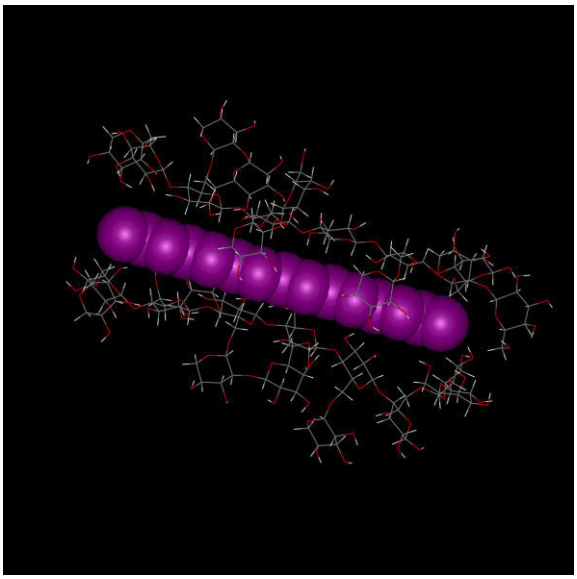

Figure 2. The molecular model for complexes of xyloglucan and iodine and/or iodide ions.