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Title	Mechanical properties of topological gel. - Molecular dynamics simulation -
Researchers	Fumio Sawa, Takeshi Aoyagi and Masao Doi
Purpose of this study	Topological gel is a new type of a gel which has cross-links that can slide along the backbone of the polymer chain composing the gel network. We have carried out molecular dynamics simulations of topological gel to study the effect of sliding cross-links on the mechanical properties.
System (Material)	This system consists of linear polymers end-capped by large molecules and connected by cyclic molecules.
Program	COGNAC ver.3.08
Method & Some important input parameters	(Method) COGNAC ver.3.08 was used for current simulation, however, initial coordinates and topology of system was made by a Python script. And also, some of analysis was done by hand made script(Python). (Inputs) System: Number of linear polymers and cyclic molecules. Potentials: Bonding (bond and angle) and Nonbonding(Lennard-Jones and Lennard-Jones-Gay-Berne) potential was used. Simulation: Temperature, density and other parameters.
Advance & Problem	(Advance) By COGNAC simulation, it was clarified that topological gel has characteristic mechanical properties. Moreover, by comparison with chemical gel, topological gel is thought to have higher entropical elasticity than chemical gel. (Problem) The examined rate of elongation is much higher than that of experimental condition. The ratio of the elongation rate and velocity of the cyclic molecules sliding on each linear polymer is thought to be the main factor of elasticity. However, comparison between simulation results and experiments can be possible with taking account of its ratio.
References	[Manuscript] Submitted/Accepted(/) [Presentation at conferences (Meetings)] 39'th Kobunshi-Zairyou-Jiyuu-Toronkai (2001) 50'th Symposium on Macromolecules (2001)
KeyWords (in English)	molecular dynamics, topological gel, mechanical properties

Results (Remarks)

<Results>

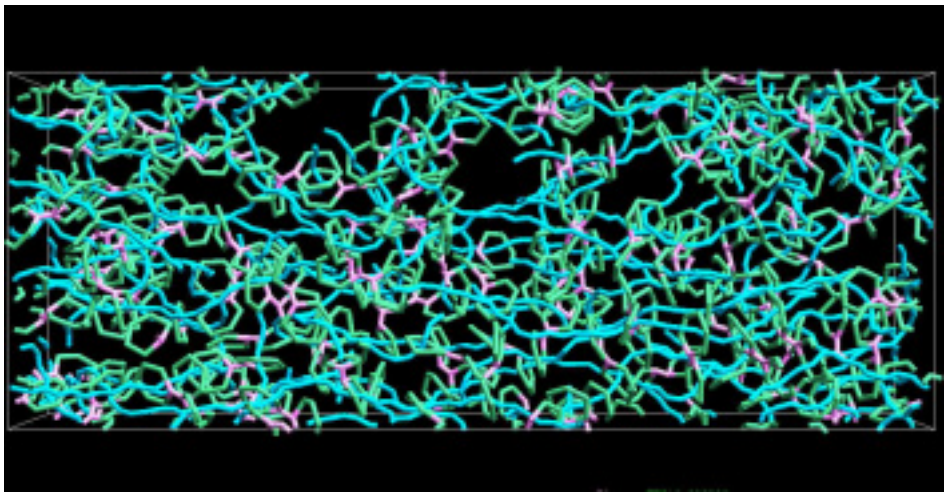

Fig.1

Fig.1)
A snapshot of the system. Linear polymers are colored blue, and cyclic molecules are green. Red objects are cross-links.

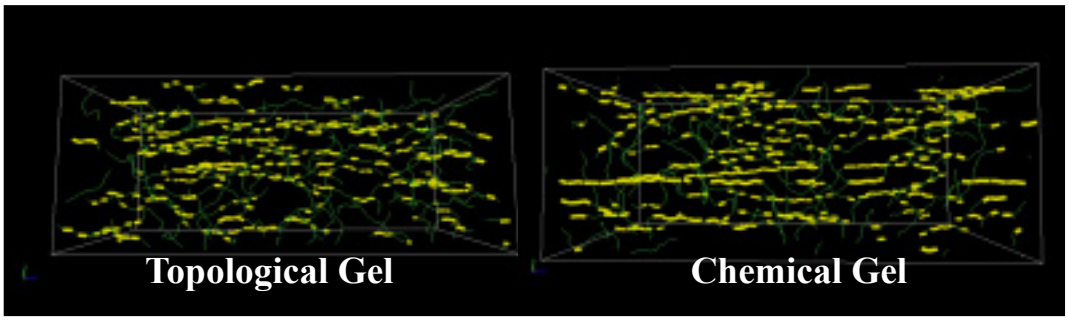

Fig.2

Fig.2)
Snapshots of gels(left: topological gel, right: chemical gel) at the conditions at elongation of 1.75. The elongational direction is horizontal. Chemical gel has some specific polymers aligning to elongation.

Fig.3)
Stress(σ) versus elongation(λ).
(cd7:topological gel,
cd7c: chemical gel)
Topological gel seems to have higher capacity of elongation more than chemical gel.

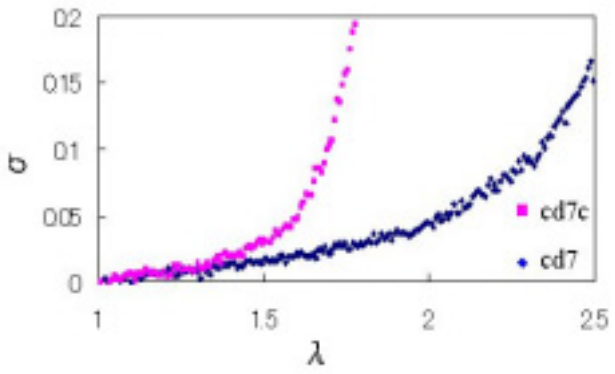

Fig.3