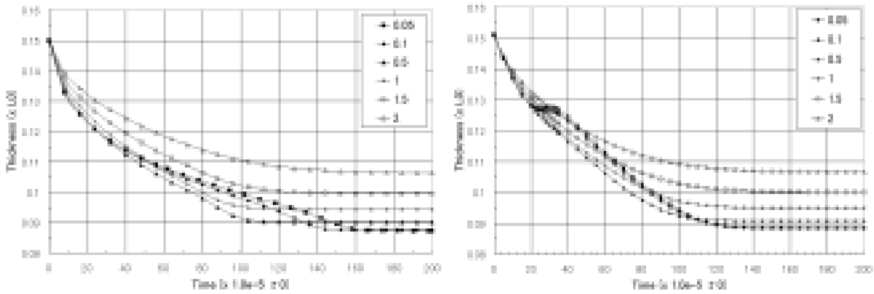
No. EAR2-018-01 First registration:2000/ 9/12 New:2000/ 9/12

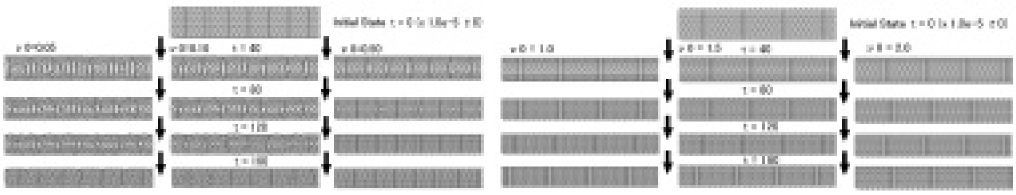
Title	The simulation of the shrinking process of NIPA gels - the stress-diffusion coupling model for dynamics of gels -
Researchers	Tatsuya Yamaue, Takashi Taniguchi, and Masao Doi
Purpose of this study	Many kinds of external stimuli, such as, temperature, pH, photons, ions, electric current (field), e.t.c. , can control the volume of the gel. In the case of volume phase transition, an enormous change in volume can be induced by an infinitesimal change of one of the these stimuli and this is of great importance in its application, as an actuator, sensor, switching device, DDS and so on. The dynamics of the volume-phase transition process of gels has been described by the collective diffusion model of gel networks, which well reproduces the liner phenomena. But, it was found experimentally that the shrinking process is strongly decelerated and stopped transiently in a "plateau period" due to the formation of surface skin. In the end of the "plateau period", various patterns appear and the gels restart to shrink. The collective diffusion model of gel networks can't reproduce these non-liner phenomena, such as surface skin which functions in DDS. Here we have constructed the Stress-Diffusion Coupling Model of gels, in which the general deformation of polymer networks, the continuity of solvent and the coupling between solvent diffusion and network stress are considered, and formulated the simulation scheme for large deformation of gels. Using this model we have simulated the shrinking process of slab NIPA(N-isopropyl-acrylamide) thermo-responsive gels undergoing spinodal decomposition by finite element method with delaunay triangulation in comparison with the collective diffusion model of gel networks.
System (Material)	NIPA(N-isopropyl-acrylamide) Gels [experiments] E.S.Matsuo and T.Tanaka, J.Chem.Phys. **89**, 1695 (1988) A.Suzuki, S.Yoshikawa and G.Bai, J.Chem.Phys. **111**, 360 (1999)
Program	MUFFIN – GELS - , ver1.0
Method & Some important input parameters	(Method) Model1: Stress-diffusion coupling model Model2: Corrective diffusion model of polymer networks (Inputs) Standard NIPA(N-isopropyl-acrylamide) gels with water solvent. polymer volume Fraction in reference state = 0.5 crosslinking number density in reference state = 0.05 - 0.20 Ginzburg-Landau free energy for mixing free energy
Advance & Problem	(Advance) The stress-diffusion coupling model, which can describe the actual solvent diffusion of gels, can reproduce the non-liner phenomena in the volume phase transition process, which related to the constraint phenomena of the solvent diffusion. (Problem) Furthermore, we will start the research of 3D simulation , electric field effects for ionic gels and another simulation scheme of the stress-diffusion coupling model, in which we consider the direct simulation of two fluids model among analysis of the velocity of solvent flow.

References	[Manuscript] Submitted/Accepted(/) T.Y,et.al.,Progress of Theoretical Physics Supplement138(2000),416. T.Y,et.al.,AIP Conference Proceedings 519 (2000), 423. T.Y,et.al.,Transactions Material Research Society of Japan, in Press. [Presentation at conferences (Meetings)] Jul 1999,NATO-ASI, Soft & Fragile matter, Summer Seminar. Oct 1999, 48^{th}. Kobunshi-Toronkai. Oct 1999, ICCP5. Nov 1999, The 3rd. Tohwa University International Conference. Dec 1999, 11^{th}. Material Research Society, Japan. Jan 2000, 11^{th}. Kobunshi-Gels Kenkyu-Toronkai
KeyWords (in English)	NIPA(N-isopropyl-acrylamide) thermo-responsive gels, stress-diffusion coupling model, corrective diffusion of polymer networks, shrinking process, plateau period, surface skin layer, pattern formations, finite element method(FEM), lagrange picture

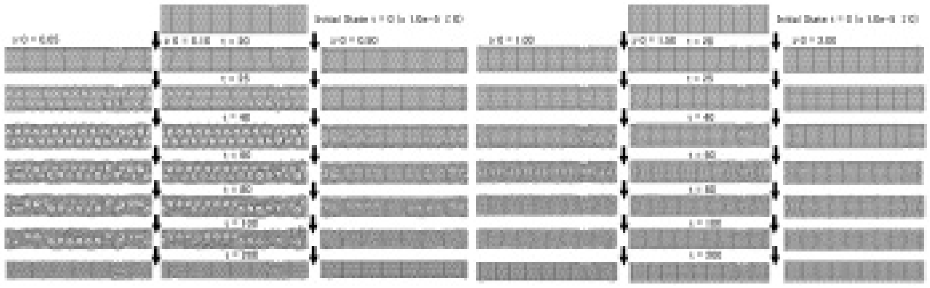
Results (Remarks)



Left : Model2, Right : Model1



Model2, Left : Soft Cases (spinodal region), Right : Hard Cases



Model1, Left : Soft Cases (spinodal region), Right : Hard Cases

By the stress-diffusion coupling model, in the spinodal region, we have reproduced the "plateau period" in the shrinking process of thermo-responsive gels. During the "plateau period", the instability grows and the "bubble-like" inner patterns due to the phase separation appear. After finishing the formation of inner patterns of gels, the gels restart to shrink. Those results nicely reproduce the phenomena which were experimentally observed. In the liner shrinking process, in which gels shrink uniformly, the results of the collective diffusion model of gel networks and the stress-diffusion coupled model equal.