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**Research Article**
**Reversible gel formation of triblock copolymers studied by molecular dynamics simulation**

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**KEYWORDS**

molecular dynamics • percolation transition • simulations • sol-gel transition • triblock copolymers • hydrogels

**ABSTRACT**

Molecular dynamics simulations have been employed to study the formation of a physical (thermoreversible) gel by amphiphilic A-B-A triblock copolymers in aqueous solution. To mimic the structure of the hydrogel-forming polypeptides employed in experiments [W.A. Petka *et al.*, *Science* **281**, 389 (1998)], the end blocks of the polymer chains are modeled as hydrophobic rods representing the  $\alpha$ -helical part of the polypeptides, whereas the central B block is hydrophilic and semiflexible. We have determined structural properties, such as the hydrophobic cluster-size distribution function, the geometric percolation point, and pair correlation functions, and related them to the dynamic properties of the system. Upon a decrease in the temperature, a network structure is formed in which bundles of end blocks act as network junctions. Both at short and medium distances, increased ordering is observed, as characterized by the pair correlation function. Micelle formation and the corresponding onset of geometric percolation induce a strong change in dynamic quantities (e.g., in the diffusion constant and the viscosity) and cause the system to deviate from the Stokes-Einstein relation. The dynamic properties show a temperature dependence that is strongly reminiscent of the

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behavior of glass-forming liquids. The appearance of a plateau in the stress autocorrelation function suggests that the system starts to exhibit a solid-like response to applied stress once the network structure has been formed, although the actual sol-gel transition occurs only at a considerably lower temperature. © 2005 Wiley Periodicals, Inc. J Polym Sci Part B: Polym Phys 43: 959-969, 2005

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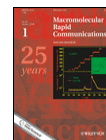


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