Understanding Phase Miscibility of Aqueous PEO Solutions: Molecular Dynamics Study

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Closed-loop (CL) phase miscibility behavior of aqueous poly(ethylene oxide) (PEO) solutions were studied by means of molecular simulations. We have performed a molecular dynamics (MD) simulation of PEO-water solutions. We computed radial distribution functions, number of hydrogen bonds, energy of mixing, mean-squared displacements, and radius of gyration with respect to the temperature. We found that hydrogen bonds between PEO and water decrease more rapidly than those of water and water with increasing temperature, indicating lower critical solution temperature (LCST) behavior. In the heterogeneous phase temperature range, both mixing energy and radius of gyration showed lower values than those of the homogeneous phase, which corresponds well with the CL type miscibility behavior. CL phase miscibility of PEO-water solutions is understood successfully by MD study.