Detailed analysis of inhomogeneous cross-linked structure model of phenolic resins cooperated with SPring-8 and J-PARC

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Objectives

The crosslink inhomogeneity has been recognized as a dominant factor on mechanical property in cured phenolic resins. Therefore, it is necessary to characterize the crosslink inhomogeneity and to clarify the structural inhomogeneity-mechanical property relationships. Experimentally the crosslink inhomogeneity in phenolic network after gelation can be well characterized by small-angle scattering experiments by X-ray or neutron with solvent swelling technique. In this study, we performed atomistic molecular dynamics simulation for construction of model gel structures of phenolic resin with inhomogeneous crosslink and calculated the scattering function to compare scattering profiles.

Outline of Results

Atomistic molecular dynamics simulation and scattering function calculation were performed for construction of swollen gel structure of crosslinked phenolic resins using LAMMPS. Swollen gel structures were constructed by solvent insertion into three types of model networks with crosslink inhomogeneity, that is, random network, microgel type and defect type. The calculated scattering function (structure factor) can be compared with experimental small-angle X-ray scattering (SAXS) and small-angle neutron scattering (SANS) profiles performed at SPring-8 and J-PARC, respectively. The scattering function of swollen network of microgel type network, for example, was well consistent with that of SAXS experiments.