Network analysis of a bond-percolation model of bi-functional monomers under photoirradiation and experimental validation

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Radical UV-curable resins are widely used in industry, and elucidating their curing mechanisms is essential for formulation and process design. Since cure shrinkage and residual stress, which are the fate of radical UV-curable resins, determine the long-term reliability of components, it is necessary from an engineering point of view to establish a method to predict them.

This study found experimentally that the shear modulus decreases with increasing irradiance when measurements are made at different UV intensities at the same UV exposure dose. We investigated what kind of network structure is responsible for this decrease in shear modulus. First, a simulation program was developed to construct a bond-percolation network structure based on Wen et al.'s study. Structural mechanical analysis was performed based on the developed network structure. The shear modulus for the network structure was compared with experimental results. The experimental and simulation results showed that the shear modulus decreased with increasing irradiance. The numerical values did not agree, but the order did. The network structure obtained from the simulation was studied in detail in terms of the contribution of each bond in the network to the elastic modulus. It was found that the web produced by increasing the irradiance had many sols formed in the early stages of the reaction. These sols were present after the reaction as dangling clusters. The elastic modulus decreases at high irradiance because these sols are present after the reaction as dangling clusters, which have a small contribution to the elastic modulus.

References

1. M. Wen, L. E. Scriven, A. V. McCormick, Kinetic gelation modeling: Structural inhomogeneity during cross-linking polymerization. Macromolecules, 2003. 36(11): p. 4140-4150.
2. M. Wen, L. E. Scriven, A. V. McCormick, Kinetic gelation modeling: Kinetics of cross-linking polymerization. Macromolecules, 2003. 36(11): p. 4151-4159.
3. M. Wen, L. E. Scriven, A. V. McCormick, Rigidity percolation modeling of modulus development during free-radical crosslinking polymerization, in Protective Coatings: Film Formation and Properties. 2017. p. 67-92.

The JST CREST (JPMJCR21L3) supported this study.