Nanoscale stress distribution and crack propagation in rubber-based nano-composites under stretching

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Nanoparticle-filled cross-linked rubber under tensile deformation was observed in situ by transmission electron microscopy (TEM), and the spatial distributions of the local maximum and minimum principal strains (ε_{max} and ε_{min}) under tensile deformation were experimentally determined. The local ε_{max} showed that deformation behavior depends heavily on the local structures and their spatial arrangements. Additionally, significantly deformed rubbery regions appeared along a network consisting of silica aggregates (silica-aggregate network). The finite element method (FEM) was applied to a series of TEM images under tensile deformation to simulate the structural changes, principal strains, and von Mises stress. The simulated morphology and ε_{max} were in excellent agreement with the experimentally-obtained morphology and strain. The simulated von Mises stress distribution, obtainable only from the experimentally-results-based-FEM, revealed that significant stress propagates along the silica-aggregate network parallel to the tensile direction. This result suggests that the silica-aggregate network may be primarily responsible for providing mechanical strength to the nanoparticle-filled rubber under deformation. Because the stress concentrates along the silica-aggregate networks, cavities appeared along these “stress pathways.” The present study would pave the way to understanding the microscopic factors determining the macroscopic mechanical properties of rubber nanocomposites mainly used for automobile tires and seismic isolation rubber.