Microvoid formation and strain hardening in highly cross-linked polymer networks

DEBASHISH MUKHERJI, CAMERON ABRAMS, Drexel University — Highly cross-linked polymer (HCP) networks are becoming increasingly important as high-performance adhesives and multifunctional composite materials. Because of their cross-linked molecular architectures, HCP’s can be strong but brittle. One key goal in improving the performance of HCP is to increase their toughness without sacrificing their strength. We use molecular dynamics simulations to study the mechanical properties of HCPs. We observe strain hardening in HCP glasses under tensile deformation. We show that formation of micro-voids, without bond-breaking, constitutes the microscopic origins of strain hardening. Micro-void-based strain hardening is not observed in a separate model by imposing a tetrahedral bond angle constraints. Strain hardening makes HCP networks ductile, thus indicating that flexible cross-linkers may be a possible means to control toughness of an HCP without sacrificing its strength.

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