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Molecular dynamics simulation of crack propagation in highly cross-linked polymers under uniaxial deformation[1] MESFIN TSIGE, MARK J. STEVENS, Sandia National Laboratories — The strength of the interface between a structural adhesive and a solid surface is a fundamental issue. We study fracture in highly cross-linked polymer networks (e.g. epoxy) bonded to a solid surface using large-scale molecular dynamics simulations. An initial crack is created by forbidding bonds to occur on a fraction of the solid surface up to a crack tip. The time and length scales involved in this process dictate the use of a coarse grained bead-spring model of the epoxy network. In order to avoid unwanted boundary effects, large systems of up to a million particles are used. Stress-strain curves are determined for each system from tensile pull molecular dynamics simulations. Comparison with standard fracture mechanics will be presented. The dependence of the interfacial fracture energy on film thickness and on the ratio of the width of the unbonded solid surface to film thickness will be described.

[1]Sandia is a multiprogram laboratory operated by Sandia Corp., a

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