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Role of the Entanglements and Bond Scission in High Strain-Rate Fracture of Polymer Melts[1] YELENA SLIOZBERG[2], Bowhead Science and Technology LLC, ROBERT HOY[3], University of South Florida, RANDY MROZEK, JOSEPH LENHART, JAN ANDZELM, Army Research Laboratory — We present coarse-grained molecular dynamics simulations of the effects of solvent molecular weight on the toughness of entangled and non-entangled polymer gels. Our results demonstrate that higher molecular weight solvents enhance gel toughness, and that mechanical properties including strength and toughness can be related to bond scission. We find a remarkable two-step gel fracture mechanism: network chains undergo scission first (and well before fracture), followed by scission of solvent chains. Even after the network chains break, long highly entangled solvent chains provide fracture resistance by effectively increasing the number of chains that must be broken as a crack propagates

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