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Test of the “radical-like polymerization” scheme in molecular dynamics on the behavior of polymers under shock loading CLAIRE LEMARCHAND, DAVID BOUSQUET, CEA-DAM-DIF, F-91297 Arpajon, France, BENOT SCHNELL, Manufacture Franaise des Pneumatiques Michelin, Site de Ladoux, 23 Place des Carmes Dcheaux, France Cedex 9, 63040 Clermont-Ferrand, France, NICOLAS PINEAU, CEA-DAM-DIF, F-91297 Arpajon, France — The behavior of polymer melts under shock loading is a question attracting more and more attention because of applications such as polymer-bonded explosives, light-weight armor and civilian protective equipment, like sports and car equipment. Molecular dynamics (MD) simulations are a very good tool to characterize the microscopic response of the polymer to a shock wave. To do so, the initial configuration of the polymer melt needs to be realistic. The “radical-like polymerization” scheme [Perez *et al*, J. Chem. Phys. **128**, 234904 (2008), Wu *et al*, Polymer **47**, 6004 (2006)] is a method to obtain near equilibrium configurations of a melt of long polymer chains. It consists in adding one neighboring monomer at a time to each growing chain. Between each polymerization step an MD run is performed to relax the new configuration. We test how details of our implementation of the “radical-like polymerization” scheme can impact or not Hugoniot curves and changes of chain configuration under shock. We compare our results to other simulation and experimental results on reference polymers.

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