Molecular dynamics simulations of polymers under shock loading: the importance of the local stress trensor

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Abstract

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Understanding the behavior of polymers under shock loading is essential for their applications in car equipment, aircraft, space structure and plastic bonded explosives. Despite much effort, both experimentally and numerically over the last twenty years (1,2), there are specificities of the shock behavior of polymers that are still unclear. These include the relation of the shocked state to the dynamic glass transition. Direct shock simulations of three different polymers, cis-1,4-polybutadiene, polystyrene and phenoxy resin, with different glass transition temperatures, were performed (3). First, I will show that the polymer melts created in this work have a structure factor and a Hugoniot locus very close to their experimental counterparts. Second, I will focus on the shear stress relaxations behind the shock front. It is found that the polymers with the highest glass transition temperature have the most slowly relaxing shear stress behind the shock front. Finally, to refine the local stress behavior around the shock front, I will present a new expression of the local stress tensor for molecular systems which verifies by construction the local balance of linear momentum (4,5).

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