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Shock wave energy dissipation behavior (SWED) in Network forming ionic liquids (NILs): A Molecular dynamics study KARTHIK GUDA VISHNU, ALEJANDRO STRACHAN, Purdue University — SWED materials play a crucial role in protecting both personnel and structures in close proximity to blasts or ballistic impact. Exposure to shock waves with intensities as low as 1 MPa can cause brain injury in personnel and, hence, it is extremely important to understand the mechanisms operating in SWED materials and help design improved formulations. Recent experimental studies show that NILs containing di-ammonium cations and citrate anions with glass transition temperatures (T_g) below room temperature exhibit shockwave absorption characteristics that outperform polyurea (PU), a benchmark SWED assessment material. The experimentalists further hypothesized that the increased SWED ability in NILs with longer side chains (in di-ammonium cation) is due to a permanent structural ordering and nano-scale segregation. We use molecular dynamics simulations with the Dreiding force field to study shock propagation mechanisms in NILs. Shock propagation mechanisms in these materials are explored by performing both Hugoniostat and large scale non-equilibrium molecular dynamics (NEMD) simulations at 300 K. The simulation results show that the NIL 5-6 (5 C atoms (back bone) and 6 C atoms (side chain)) attenuates shocks better than NIL 5-3 (3 C atoms (side chain) and higher Tg) and PMMA in agreement with experimental observation. The simulations show that under shock loading the structures lose long range order; we find no evidence of nano-segregation nor or permanent structural changes.

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