

Abstract Submitted
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Towards Accurate Molecular Modeling of Plastic Bonded Explosives T.L. CHANTAWANSRI, J. ANDZELM, U.S. Army Research, RDRL-WMM-A, D. TAYLOR, E. BYRD, B. RICE, U.S. Army Research, RDRL-WMB-D — There is substantial interest in identifying the controlling factors that influence the susceptibility of polymer bonded explosives (PBXs) to accidental initiation. Numerous Molecular Dynamics (MD) simulations of PBXs using the COMPASS force field have been reported in recent years, where the validity of the force field in modeling the solid EM fill has been judged solely on its ability to reproduce lattice parameters, which is an insufficient metric. Performance of the COMPASS force field in modeling EMs and the polymeric binder has been assessed by calculating structural, thermal, and mechanical properties, where only fair agreement with experimental data is obtained. We performed MD simulations using the COMPASS force field for the polymer binder hydroxyl-terminated polybutadiene and five EMs: cyclotrimethylenetrinitramine, 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclo-octane, 2,4,6,8,10,12-hexantirohexaazasisowurzitane, 2,4,6-trinitro-1,3,5-benzenetriamine, and pentaerythritol tetranitate. Predicted EM crystallographic and molecular structural parameters, as well as calculated properties for the binder will be compared with experimental results for different simulation conditions. We also present novel simulation protocols, which improve agreement between experimental and computation results thus leading to the accurate modeling of PBXs.

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