

**New Reactive Molecular Dynamics Algorithm. Modeling the Thermal
Decomposition of Polymers.**

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A new version of the novel reactive molecular dynamics algorithm (MD_REACT) has been developed as a result of collaboration between researchers at the University of Massachusetts, Amherst, and the Building and Fire Research Laboratory of NIST. The method is designed to serve as a versatile tool for modeling of thermal decomposition of polymeric materials. The algorithm is based on classical molecular dynamics. A dynamic force field is employed to simulate potential energy surfaces of a wide range of elementary chemical transformations. The parameters of the forcefield have been calibrated against the results of CBS-QB3 quantum chemical calculations performed on model compounds. Thermal degradation of PMMA has been studied using the reactive molecular dynamics approach. The results of these simulations are compared with experimental observations.