

Chemical Reactions of a CL-20 Crystal under Heat and Shock determined by ReaxFF Reactive Molecular Dynamics Simulations

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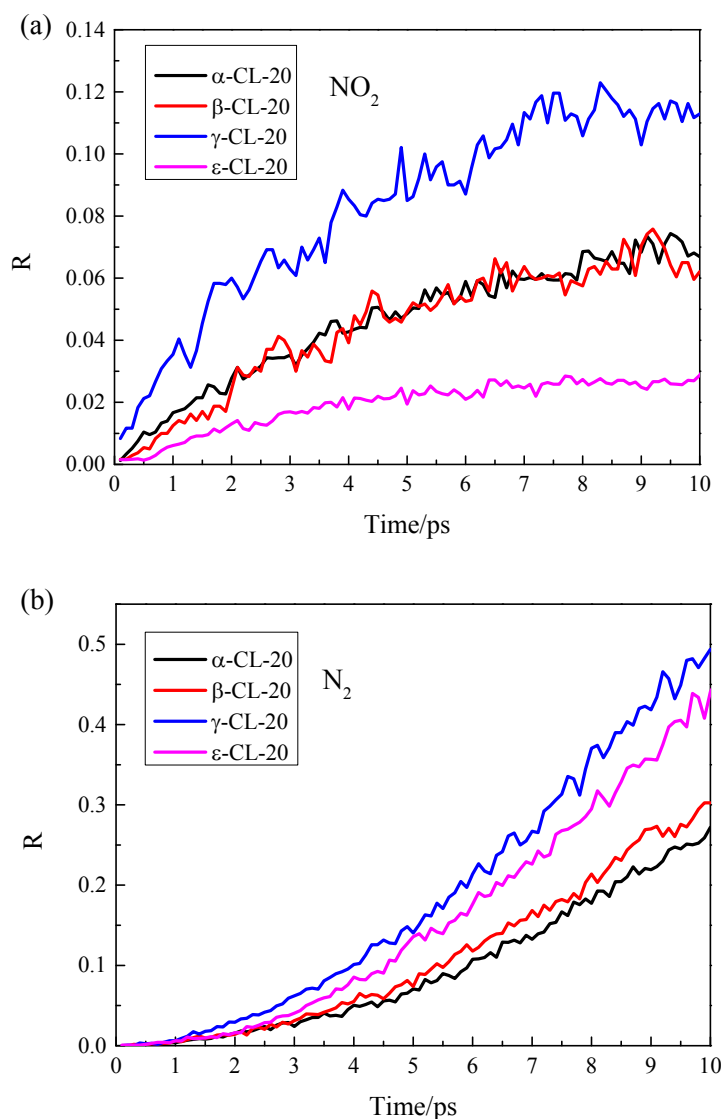


Fig.1 Evolution of generation rates of NO_2 and N_2 for α , β , γ , and ϵ -CL-20 crystals under the shock (R is the ratio of molecules numbers between the products and the reactants in the supercell)

* The type of article: Research paper

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