

Abstract Submitted
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Non-Equilibrium Chemical Bonding of Shock-Induced Chemical Reactions. ANGUANG HU, Defence Research and Development Canada — Using multiresolution and multiscale quantum chemistry simulations recently developed, we demonstrated that dynamic non-equilibrium chemical bonding processes of shock-induced phase growth, mixing and detonations can take place between two Hugoniot adiabatic states of shock and detonation waves, representing reactant and product thermodynamic states. Such a process can start immediately on the onset when mechanical work couples thermal heat upon activation of reactive modes selected mainly by mechanical compression. Our preliminary results are in agreement with a number of shocked induced chemical transformations in terms of phase transition temperatures and pressures, for example, transformations of hexagonal diamond and boron nitride. Simulations also show unambiguous distinction between homogeneous and hot spot detonation reactions regarding shock leading pressure and temperature together with detonation densities. At lower pressure and density, it shows the hot spot mechanism with larger changes of bond lengths, leading to extremely higher temperature. In contrast, at larger pressure and density it shows homogeneous mechanism with small changes of bond lengths, resulting in relatively lower temperature. This is in good agreement of experimental observations.

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