

Abstract Submitted
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A possible crystal defect mediated mechanism governing energy release in solid organic secondary explosives BRYAN HENSON, LAURA SMILOWITZ, Los Alamos National Laboratory — Work has been ongoing in our group for several years to produce a global chemistry model of thermal ignition for the solid organic secondary explosive octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) valid over the entire temperature range of energetic response from thermal ignition to detonation. We have made considerable progress recently, resulting in the first broadly accurate model of this type for HMX. We have also recently provided the first theory of the phenomenon of melt acceleration in the thermal decomposition which indicates a universal mechanism applicable to this entire class of materials. The success of these models derives from the kinetic rate equations used, which are based upon rates activated by energies of vaporization and sublimation. The equations can be reduced to dimensionless form, yielding melt accelerated rates of thermal decomposition, ignition and detonation which are functions of two rate constants, one proportional to the liquid activity and another that can be interpreted as the simultaneous occupation of two defect states of the crystal. In this reduced form, data from a number of secondary explosives may be superposed on common curves. In this talk we explore the possibility that the underlying mechanism responsible for this behavior is linked to the equilibrium population of a crystal defect described by a vacancy in contact with local disorder.

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