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Reaction rate model of energy release in shocked RDX[1] IGOR SCHWEIGERT, United States Naval Research Laboratory — Shock-to-detonation transition in secondary explosives is driven by energy localization at microstructural heterogeneities, wherein local temperature spikes ("hot spots") trigger chemical reactions and formation of self-sustained reaction fronts. Emerging mesoscale methods, including sub-scale hydrodynamics and coarse-grained particle methods, can explicitly model these processes but require reaction rate models as input. I will present the development of such a model for RDX that combines first-principles predictions for condensed-phase decomposition under GPa pressures with a reduced model of thermal oxidation of RDX decomposition products. I will also discuss inherent shortcomings of the model due to uncertainties in the first-principles predictions and the scarcity of kinetic data for high-temperature and high-pressure conditions.

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