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Homogeneous initiation in single crystal PETN from shock induced bulk heating

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Calculations of shock initiation in polycrystalline explosives convolve several phenomena. An input shock pressure P generates compression and temperature (V, T) . The temperature, T (and possibly P), determines the time to thermal ignition and the resulting rate of decomposition through a thermally activated Arrhenius rate and mechanism. The resulting rate of pressurization is further determined by the state of solid compression V and the product pressure through the fluid equation of state (EOS). This pressurization then determines the resulting shock physics that follows ignition, *e.g.* wave coalescence, initiation. The simplest version of this problem in the solid state is the shock initiation of single crystal samples by homogeneous initiation. Here the relationship of (V, T) in the reactant crystal is simplified by the absence of free volume and a quantitative relationship amongst (P, V, T) through the solid EOS. In particular the possible states (V, T) as a function of P are constrained by the EOS. We present calculations of the time and distance to initiation as a function of input pressure in single crystal PETN. We use a JWL EOS for the solid to constrain the bulk temperature and compression as a function of impact pressure. We calculate the thermal ignition time as a function of temperature from a model of PETN thermal decomposition and the pressurization in the far field using a product fluid EOS and a simple application of the method of characteristics. We determine the unique (V, T) state at each pressure by solving for the intersection of characteristics generated by the ignition and the input shock at the time and distance to initiation observed in experiments. Interesting results include the relationship between the input $T(P)$, the observation of multiple wave phenomena at low pressure and a mechanism for the nonlinearity in the measured pop-plot.