

Abstract Submitted
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Vibrational energy transfer in shocked molecular crystals JOE HOOPER, Naval Surface Warfare Center, Indian Head — The vibrational energy transfer behind a shock and its possible role in the earliest stages of explosive initiation is considered. A new theory of multiphonon energy transfer into shocked molecules is developed which expands on existing treatments and allows consideration of a range of molecular crystals and liquids. Simple analytic forms are derived for the change in this energy transfer with increasing Hugoniot pressure or near simple defects. The time required for the total shocked system to come to thermal equilibrium is found to be an order of magnitude or more faster than proposed in previous work, in good agreement with recent molecular dynamics calculations. In typical energetic molecular crystals, thermal equilibration is predicted to occur two to five picoseconds following passage of the shock wave. Simple defects are introduced into the model by considering the mesoscale elastic strain fields surrounding an inhomogeneity. For straight dislocations, a region of modestly enhanced energy transfer on the scale of five nanometers is found. However, due to the rapid establishment of thermal equilibrium, we find it is unlikely these regions are related to hot spot formation. Indeed, the theory developed here suggests that the effect of nonequilibrium phonon processes on sensitivity or initiation is minimal.

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