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Deformation and excitation of molecules during shock compression of defects[1] SERGEY V. ZYBIN, Caltech Institute of Technology, MARK L. ELERT, U. S. Naval Academy, CARTER T. WHITE, Naval Research Laboratory — Shock initiation of chemical reactions in solids often starts at hot spots that are created during interaction of a shock wave with pre-existing defects and interfaces in the material. The formation of hot spots can involve the vaporization of material into a pore (or crack) followed by recompression of the ejected gas during the collapse of the pore with fast temperature increase (local overheating). However, in presence of large temperature gradients and non-equilibrium energy transfer at the front, the analysis of molecule deformation and excitation should not be limited to the Arrhenius kinetics only, but can also involve non-thermal mechanisms. Here, we report results of molecular dynamics simulations of shock passage through the planar gap (crack) in hydrocarbon molecular solids and analyze the temperature rise, energy distributions, and bond deformations. Our analysis shows that the region of most intense molecular deformation is located in vicinity of the collision front of the rarefaction and reflected (from the opposite side of the crack) waves, where the velocity distributions deviate widely from the equilibrium Maxwellian.

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