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Instability of planar detonation front in energetic materials
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OLEYNIK, University of South Florida — Detonation wave propagation in solid en-
ergetic materials (EMs), as described by the standard AB model, was studied using
a novel moving window molecular dynamics (MW-MD) technique. Parameters of
the AB model were modified to investigate the mechanisms of detonation propaga-
tion in EMs as a function of the activation barrier for the chemical reaction $AB+B$
 $\rightarrow A+BB + 3 \text{ eV}$. For barriers below 0.2 eV, the detonation front structure re-
mained planar irregardless of the cross-section of the sample. For higher activation
barriers, the one-dimensional planar detonation evolves into a cellular detonation
upon increase of one of the transverse dimensions of the sample. The cellular det-
onation transforms into a stable three-dimensional turbulent-like detonation upon
simultaneous increase of both transverse dimensions of the sample. These various
instabilities of the planar detonation front in solid EMs observed in our MW-MD
simulations mirror the major regimes of gas-phase detonation, thus confirming the
universal nature of detonation phenomena.

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