

Abstract Submitted  
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**Simulating phase formation during exothermic reactions in Al/Ni and Al/Zr multilayered foils**<sup>1</sup> RONG-GUANG XU, Department of Physics and Astronomy, Johns Hopkins University, MICHAEL L. FALK, Department of Materials and Engineering, Department of Mechanical Engineering and Department of Physics and Astronomy, Johns Hopkins University, HONG-WEI SHENG, Department of Computational and Data Sciences, George Mason University, JOHNS HOPKINS UNIVERSITY TEAM, GEORGE MASON UNIVERSITY COLLABORATION — Reactive multilayered foils are composed of thousands of alternating micro- to nano- scale layers of elements which have a large negative enthalpy of mixing. When a small pulse of energy (such as an electric spark or a thermal pulse) is provided, highly exothermic, self-propagating chemical reactions can be triggered. Both theoretical models and experimental data indicate that even a relatively small amount of premixing can have a dramatic effect on the heats and velocities of the propagating reaction front. We have implemented molecular dynamics simulation to study the phase transformation sequence during multilayered reactions and to elucidate how premixing can affect the sequence of phase formation during such reactions.

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