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Dynamic evolution of aluminum nanoparticle impacted by RDX slab

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A modified ReaxFF force field was used to study dynamic deformation of Al nanoparticles (ANPs) and chemical evolution of RDX/Al mixtures. When small ANPs impact RDX crystal planes, the interaction between RDX and Al at the initial stage does not affect the order of shock-induced anisotropic response of RDX crystal and different thickness of alumina shell on ANPs exhibits different capacity to resist structural deformation. When Al slab with 30 wt% is coated with a 3 nm thickness of alumina, Al slab exhibits inert characteristics and provides high compression condition to enhance decomposition of RDX molecules during the initial impact stage.

I . INTRODUCTION

Aluminum (further “Al”) is common ingredient in rocket propellants and various explosives. It is generally recognized that micrometric aluminum powder (further “ μ -Al”) hardly participates in the reaction zone, so aluminized explosives are often used as thermobaric weapons for their late-time blast effect or underwater weapons for their significant bubble energy.^[1] Meanwhile, nanometric spherical aluminum particles (further “ANPs”), because of their high reaction rate, the complete reaction with oxidizer, large surface area, have been expected to increase the detonation performance of high explosives in the recent thirty years.^[2] However, some serious shortcomings confine their industrial application,^[2] so more work is still needed to understand the effect of ANPs on the detonation characteristics and sensitivity of explosives.

From the Nonequilibrium Zeldovich-von Neumann-Doring theory,^[3] we know that key features of shock initiation of explosives contain the von Neumann pressure spike, reaction zone and isentropic expansion region. Several nonequilibrium chemical

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