Anisotropic Mechanical Response and Phase Transition of Cooked HMX

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Abstract: The crystal plasticity constitutive model is developed to investigate the role of solid-solid phase transformation on the deformation mechanism of the HMX single crystal, with accounting for nonlinear elasticity, crystalline plasticity and temperature-controlled phase transition ($\beta \rightarrow \delta$ phase transition). The phase transition of HMX at various heating rates was simulated using a finite element software ABAQUS and a subprogram VUMAT. It shows that the phase transition is reversible, while the paths for $\beta \rightarrow \delta$ and $\delta \rightarrow \beta$ transitions are different from each other. Residual strain and stress occur when the crystal converts back into the β phase. In addition, cracks are generated during the $\beta \rightarrow \delta$ phase transition, and maintain after the $\delta \rightarrow \beta$ phase transition. Moreover, the temperature homogenization can facilitate the phase transition, and the propagation of the phase transition and the heating proceed in a same direction. Furthermore, the $\beta \rightarrow \delta$ phase transition can lead to crystal expansion. Because the thermal expansion coefficient of the δ phase is larger than that of the β phase, the crystal volume is expanded more quickly after the $\beta \rightarrow \delta$ phase transition, causing a rapid increase in internal stress and slipping. Due to the anisotropic thermal expansion of the HMX single crystal, cracks occur most readily along the third principal axis after the phase transition, resulting in ready formation of hot spots. Therefore, the $\beta \rightarrow \delta$ phase transition makes the HMX crystal more sensitive to cook-off.

Key words: phase transition; cook-off; chemical kinetics; thermal expansion; octogen(HMX)

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