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Theoretical study of β-HMX decomposition mechanism of the solid phase under shock loadings GUANGFU JI, Professor, NINA GE, None, XIANGRONG CHEN, Professor — Study material properties under extreme conditions is a fundamental problem in the field of condensed matter physics. The decomposition mechanisms of energetic materials under the shock wave become a hot topic in recent years. In this paper, molecular dynamics simulations combined with multi-scale shock technology (MSST) are used to study the decomposition mechanism, shock sensitivity and electronic structure ofβ-HMX. First, the decomposition mechanism of β-HMX perfect crystal were studied at different shock speeds. We found that when the shock wave at a speed 8 km / s is loaded, the decomposition reaction start at N-NO2 bond breakage; when the shock wave at a speed of 10 km / s and 11 km / s is loaded, the the first decomposition reaction is CH bond breaking, and accompanied by the formation of five-membered ring and transfer of hydrogen ions. The simulation results also show that when the shock wave velocity is increased, the higher the pressure generated in the high-pressure N-NO2 bond cleavage was inhibited significantly. Secondly, the impact of its initial chemical reaction process along different crystal axis directions were studied, the results showed that along the a-axis and c-axis shock sensitivity is higher, and along the b-axis sensitivity is lower. We believe that the system of all sensitivity of direction is due to the rotation of the friction between the slip plane of crystals and molecules. Finally, we discussed the solid phase β-HMX electronic properties change under the shock wave loadings. We found that in the 11 km / s under the impact load, when the pressure reaches 130 GPa , zero bandgap is reached.

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