

# **Non-equilibrium molecular dynamics simulations of the shock induced failure in Al with helium bubbles**

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## **Abstract**

The effects of defects on the dynamic failure of materials have attracted considerable attention recently. Gas bubbles, representative microstructures in irradiated materials, are one of the typical heterogeneities in practical materials. Thus, non-equilibrium molecular dynamics simulations are conducted on Al with pre-existing helium bubbles to find out the dynamic evolutions under shock wave. The presence of helium bubbles has significant influence on the Hugoniot state of equation, increasing the temperature while reducing the shock velocity when shocked to a given pressure. The internal He pressure contributes the adjacent plasticity, providing the sites of nucleation of dislocations. Moreover, the microstructures under compression and tension are resolved. It's found that the void growth and coalescence process during spallation is remarkably affected by helium bubbles.

**Keywords:** Helium bubbles; Shock wave; Plasticity; Molecular dynamics simulations