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3D Fragmentation of Nanocrystals by Molecular Dynamics

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ABSTRACT

The dynamic fragmentation of brittle materials has long been investigated both from scientific and engineering view points. Numerical modelling has proven to be an indispensable tool for understanding this process, yet its application has been limited to models of reduced dimensionality due to computational cost. In this work we exploit recent computational and algorithmic advancements to investigate dynamic fragmentation in three dimensions using a massively parallel molecular dynamics approach. The relationship between strain rate and fragment size in three dimensions is analyzed with respect to prior atomistic and continuum models for lower dimensions.

To best address some key outstanding questions of the dynamic fragmentation process, a simple atomistic material model is employed where the interatomic forces are described as

$$f(r) = k(r - r_0)\left[\exp\left(r \frac{\Xi}{r_{break}} - \Xi \right) + 1 \right]^{-1}$$

with k being the spring constant, r_0 the nearest-neighbour equilibrium spacing of the atoms, r_{break} the critical separation for the breaking of bonds, and Ξ the amount of smoothing at the breaking point. This material model enables the investigation of the role of material nonlinearity and the interplay between crack branching and the fragment size distribution by varying the values of Ξ and r_{break}. When Ξ and r_{break} are small, nucleated cracks quickly reach their unstable speed and crack branching is prominent. When these values are large, cracks remain stable until they reach the Rayleigh-wave speed. We speculate that our simulations will reveal that the fragment size distribution changes abruptly at very high strain rates due to cracks interacting before they reach their unstable speeds.

The prospect of using three dimensional continuum models will be discussed by examining the role of r_0 in our atomistic model. For a fully convergent continuum model to be brought to fruition, the mesh size must not influence the energy dissipated during fragmentation, and thus, rate and length-scale dependent cohesive laws may be required.