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COLLISION AND FRAGMENTATION OF NANOGRAINS

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Abstract

Collision and fragmentation of nanograins can be of interest in various fields, from the dynamics of interstellar dust, to spall in strong shocks. Atomistic molecular dynamics (MD) simulations of grain-grain collisions have been carried out for spherical grains of up to 5 nm, with relative velocities of few km/s and a number of random impact parameters. We have simulated both copper FCC grains using an Embedded Atom Model (EAM) potential, and carbon diamond grains using the Reactive Empirical Bond Order (REBO) potential. For the carbon grains, grain fusion is often observed even at these high velocities. High pressures and temperatures generated by the collision lead to hybridization changes in the carbon grains, and melting in the copper grains. Spall and fragmentation of the grains results in a complex grain size distribution, which does not follow a single power-law distribution.

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