High Strain Rate Deformation in α-Alumina: 540 Million Atom Molecular Dynamics Simulation

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I have carried out a 540-million atom molecular dynamics (MD) simulation to investigate deformation mechanisms in α-alumina under hypervelocity impact. In the simulation, aluminum oxide target is impacted by a projectile normal to the (0001) surface. The simulation reveals large temperature and pressure gradients around the projectile, which cause local amorphization of the substrate. In the crystalline regime away from the projectile, several types of deformations emerge and disappear under the influence of local stress fields. Deformation mechanisms such as slips and twins along {0001} and {012} planes, and a few new deformation patterns are observed, e.g., rhombohedral twinning along {012}, slip-twin-slip structure along {011}, and crystalline structural change under shear stresses. In the unloading phase, extensive cracking happens at the intersection of deformations within an hourglass-shaped volume. The substrate eventually fails along the surface of the hourglass.