Atomistic simulation of Richtmyer-Meshkov instability in solids using the IBM Blue Gene Computer

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Recent advances in the computing power have created great opportunities for modeling non-equilibrium phenomena via molecular dynamics (MD) simulations. With a few billions of simulated atoms, MD can grasp at the atomic level the essentials of many non-equilibrium processes in shock physics and hydrodynamics. In laser ablation, a shock wave induced by laser irradiation interacts with the target imperfections and results in the Richtmyer-Meshkov (RMI) and Rayleigh-Taylor (RTI) instability of the ablation front. On the other side, high-velocity impact can lead to shock-induced RMI at the interface of two different solids resulting in the nanoscale material mixing and penetration.

Development of instabilities at the solid interfaces is of great interest in inertial confinement fusion (ICF), detonations in heterogeneous (e.g. polymer-bonded) explosive materials (where a “jetting” effect at the interface between polymer and explosive crystal can initiate a detonation), and many other applications. The atomistic dynamics of a solid under deformations of very high strain rate is also one of key issues for theories and models, which study the material strength and phase transitions under a high strain rates.

Here we report the results of large-scale molecular dynamics simulations of the Richtmyer-Meshkov instabilities performed on the Blue Gene/L (BG/L) supercomputer at the LLNL. Using 1/8th size of BG/L (16,000 processors) for a typical simulation time of ~100 ps (~3-4 days run) we were able to achieve ~1/100th of the interface perturbation wavelength usually used in experiment. Simulation code (MDCASK) exhibited excellent scaling up to 32K nodes (64,000 processors) making possible even bigger/longer simulations. The results of the simulation provided an important insight into atomistic mechanisms of instability growth, plastic flow, and vorticity at the interface, paving a way to better continuum models of RMI in condensed phase.