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A quasi 2-D molecular dynamics study of the initiation and evolution of the Kelvin-Helmholtz instability KYLE CASPERSEN, ROBERT RUDD, DAVID RICHARDS, JIM GLOSLI, Lawrence Livermore National Laboratory, JOHN GUNNELS, IBM, FREDRICK STREITZ, Lawrence Livermore National Laboratory — Typically hydrodynamic phenomena are modeled with continuum mechanics via integration of the Navier-Stokes (NS) equation or a closely related variant. However, as fluids are studied at smaller and smaller length scales atomistic effects can, and will, ultimately dominate; furthermore, even at micron scales it is not clear that the NS equation provides a complete description of the fluid, e.g. due to the initiation of instabilities at the molecular scale in initially quiescent fluids. To assess the effect of atomistic behavior on one particular hydrodynamic phenomenon–the Kelvin-Helmholtz instability–we have performed a very large molecular dynamics simulation of molten metals undergoing shear flow. Nine billion copper and aluminum atoms were sheared at a speed of 2000 m/sec for a total simulated time of more than a nanosecond. We present here results showing the initiation of the instabilities, the crossover to hydrodynamics, and the evolution and scaling behavior of the KH instability in a quasi 2-D geometry. Prepared by LLNL under Contract DE-AC52-07NA27344.

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