Abstract Submitted
for the SHOCK07 Meeting of
The American Physical Society

Atomistic Simulations of Detonation Instabilities in Condensed Phase Systems EDWARD KOBER, ANDREW HEIM, TIMOTHY GERMANN, LANL, NIELS JENSEN, UC Davis — We report the results of simulations of condensed phase detonation phenomena using a model diatomic system: 2AB -> A_2 + B_2. The initial set of parameters for this system corresponded to the Model 0 set of C. White et al, which exhibits a steady, Chapman-Jouget (CJ) detonation structure with a reaction zone length of 30-100 Å. This has a highly compressed CJ state (V/V_0 ~0.5) that does not consist of discrete molecular species. The potential form was modified so that a more molecular CJ state resulted, consistent with the models for conventional organic explosives. The new system has a less dense CJ state (V/V_0 ~0.8), and the reaction zone was substantially extended. The reaction rate fits Arrhenius-type kinetics with an activation energy of ~2 eV, with a minor density dependence. In contrast, the original Model 0 system had a lower activation energy (~1 eV) with a stronger density dependence. The new system exhibits quite marked two dimensional instability structures with well-defined wavelengths similar to what has been observed for gas-phase detonations and for nitromethane. Depending on the exothermicity and the width of the periodic simulations, these instabilities can result in either detonation failure or quasi-steady propagation. The observed propagation velocities are several per cent higher than CJ values derived from thermodynamic analyses.

Edward Kober
Los Alamos National Laboratory

Date submitted: 27 Feb 2007 Electronic form version 1.4