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Campaign 2 Level 2 Milestone Review 2009: Milestone # 3131 Grain Scale Simulation of Pore Collapse

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Disclaimer

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Campaign 2 Level 2 Milestone Review 2009:

Milestone # 3131

Grain Scale Simulation of Pore Collapse

Summary report

30 September 2009

Committee members:

Richard Becker

Robert Cavallo

Rose McCallen

Eric Schwegler

Craig Tarver

Summary report on the review of the L2 Milestone #3131 (Q4FY09):

Grain Scale Simulation of Pore Collapse

Review held 16 September 2009

Committee members: Richard Becker
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The milestone reviewed on Sept. 16, 2009 was "High-fidelity simulation of shock initiation of high explosives at the grain scale using coupled hydrodynamics, thermal transport and chemistry." It is the opinion of the committee that the team has satisfied the milestone. A detailed description of how the goals were met is provided below.

The milestone leveraged capabilities from ASC Physics and Engineering Materials program combined with experimental input from Campaign 2. A combined experimental-multiscale simulation approach was used to create and validate the various TATB model components. At the lowest length scale, quantum chemical calculations were used to determine equations of state, thermal transport properties and reaction rates for TATB as it is decomposing. High-pressure experiments conducted in diamond anvil cells, gas guns and the Z machine were used to validate the EOS, thermal conductivity, specific heat and predictions of water formation. The predicted reaction networks and chemical kinetic equations were implemented in Cheetah and validated against the lower length scale data. Cheetah was then used within the ASC code ALE3D for high-resolution, thermo-mechanically coupled simulations of pore collapse at the micron size scale to predict conditions for detonation initiation.

At the lowest length scale the main atomistic simulation technique used is based on self-consistent charge density functional tight-binding (SCC-DFTB). It is an approximate density functional theory method that is several orders of magnitude faster while still being able to quantitatively account for the various bond making and breaking processes that are central to the chemistry of a high-explosive. Here, the SCC-DFTB method has been used to examine directly the thermal decomposition mechanics of nitromethane and TATB under extreme temperature and pressure conditions. The data from these simulations were used to formulate a set of simplified decomposition reaction mechanisms which were used in the Cheetah thermochemical code. A number of comparisons between the original MD simulations results and Cheetah have been carried out, and the agreement is generally good. Cheetah does overpredict the high temperature nitrogen formation rate, indicating an opportunity for further refinements.

Diamond anvil cell experiments have been used to validate predictions of water formation from the decomposition of TATB at high pressures. At ambient pressure water is not detected and the reactions are confined to the heated portion of the specimen. At high pressure the whole sample is burned and water formation is observed. In addition, high pressure experiments were used to

validate sound speed predictions from Cheetah EOS calculations and the thermal diffusivity predicted from first principles calculations.

The material property and chemical kinetic information encoded in Cheetah provides the basis for predicting shock initiation in grain-scale hydrodynamic simulations. Specifically, initiation of reaction in TATB due to collapse of a micron-sized void is investigated as voids have been shown experimentally to play a central role in initiation of detonation. A shock impacting a representative volume element containing single air-filled void from a periodic array of voids is simulated in high resolution, 2D-axisymmetric calculations. The void volume fraction is less than 1% and void sizes are 2 μm and 4 μm diameter, which is sub-grain size for TATB. Several different shock pressures were applied to investigate the pressure threshold for initiation. The ASC finite element code ALE3D solves the hydrodynamic and thermal transport equations and Cheetah is used as a module to provide the equation of state and thermal transport properties for the finite element calculations.

The micron-scale simulations with shock pressures of several GPa show collapse of the void by a jet of TATB shooting across the void axis. The jet impinges on the opposite void surface, creating high temperature and pressure at the impact site. The air in the pore is compressed significantly and becomes very hot due to nearly adiabatic compression. Because of the main jet impacting along the void axis, the air is forced into an off-axis cavity. There was considerable attention focused on the air heating a small secondary jet which protrudes into the air cavity. This creates a small ignition point at lower shock pressures. At higher pressures the decomposition of the TATB is greatest where the primary jet impacts the opposite void surface, providing a much larger volume for the initiation site than the secondary jet.

In studies of the sensitivity to void size and pressure, when the void size is decreased the initiation is suppressed, in agreement with experimental data. The experimental data show a shock initiation threshold of 10 GPa with a 30 mm distance to detonation and a 20 GPa threshold for a 2 mm distance. The simulations predict a short-lived detonation at 10 GPa and a more sustained detonation at 25 GPa, so the predictions of threshold initiation pressure are in the right vicinity compared to the experiments. The simulation technique shows great promise for being able to predict shock initiation. Further studies will be needed to examine non-ideal pore geometries and multiple hot-spot initiation to better assess a sustained reaction.

The committee viewed this as significant progress and believes the work to be very promising. We would like to offer suggestions on several avenues to further this research:

a) With sufficient computational resources, the simulations should be run in 3D on larger volumes with multiple, nonspherical pores to better capture observed void configurations and sustained ignition from multiple initiation sites;
b) Improve the computational efficiency of simulations at all levels to facilitate a);
c) Expand the range of the fit to data and the SCC-DFTB simulation results to improve accuracy and robustness of reactions predictions;
d) Include strength and melt viscosity in the simulations to provide mechanical dissipation to the flow;
e) Provide suggestions for possible experiments to validate results from the grain scale simulations. There is currently no validation data for the details of ignition near the pores.