A Comparative Study on Impact Failure Evolution with the MPM and MD

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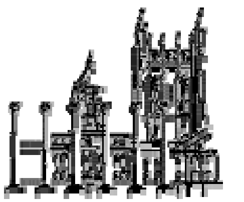
Outline

1. Introduction

2. Previous Work on Nanothermite Response

3. Comparative Study with the MPM and MD

4. Concluding Remarks and Future Tasks



1. Introduction

- Commonly used energetic materials are based on mono-molecular compounds such as TNT and RDX. The energy densities of such materials are relatively low.
- Higher energy densities could be obtained from combusting metal fuels such as Al. However, the energy release rate of such fuels is relatively low.
- Recent developments in nanoscaled metal components have demonstrated that the high energy release rate could be realized due to the very high reactive interface areas in metal-based reactive nanomaterials.
- <u>There is a lack of understanding on multi-scale interactions involved as well as physics-based modeling.</u>

Generation of Fast Propagating Combustion and Shock Waves with CuO/Al Nanothermite

(APL, Apperson et al., 2007)

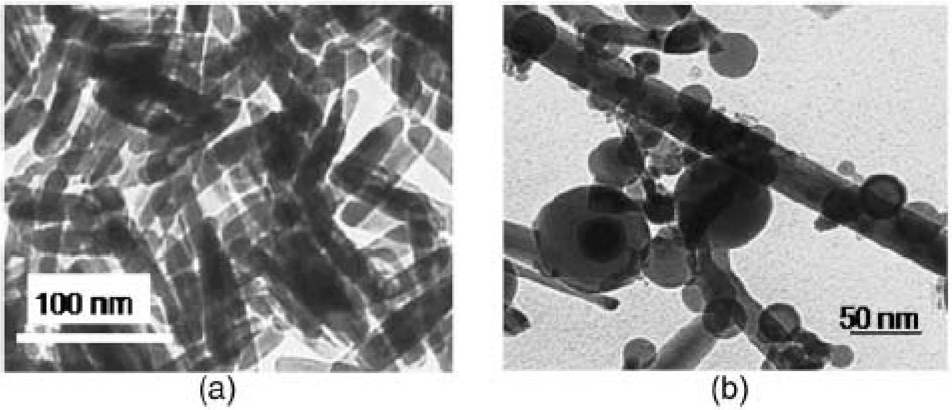
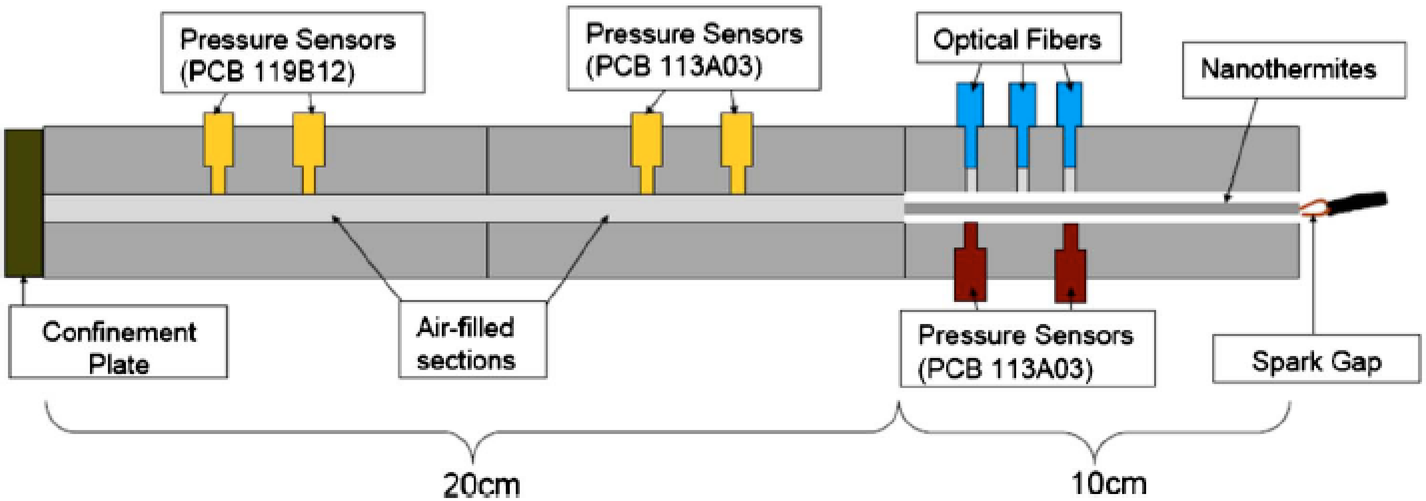


FIG. 1. TEM Images of (A) CuO nanorods and (B) self-assembled CuO nanorods/Al.



Generation of Fast Propagating Combustion and Shock Waves with CuO/Al Nanothermite

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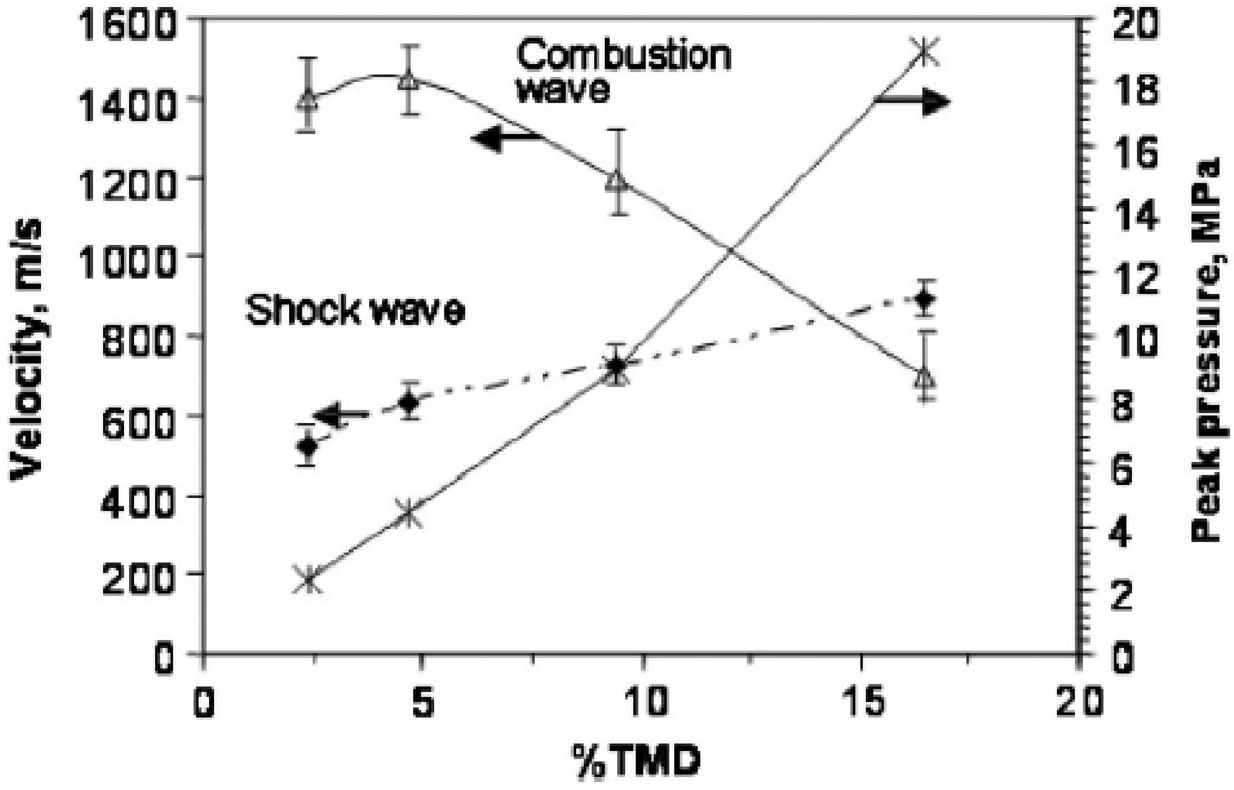
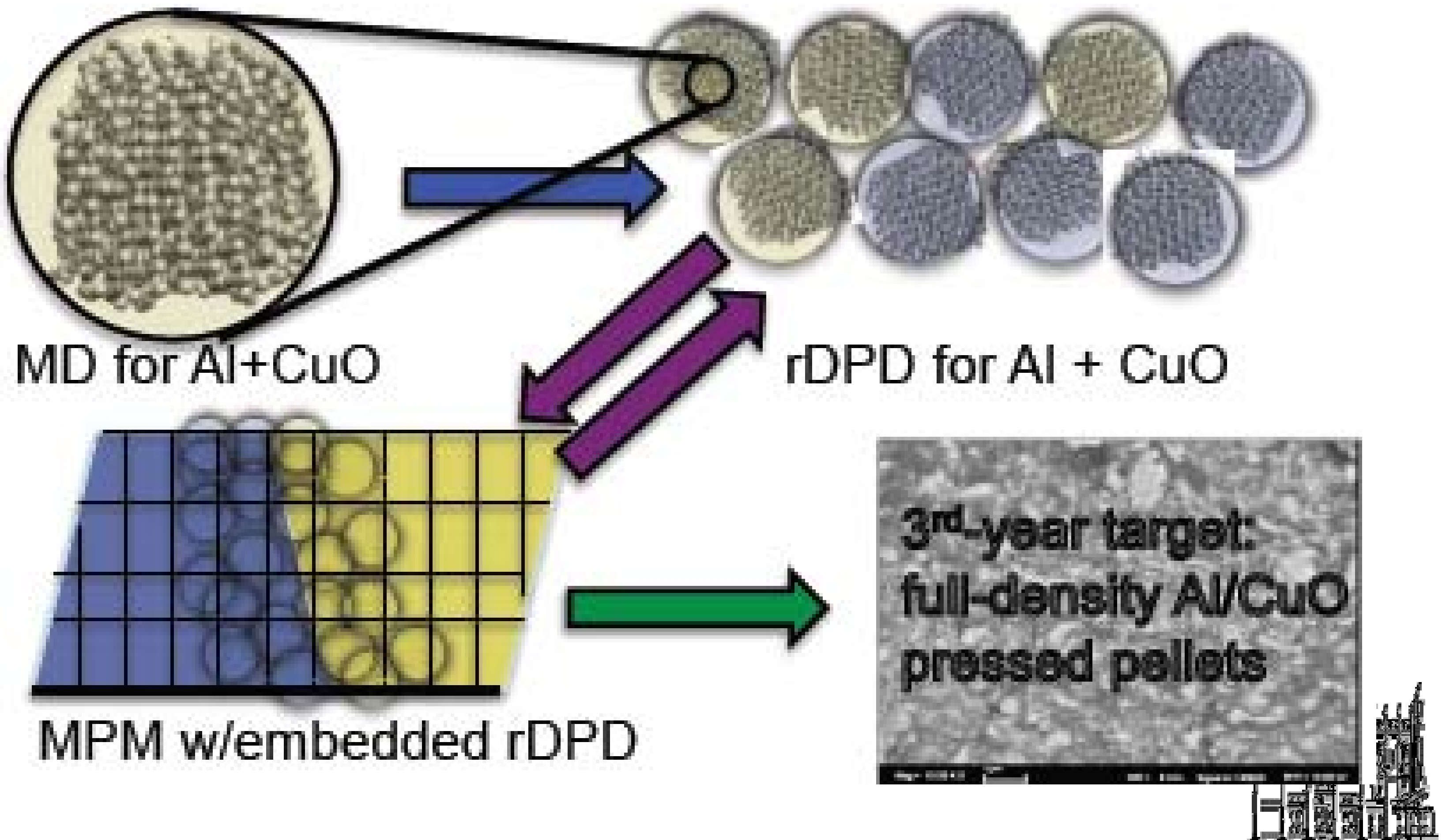


FIG. 4. Plot of combustion velocity, shock wave velocity, and peak pressure as a function of the density of physically mixed CuO/Al composite.

Particle-based multi-scale simulation procedure for predicting the coupled spatial-temporal energy-release properties

Hierarchical from MD to rDPD)

Concurrent between rDPD and MPM via Nonlocal Treatment



2. Previous Work on Nanothermite Response

(Journal of Nanoparticle Research, Gan et al., 2010)

- With the assumption for the infinite reaction rate without atomistic details, an equation of state for the detonation product of CuO/Al nanothermite composites has been developed based on the Chapman-Jouguet theory and nanothermite detonation experiment..
- The EOS has been implemented into the MPM for coupled CFD and CSD simulation of the detonation response.
- The MPM is improved with an iterative scheme for describing strong-shock wave propagation in fluids.
- The simulation results demonstrate the validity of the proposed EOS to catch the essential feature of the detonation response at continuum level.

2. Previous Work on Nanothermite Response

(Journal of Nanoparticle Research, Gan et al., 2010)

For the gaseous detonation product,

$$\boldsymbol{\sigma}_p = -\hat{p}\underline{\underline{\boldsymbol{I}}}$$

The pressure is determined via the EOS,

$$I = I(\hat{p}, \rho)$$

with the internal energy being dependent on the stress state.

An iterative procedure is designed to obtain convergent internal energy and stress values in each time increment so that strong-shock wave propagation could be better simulated.

2. Previous Work on Nanothermite Response

(Journal of Nanoparticle Research, Gan et al., 2010)

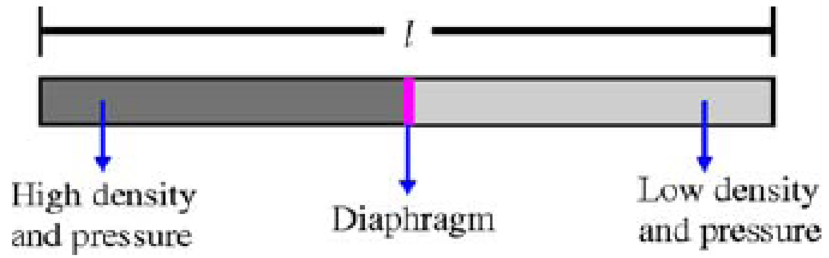


Fig. 4 One-dimensional shock tube problem

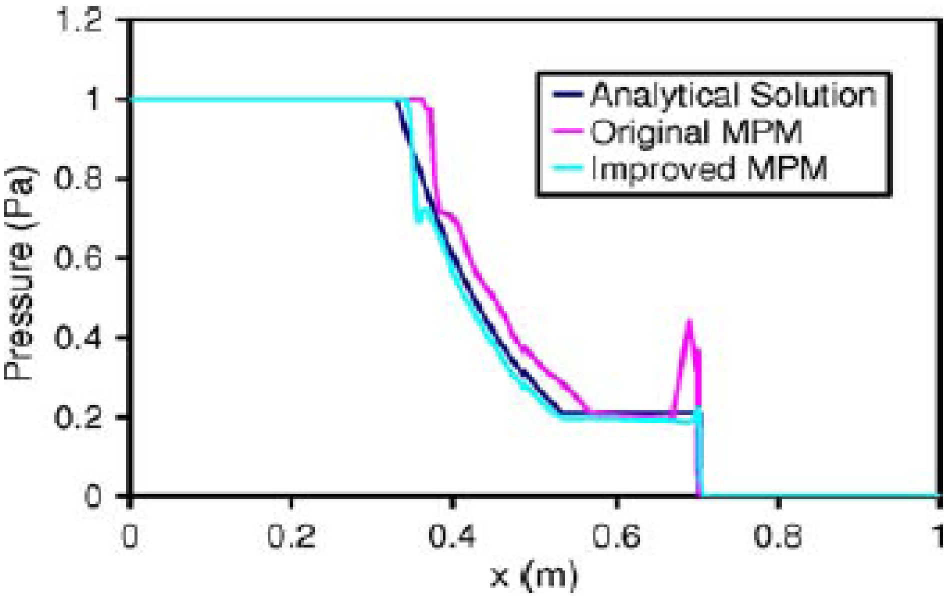


Fig. 5 Pressure profiles by the original and proposed MPM algorithms

2. Previous Work on Nanothermite Response

(Journal of Nanoparticle Research, Gan et al., 2010)

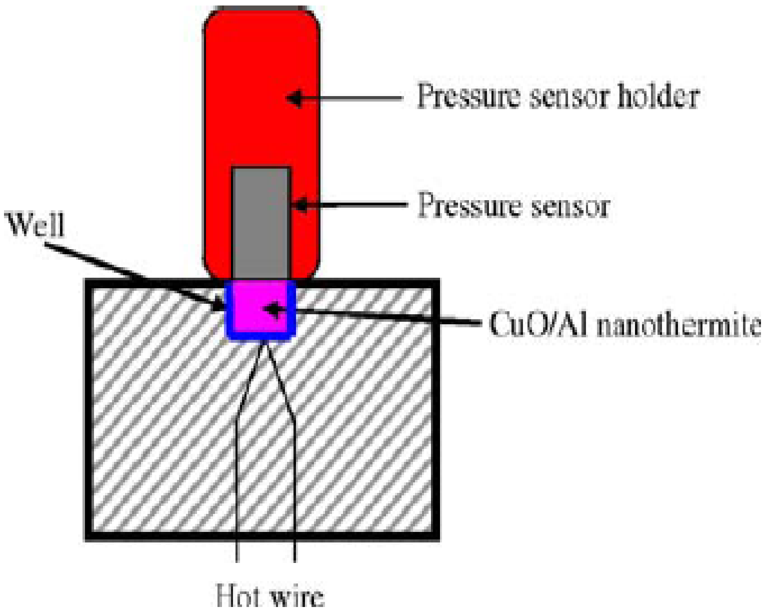


Fig. 1 Experimental setup for the detonation of the CuO/Al nanothermite material

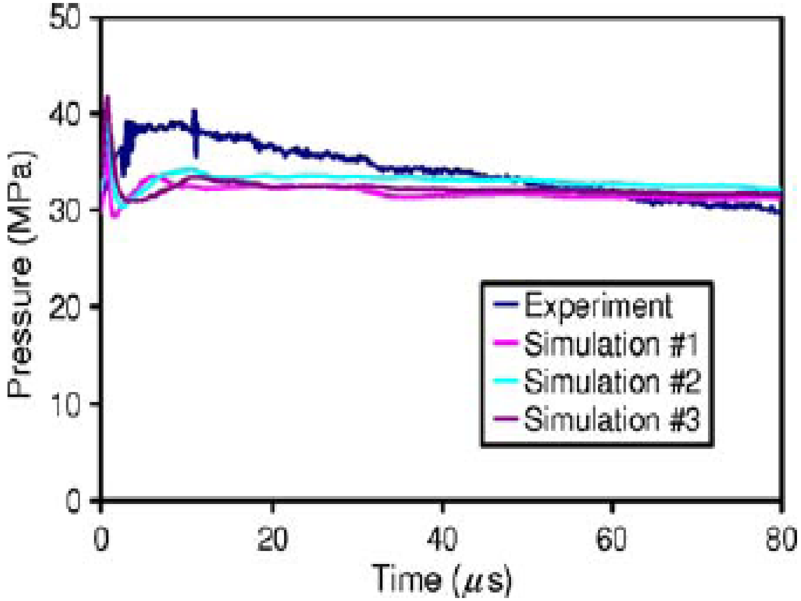
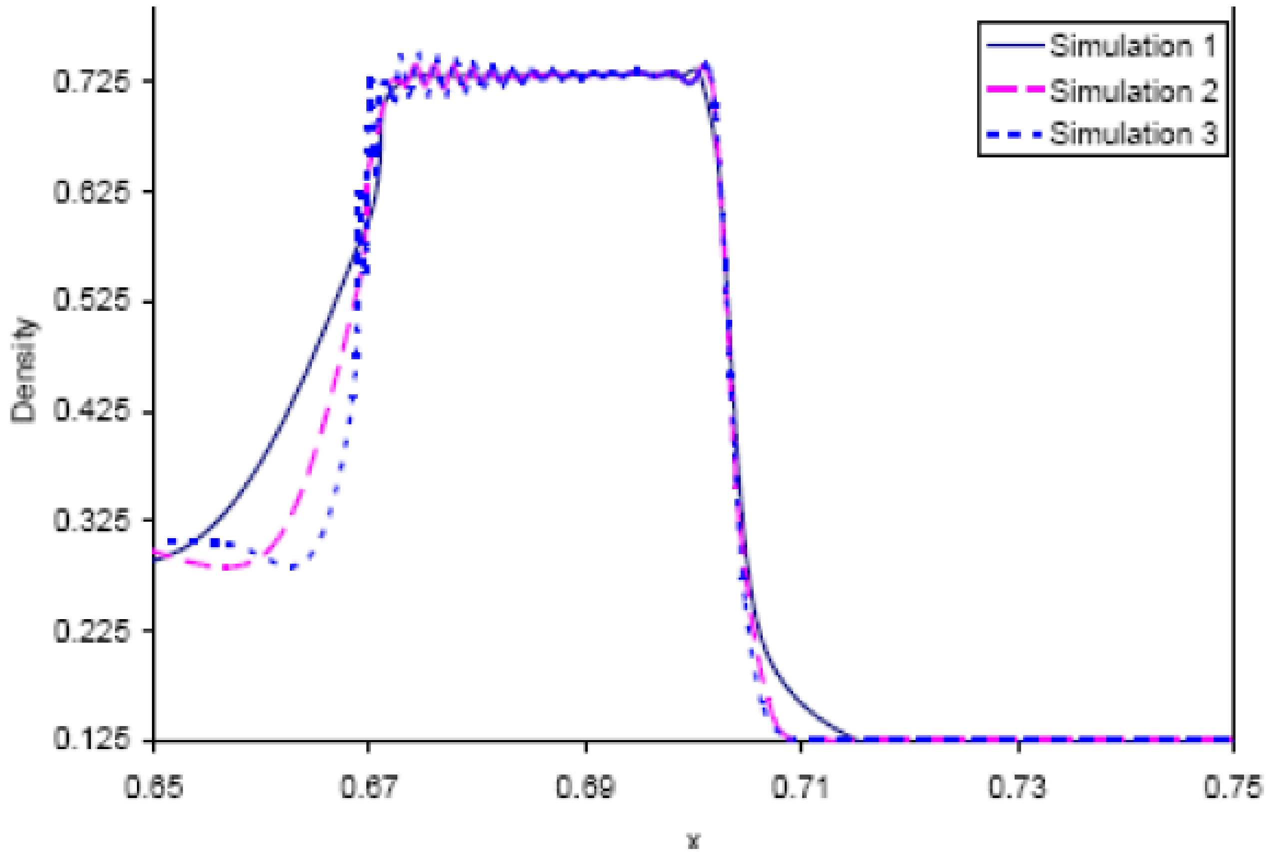


Fig. 7 Comparison of pressure–time histories obtained by the simulations and experiment

Nonlocal Treatment
With Local Artificial Viscosity



The effect of nonlocality on the wave profile in a shock tube at a given time

Particle-Based Multi-Scale Approach

- Use reactive molecular dynamics (rMD) to predict the chemical reactions involved in the detonation process of CuO/Al composites.
- Employ the rMD results to find the forcing field for the reactive dissipative particle dynamics (rDPD).
- Design a nonlocal spatial discretization scheme, via the gradient and/or integral measure of appropriate state variables, for better simulating multi-scale multi-phase interactions within the MPM framework. – *Mapping functions involving both coarse and fine information!*
- Embed the rDPD mesoscale domain into the MPM macroscale domain via the nonlocal mapping functions.

3. Comparative Study with the MPM and MD

- The onset and evolution of dislocation and shear banding under impact loading is the key to understand the initiation of the detonation process of CuO/Al nanothermite composites.

- A comparative study is being performed to investigate the link between different scales.

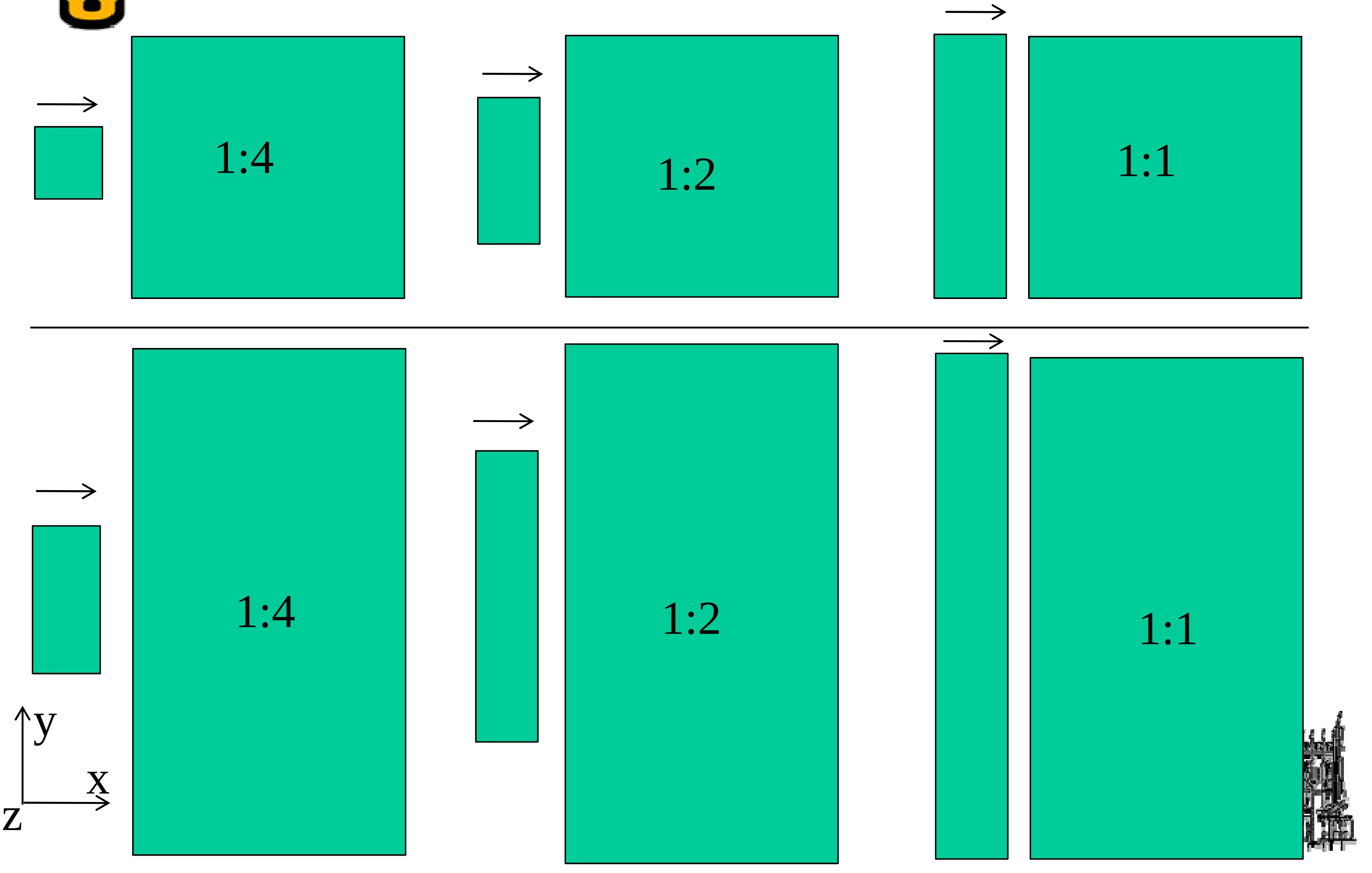
- The molecular dynamics simulation and the MPM study at continuum level have been performed to understand the effects of aspect ratio, boundary conditions, loading types, problem geometry and size on the impact failure evolution at different scales.

Part I: MD simulation

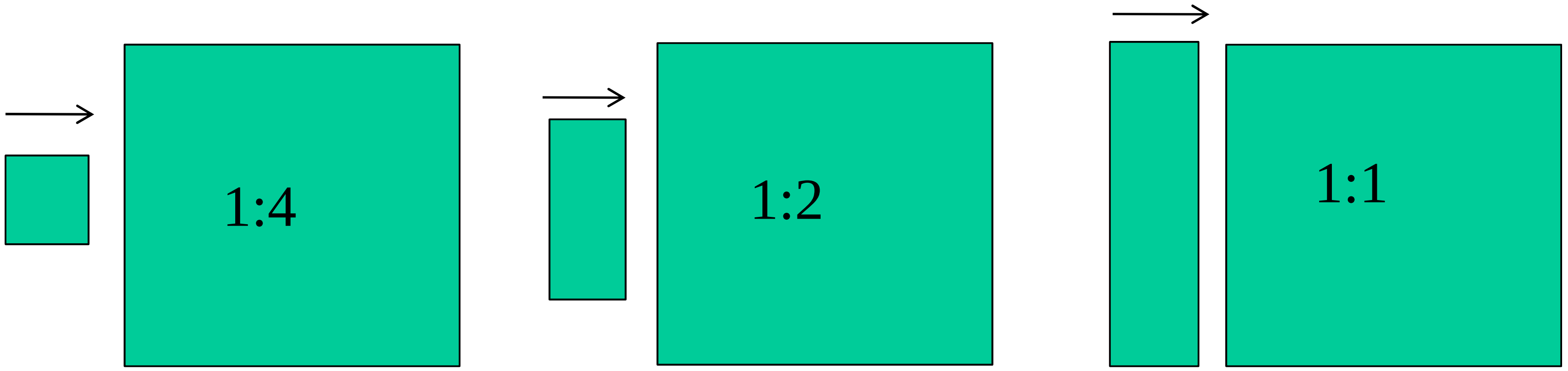
- Material: Cu
- Potential: EAM
- Lattice Constant: *a*= 0.3615 nm
- Initial Temperature: 298 K
- Boundary conditions for plate impact:

X:free; Y:free; Z: periodical

Problem Geometry for Aspect Ratio and Size Effects



1.1 Aspect Ratio Effect

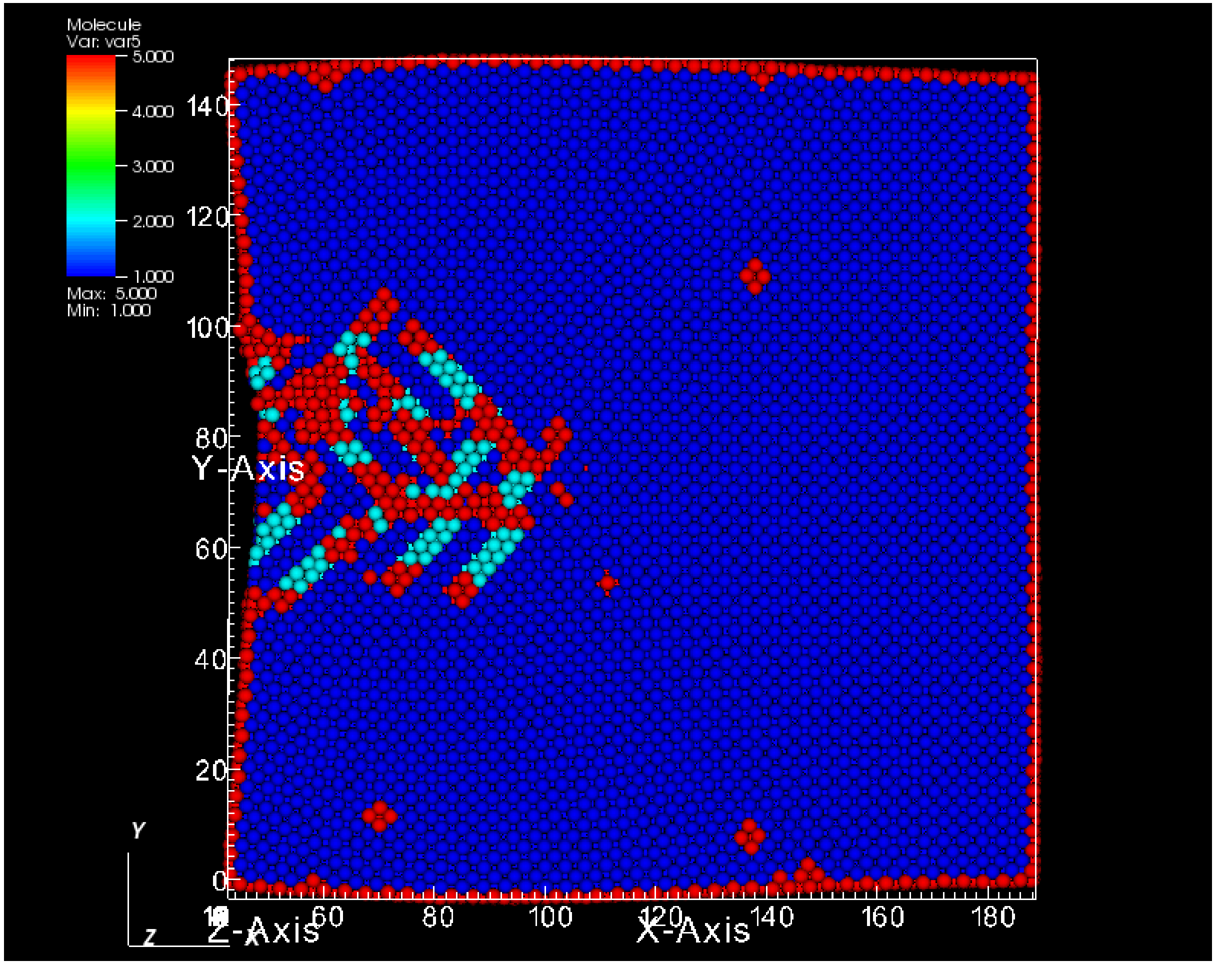


Target: $40a \times 40a = 14.46$ nm×14.46 nm

- Impact velocity : 1000 m/s or 5000 m/s

Flyer: 10a×10a×4a; Target: 40a×40a×4a

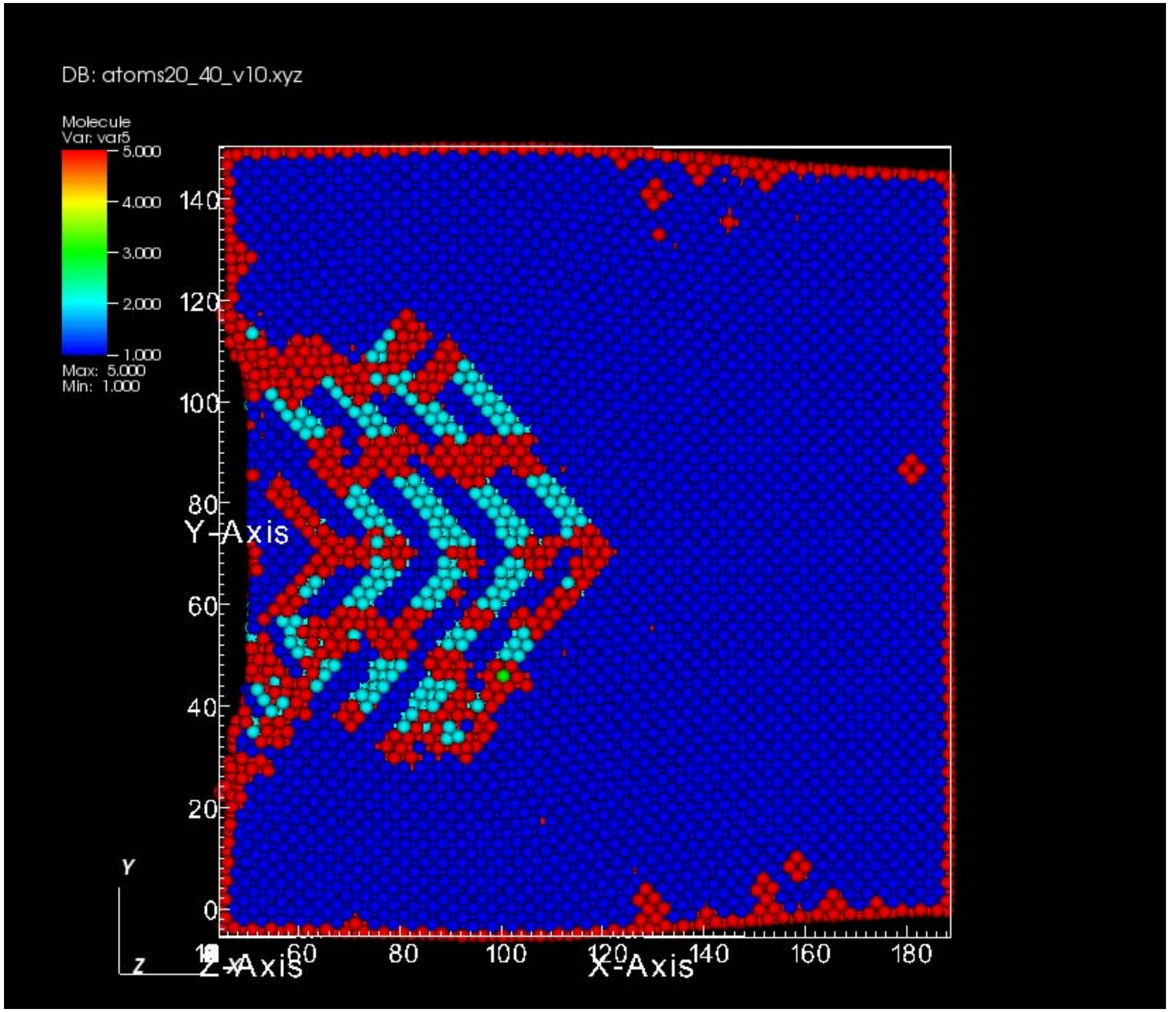
Impact velocity:1000m/s



T=2.77 ps

Flyer: 10*a*×20*a*×4*a*; Target: 40*a*×40*a*×4*a*

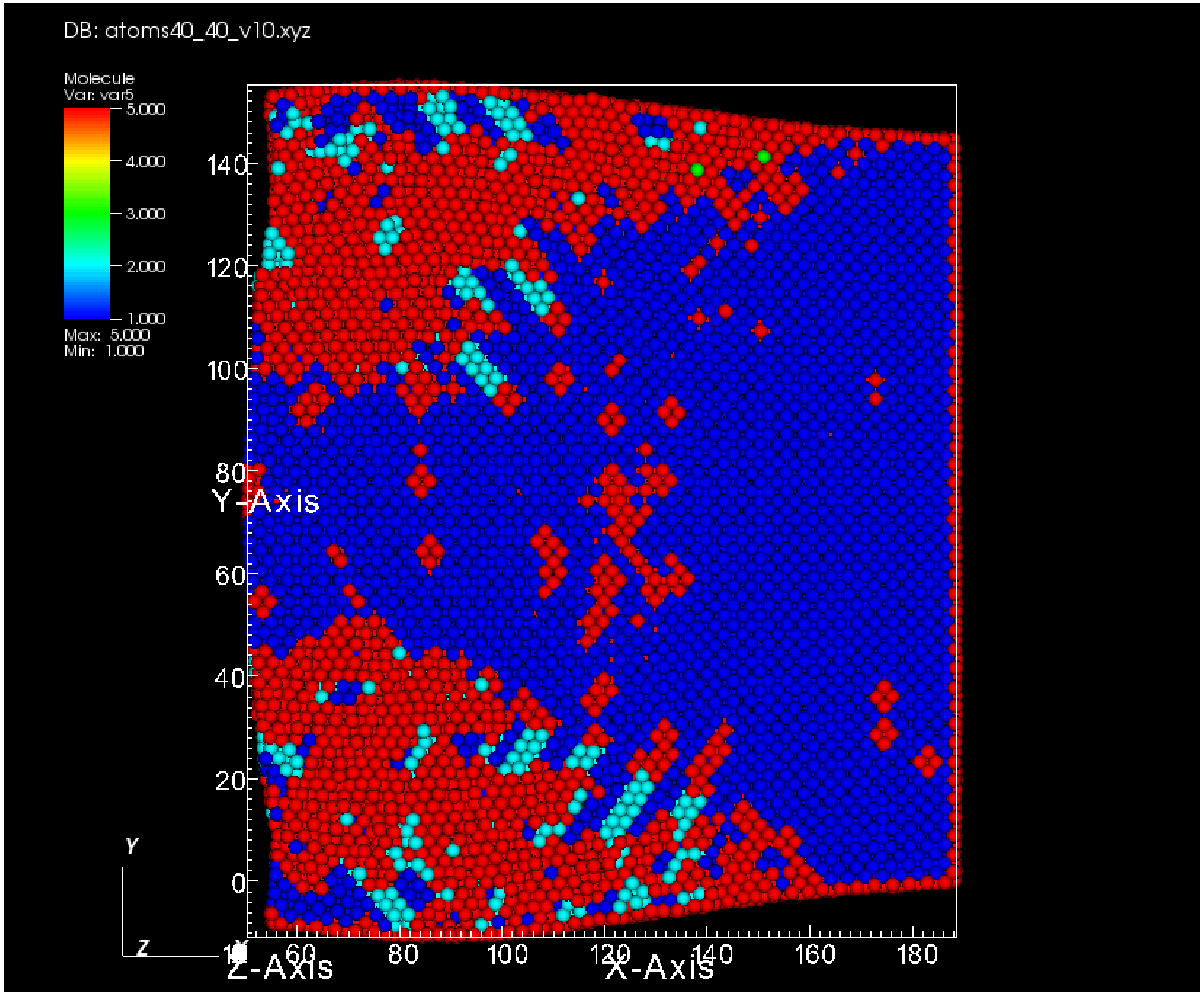
Impact velocity:1000m/s



T=2.77 ps

Flyer: 10*a*×40*a*×4*a*; Target: 40*a*×40*a*×4*a*

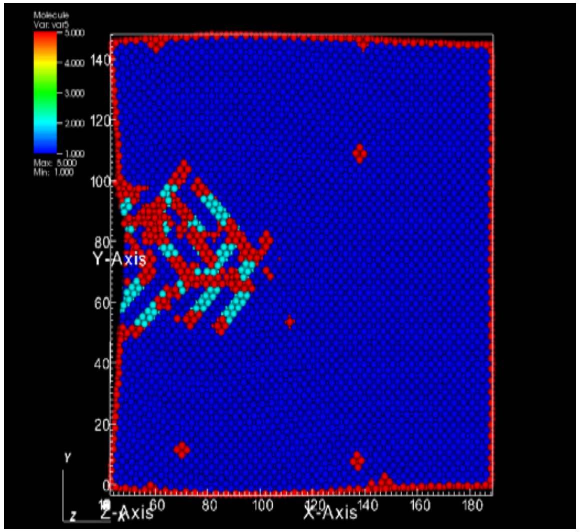
Impact velocity:1000m/s



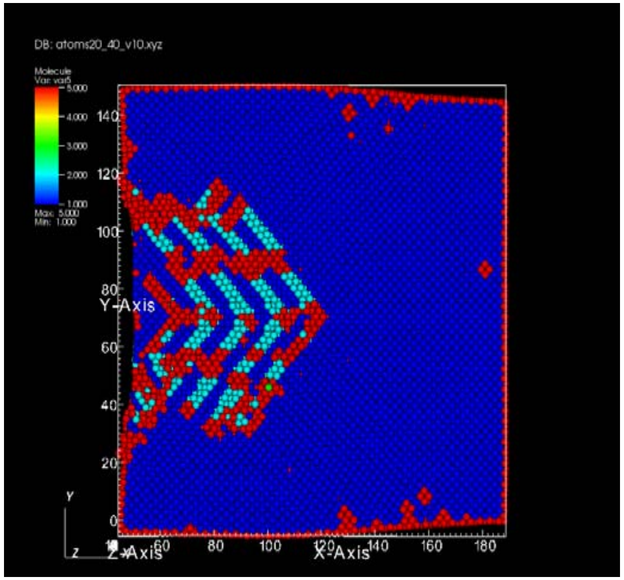
T=2.77 ps

Comparison for the Aspect Ratio Effect

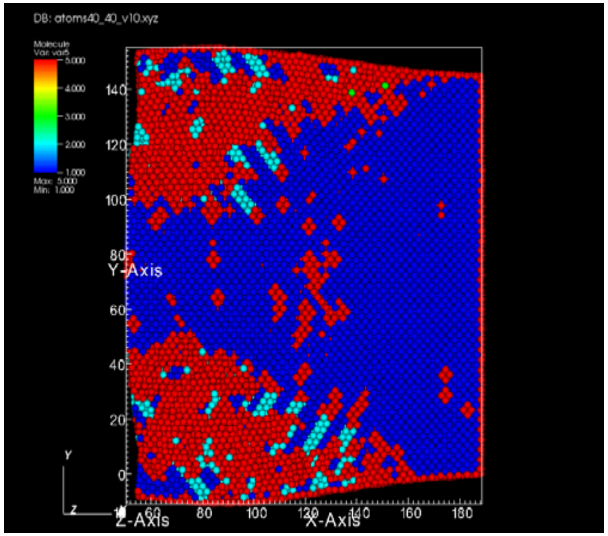
Impact velocity:1000m/s



Flyer: 10*a*×10*a*×4*a*;
Target: 40*a*×40*a*×4*a*



Flyer: 10*a*×20*a*×4*a*;
Target: 40*a*×40*a*×4*a*

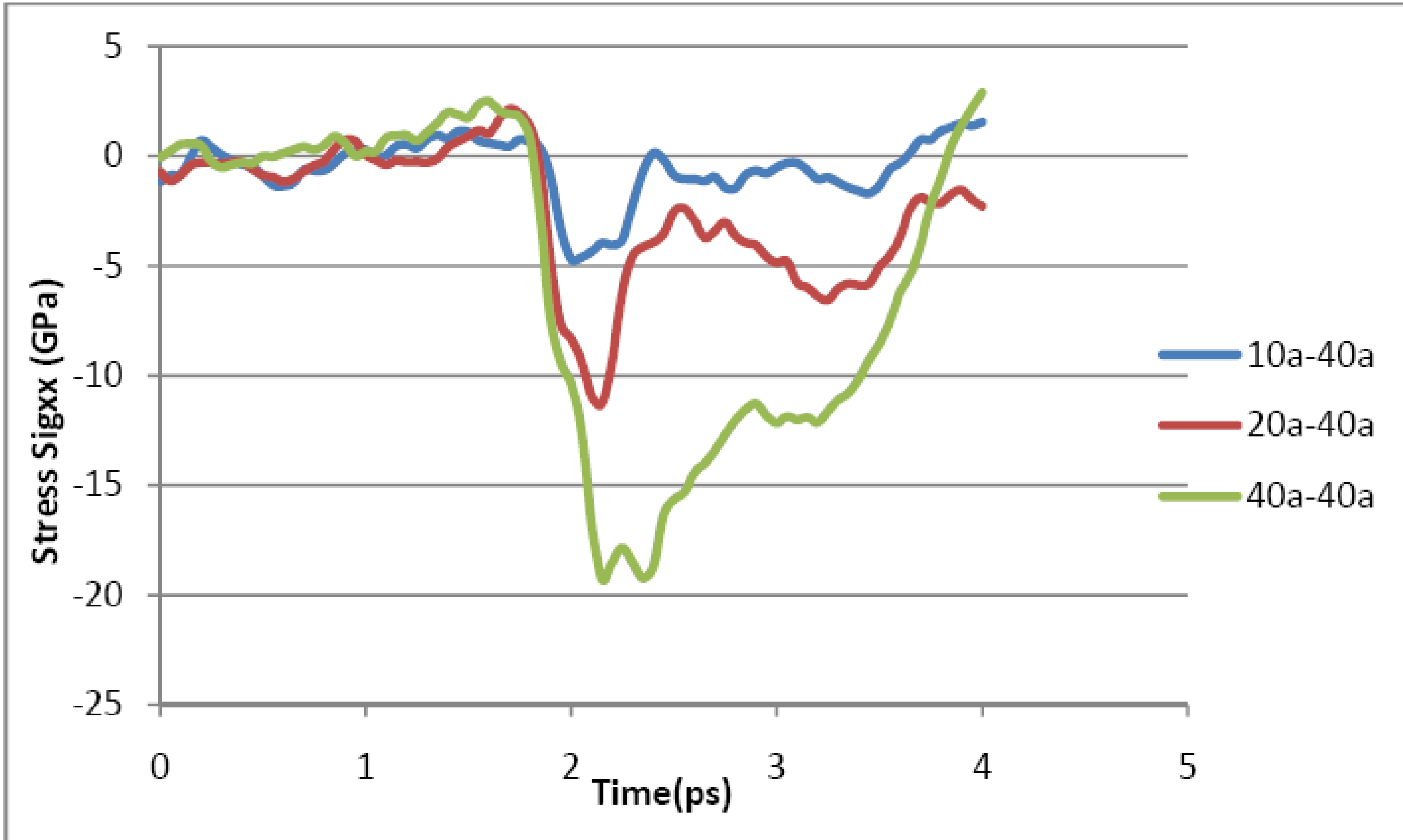


Flyer: 10*a*×40*a*×4*a*;
Target: 40*a*×40*a*×4*a*

T=2.77 ps

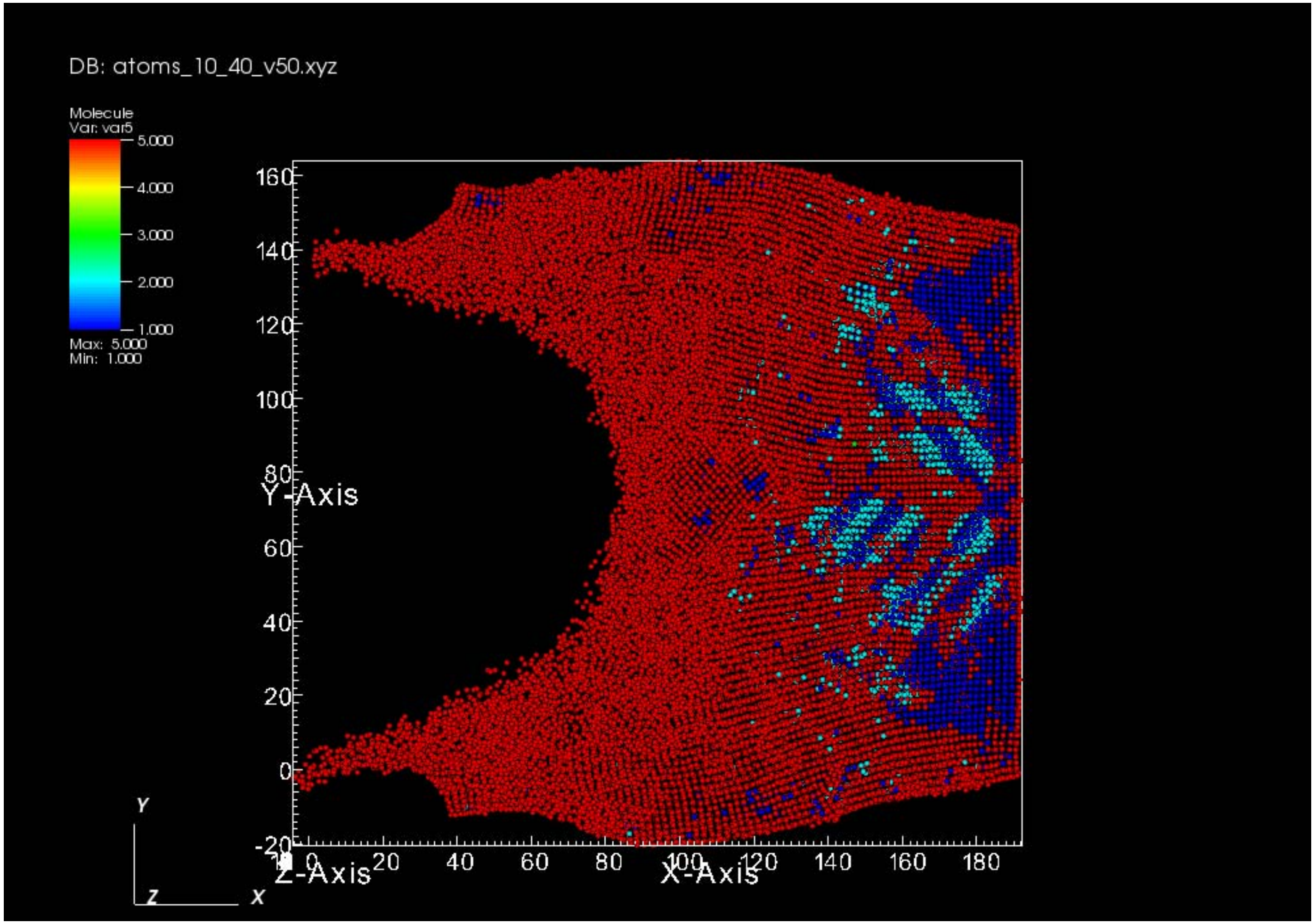
Stress Histories in the Middle of Target

Impact velocity:1000m/s



Flyer: 10a×10a×4a; Target: 40a×40a×4a

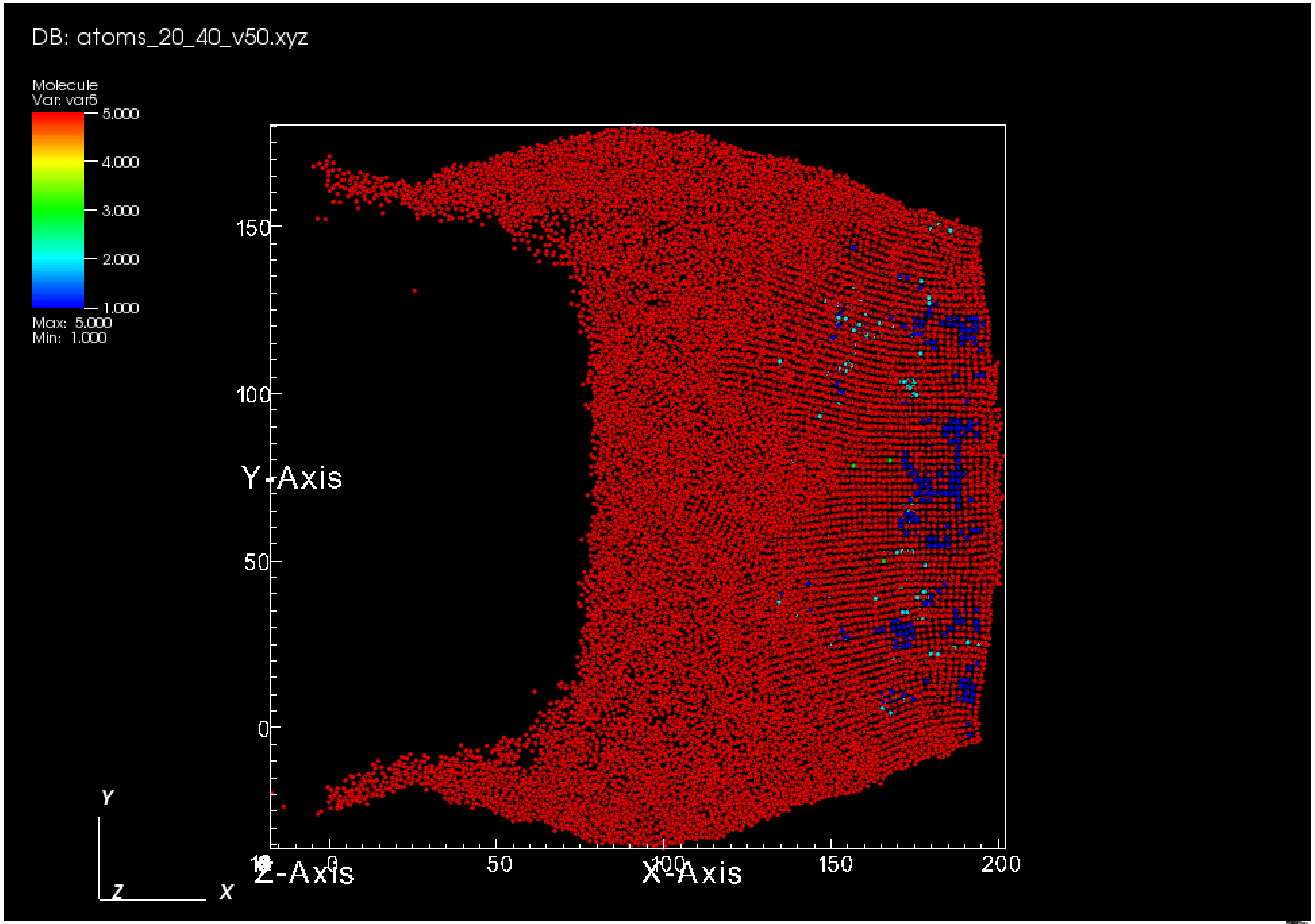
Impact velocity: 5000m/s



T=2.77 ps

Flyer: 10a×20a×4a; Target: 40a×40a×4a

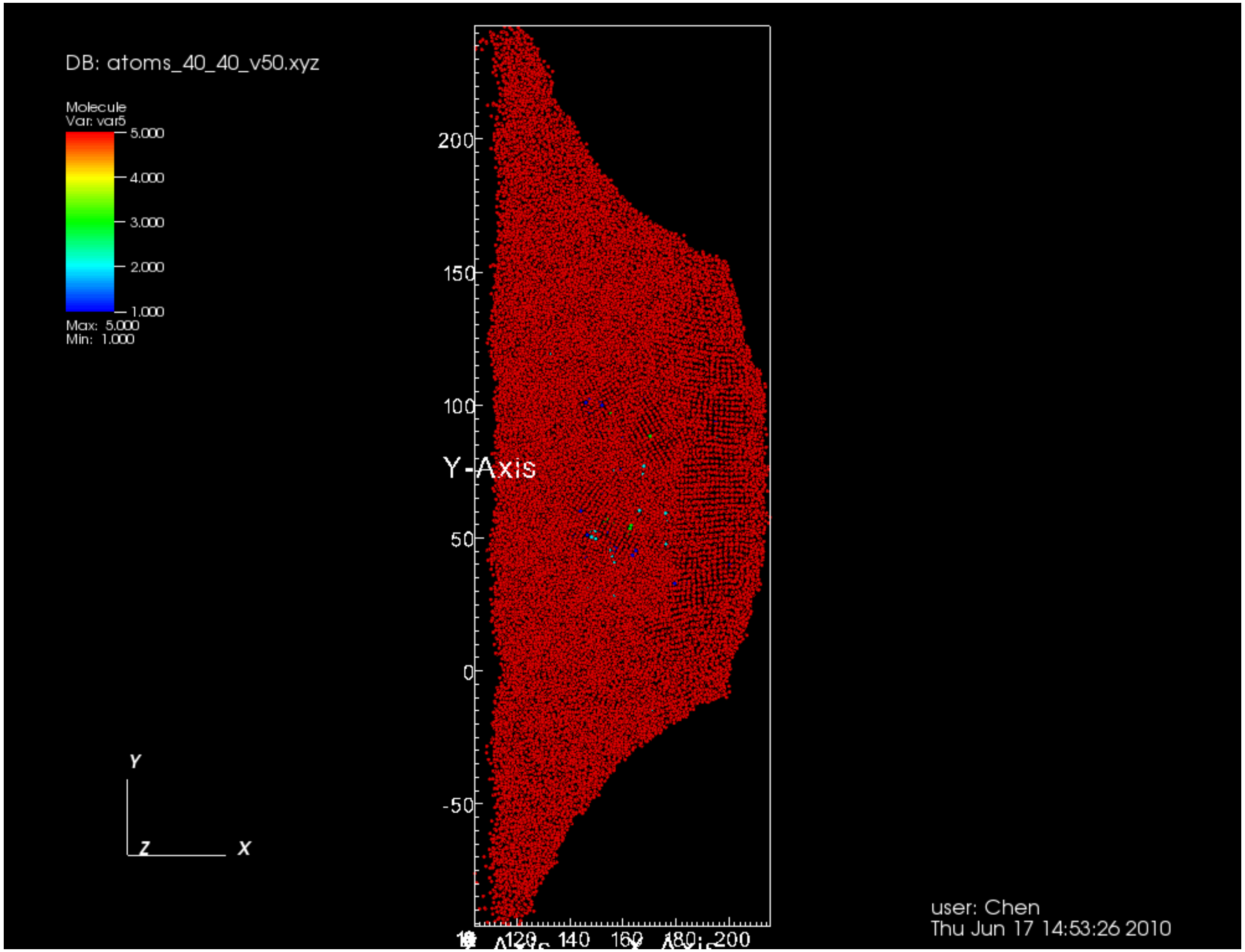
Impact velocity: 5000m/s



T=2.77 ps

Flyer: 10a×40a×4a; Target: 40a×40a×4a

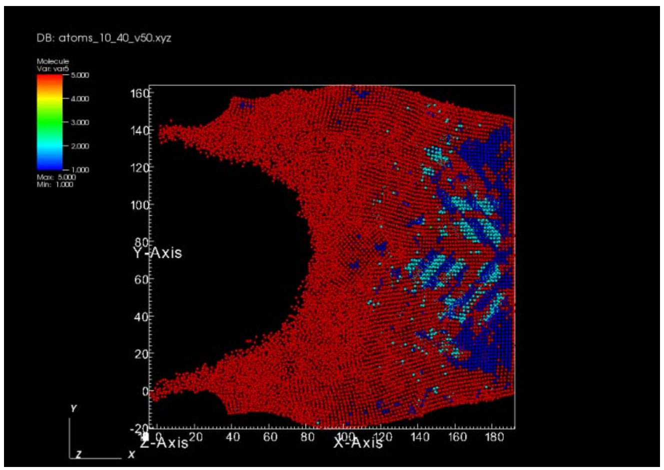
Impact velocity: 5000m/s

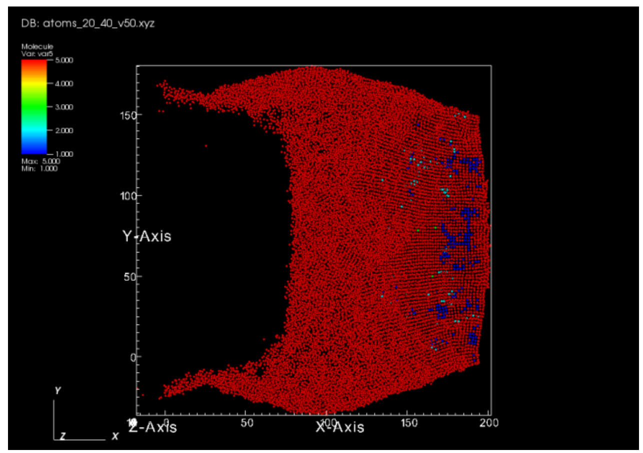


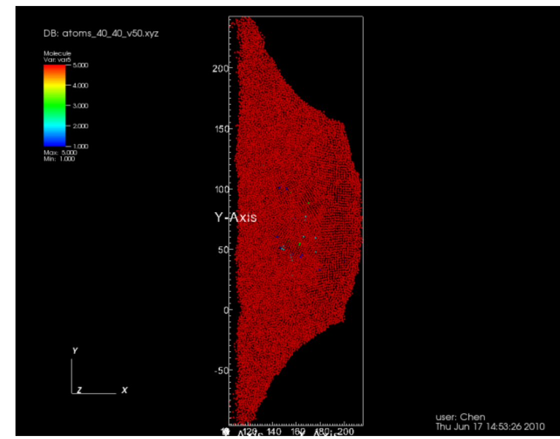
T=2.77 ps

Comparison for the Aspect Ratio Effect

Impact velocity:5000m/s







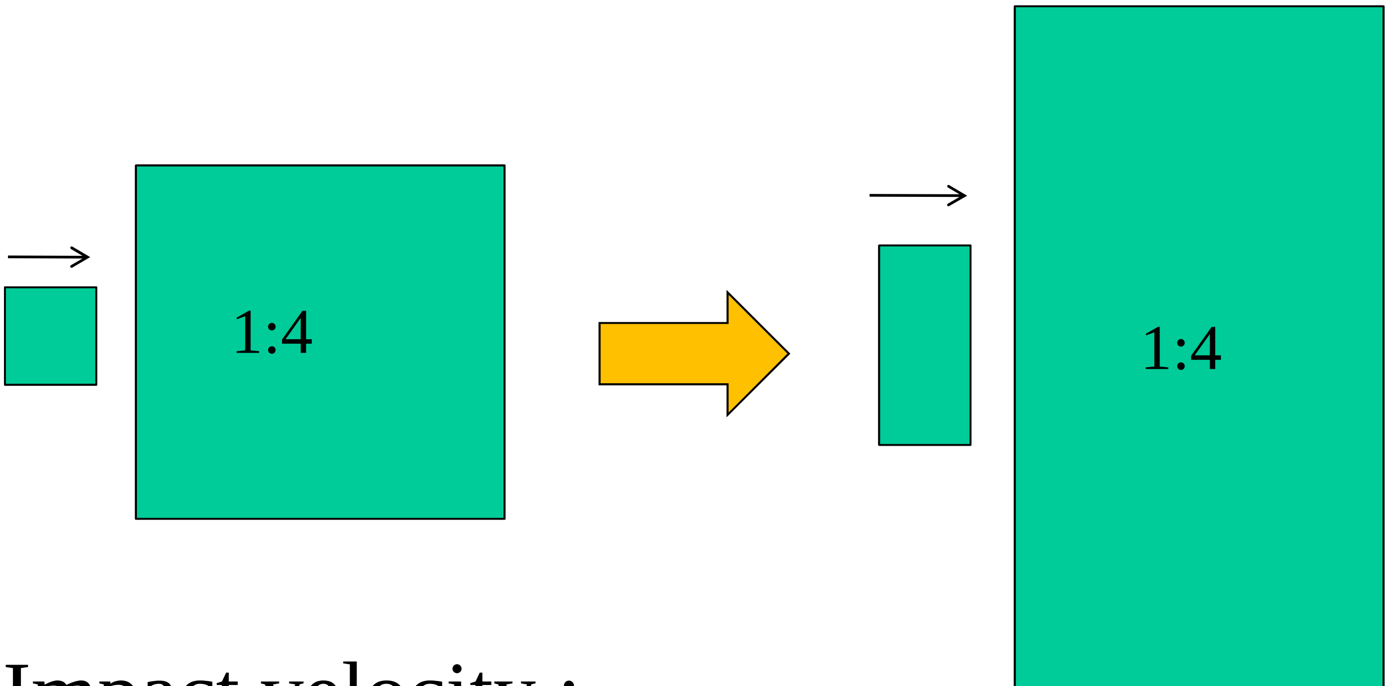
Flyer: 10*a*×10*a*×4*a*;
Target: 40*a*×40*a*×4*a*

Flyer: 10*a*×20*a*×4*a*;
Target: 40*a*×40*a*×4*a*

Flyer: 10*a*×40*a*×4*a*;
Target: 40*a*×40*a*×4*a*

T=2.77 ps

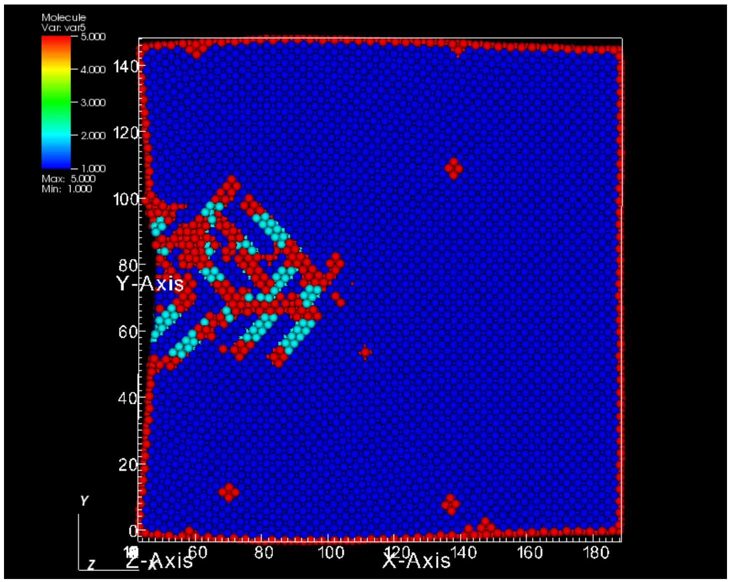
1.2 Size Effect

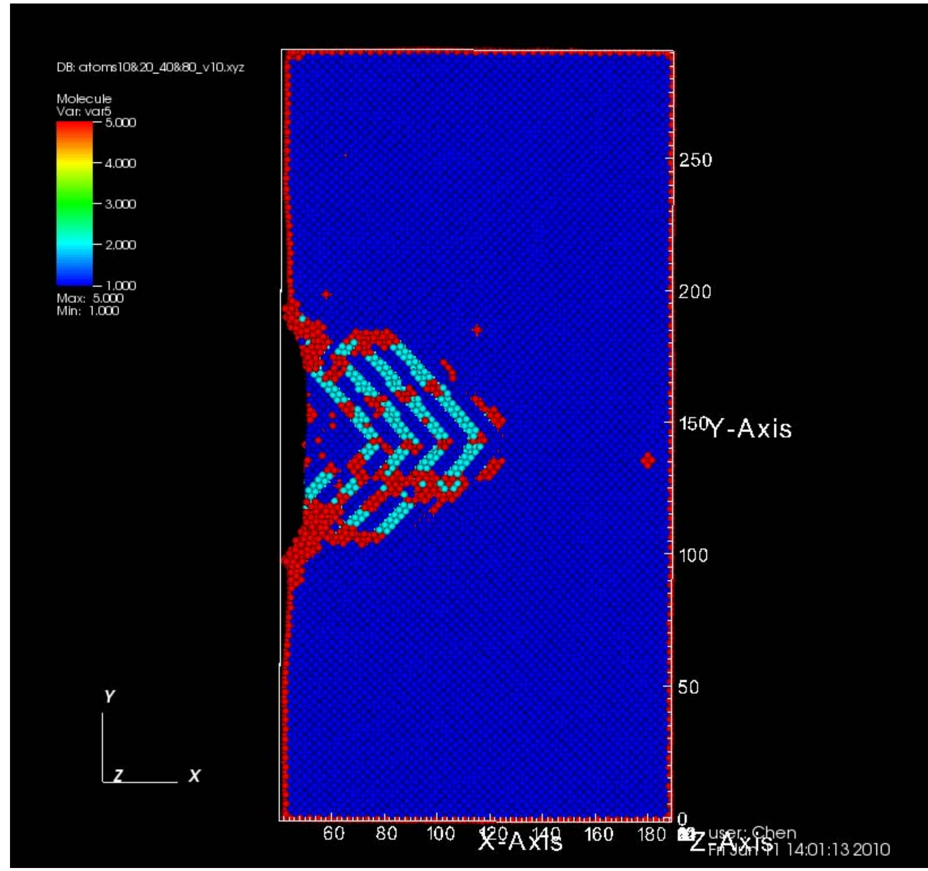


- Impact velocity : 1000 m/s

Flyer: $10a\times10a\times4a$;
Target: $40a\times40a\times4a$

Flyer: $10a\times20a\times4a$;
Target: $40a\times80a\times4a$



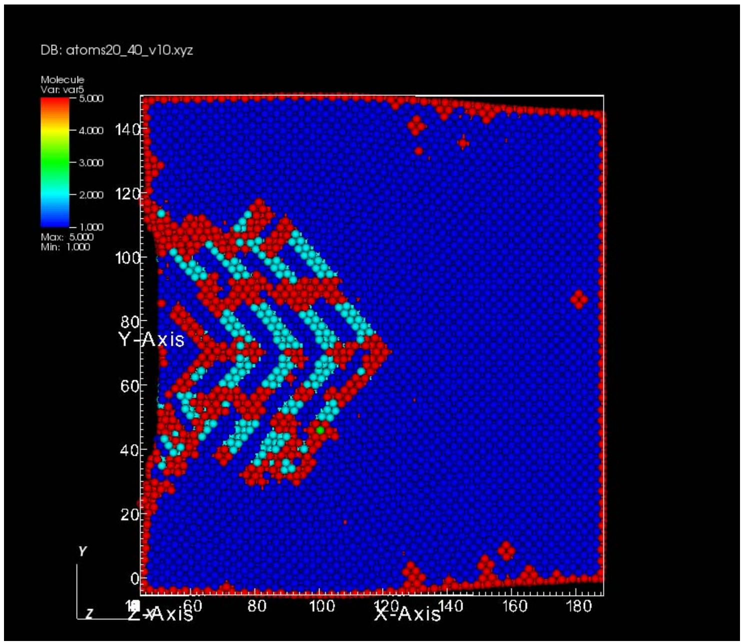


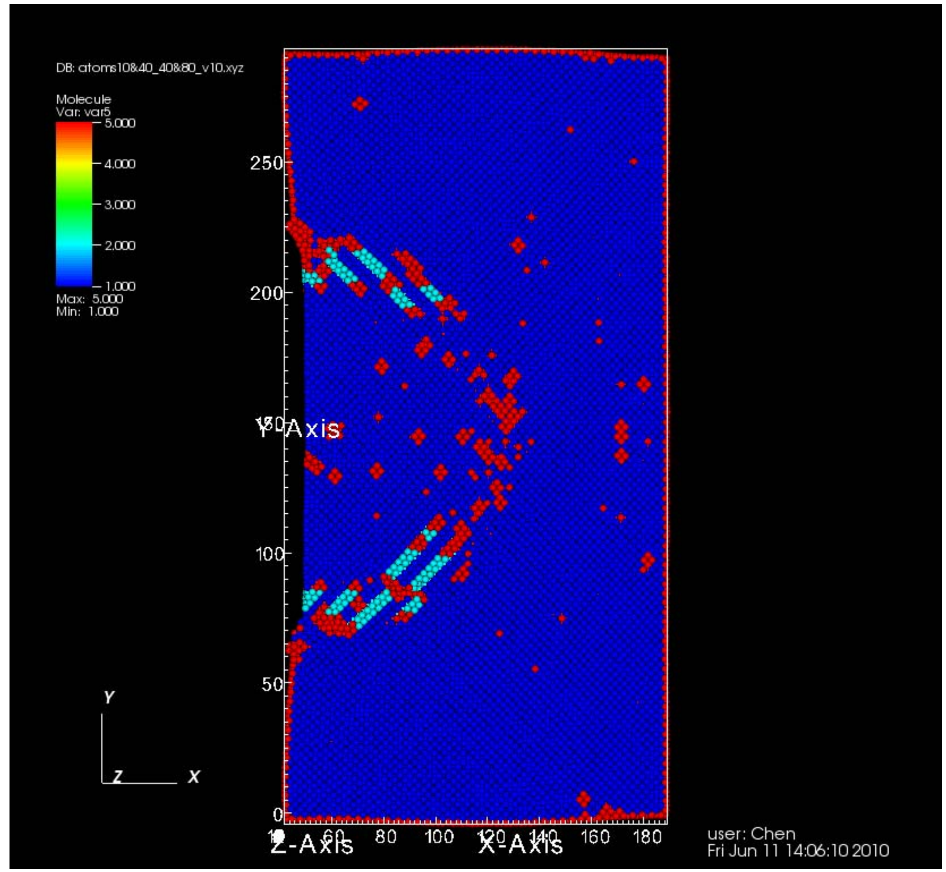
Impact velocity:1000m/s

T=2.77 ps

Flyer: $10a \times 20a \times 4a$;
Target: $40a \times 40a \times 4a$

Flyer: $10a \times 40a \times 4a$;
Target: $40a \times 80a \times 4a$



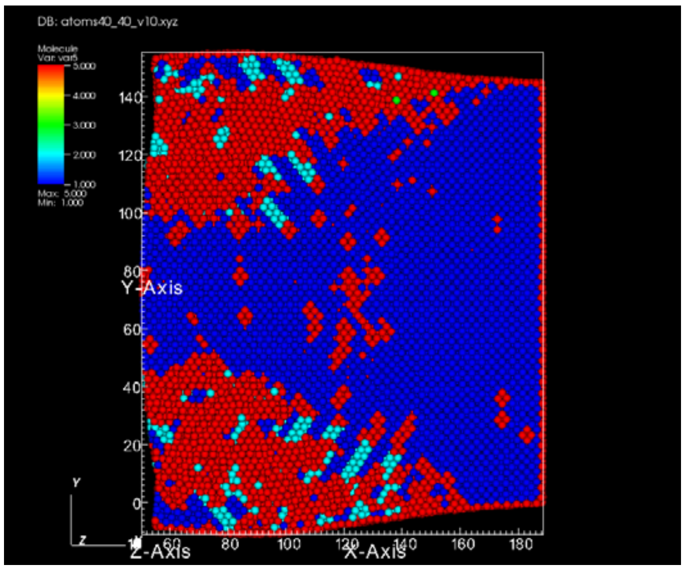


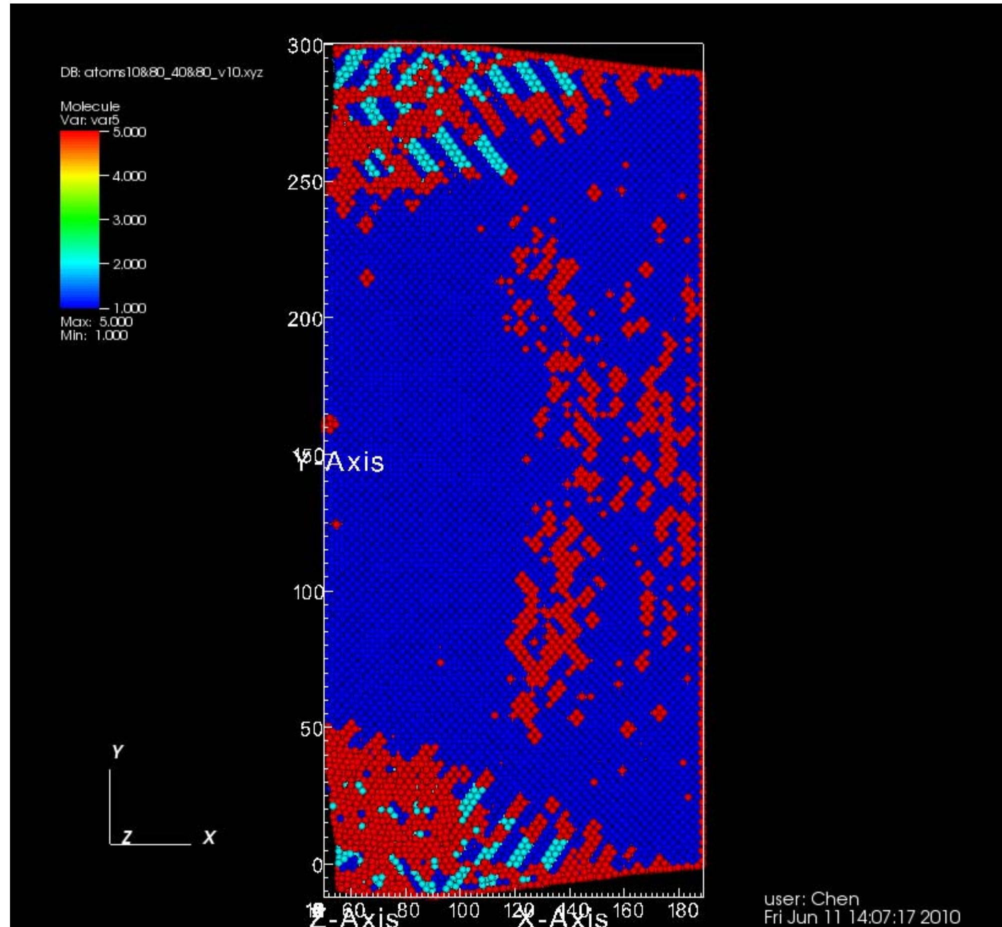
Impact velocity:1000m/s

T=2.77 ps

Flyer: $10a \times 40a \times 4a$; Target: $40a \times 40a \times 4a$

Flyer: $10a \times 80a \times 4a$; Target: $40a \times 80a \times 4a$





Impact velocity:1000m/s

T=2.77 ps

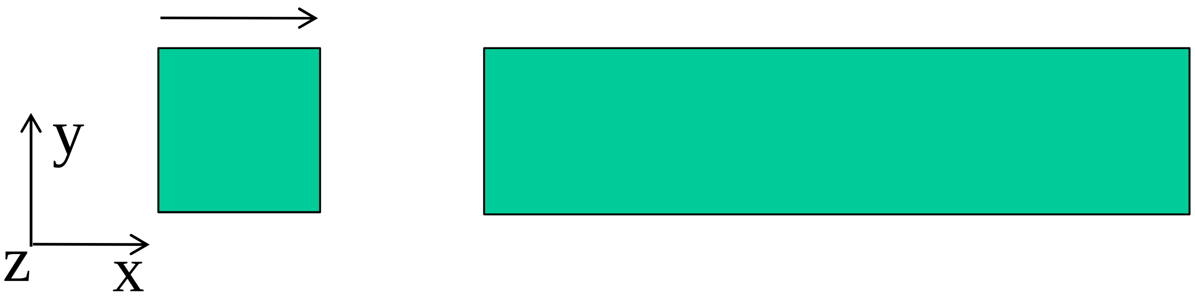
1.3 Boundary and Loading Effects

X:free; Y:free; Z: periodical → X :Free; Y: Periodical; Z: Periodical

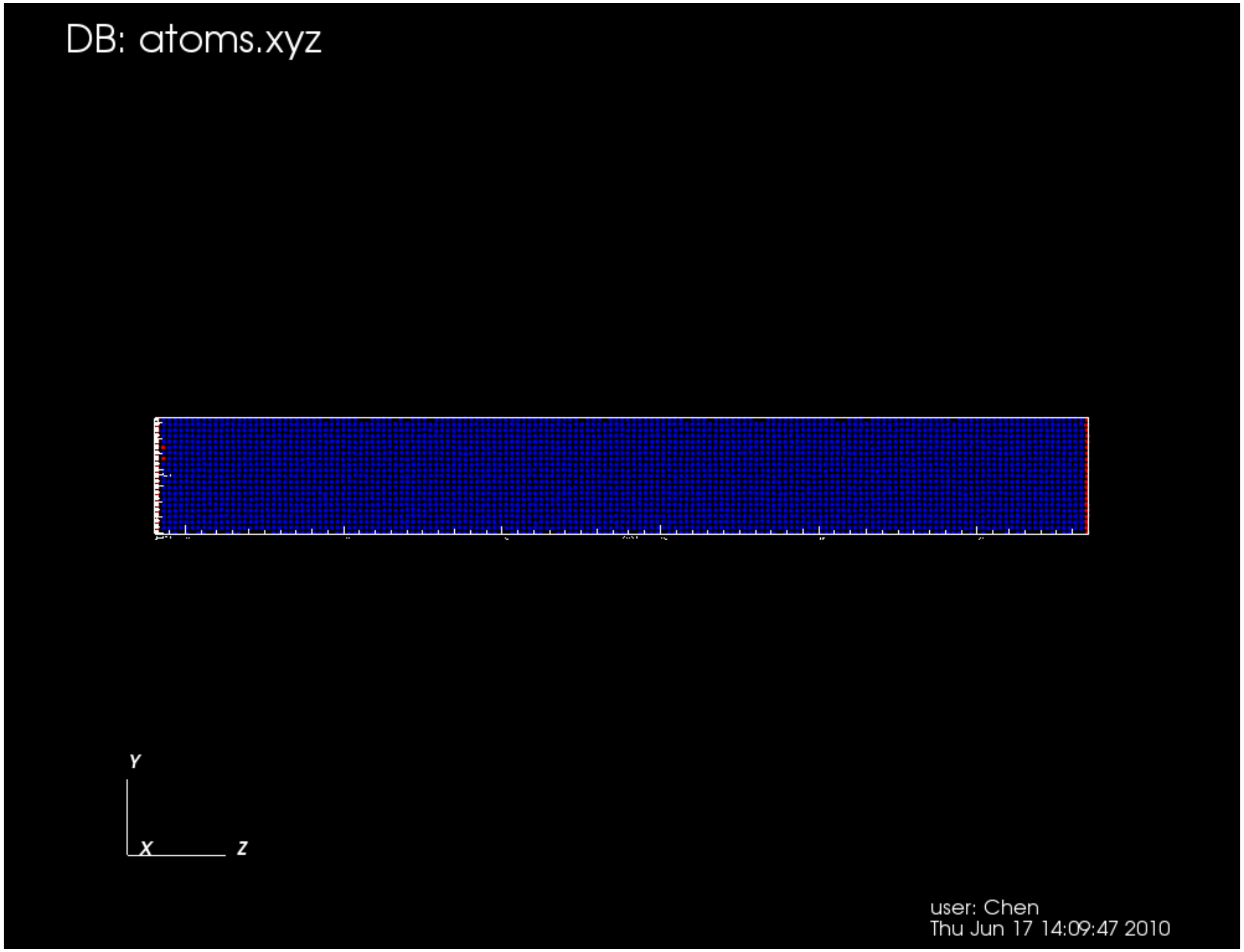
Flyer: $10a \times 10a \times 4a$;

Target: $10a \times 40a \times 4a$;

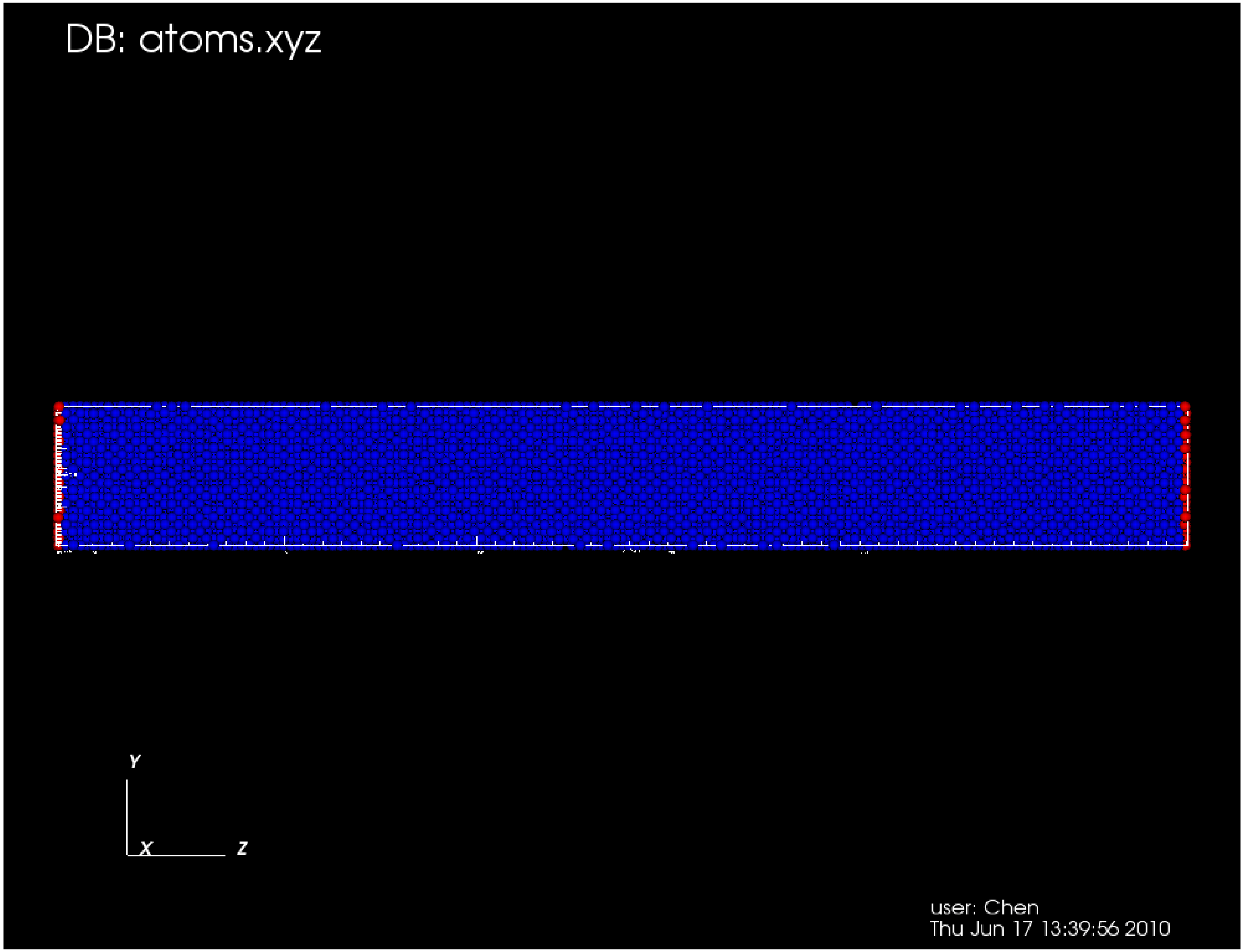
- Case1: Initial impact velocity of 1000 m/s
- Case2: Constant impact velocity of 1000 m/s



Case1: Initial impact velocity of 1000 m/s



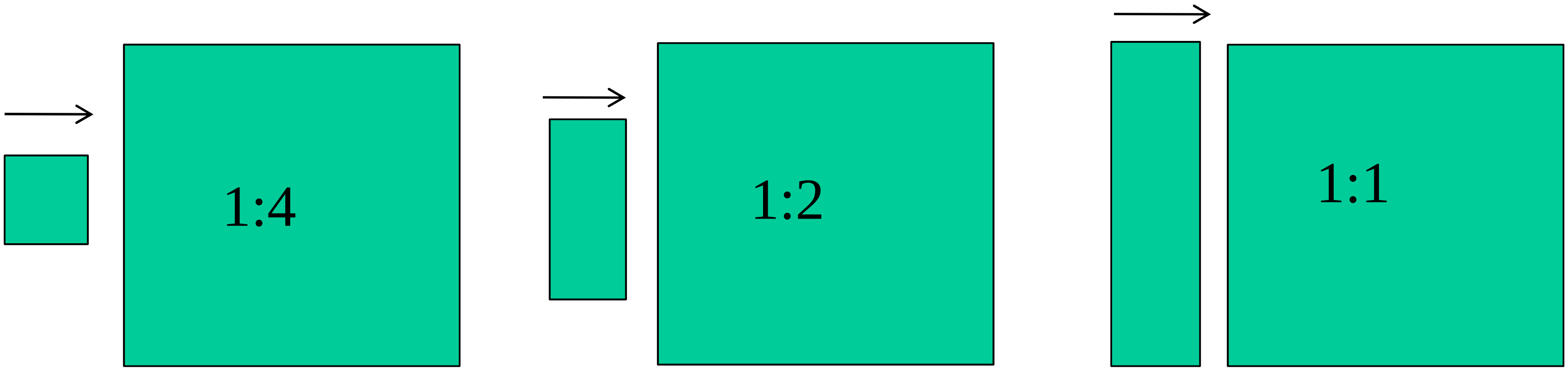
Case2: Constant impact velocity of 1000 m/s



Part II: MPM simulation

- Material: Cu
- Density: 8.92×10^3 kg/m^3
- Young's Modulus: 120 GPa
- Poisson's Ratio: 0.34
- Yield Strength: 70 MPa
- Peak Strength: 200 MPa
- Yield criterion: Von Mises Model
- Problem geometry: 2D Plane Strain, X, Y free

2.1 Aspect Ratio Effect



1.6m×1.6 m

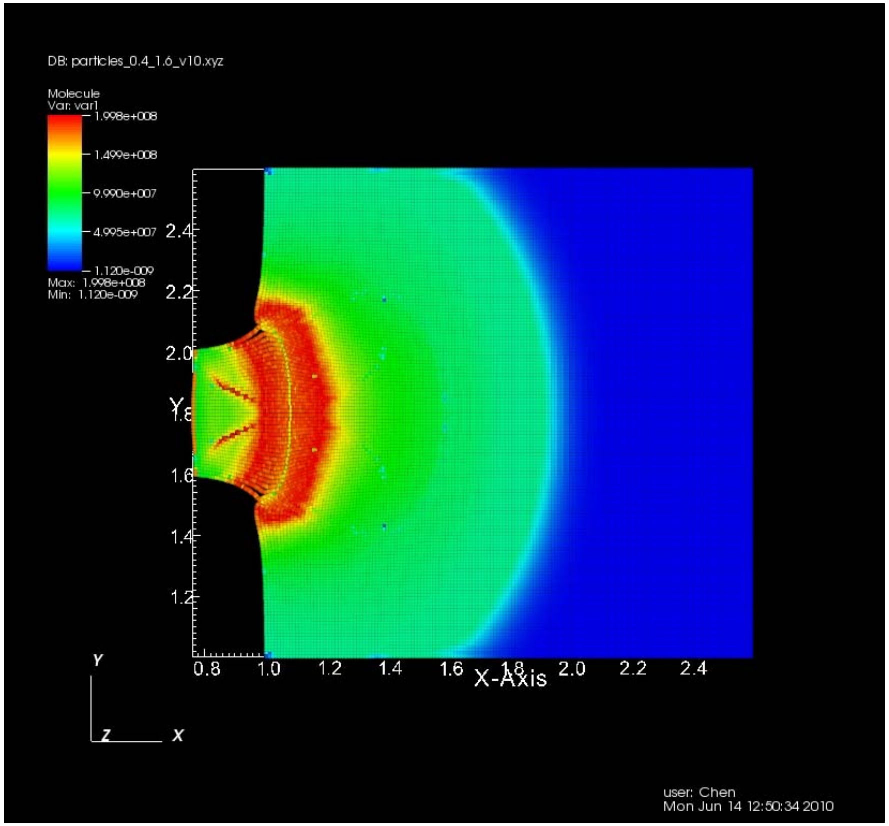
- Impact velocity : 1000 m/s or 5000 m/s

2.1 Aspect Ratio Effect

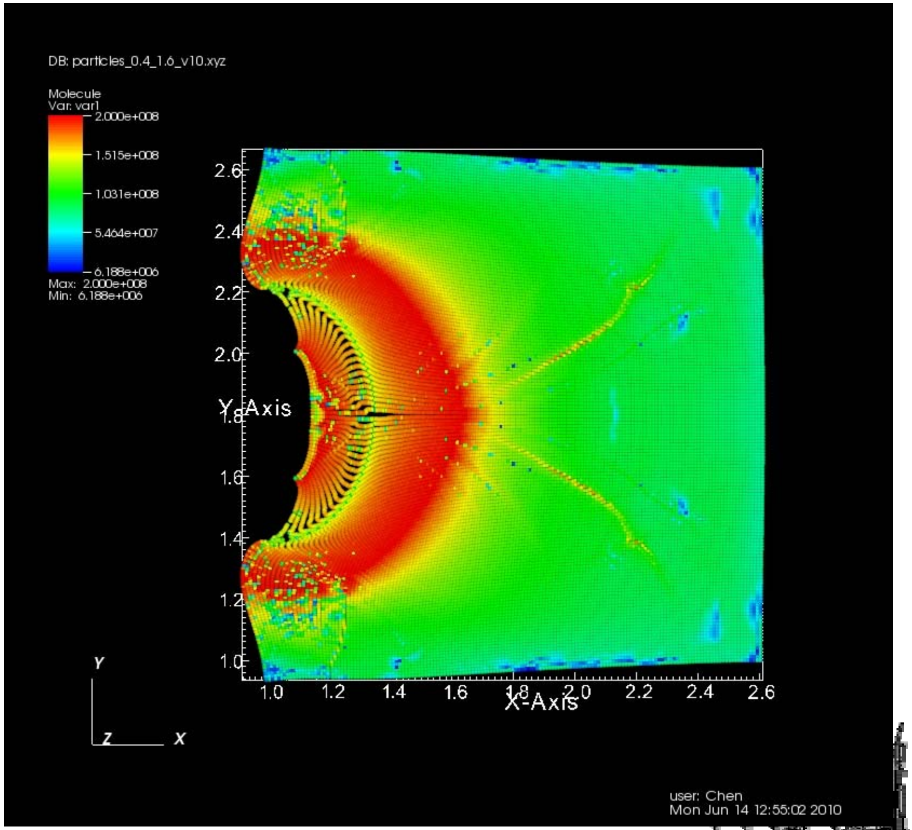
Flyer: 0.4m×0.4m; Target: 1.6m×1.6m

Impact velocity:1000m/s

Stress Distribution



T=0.18 ms

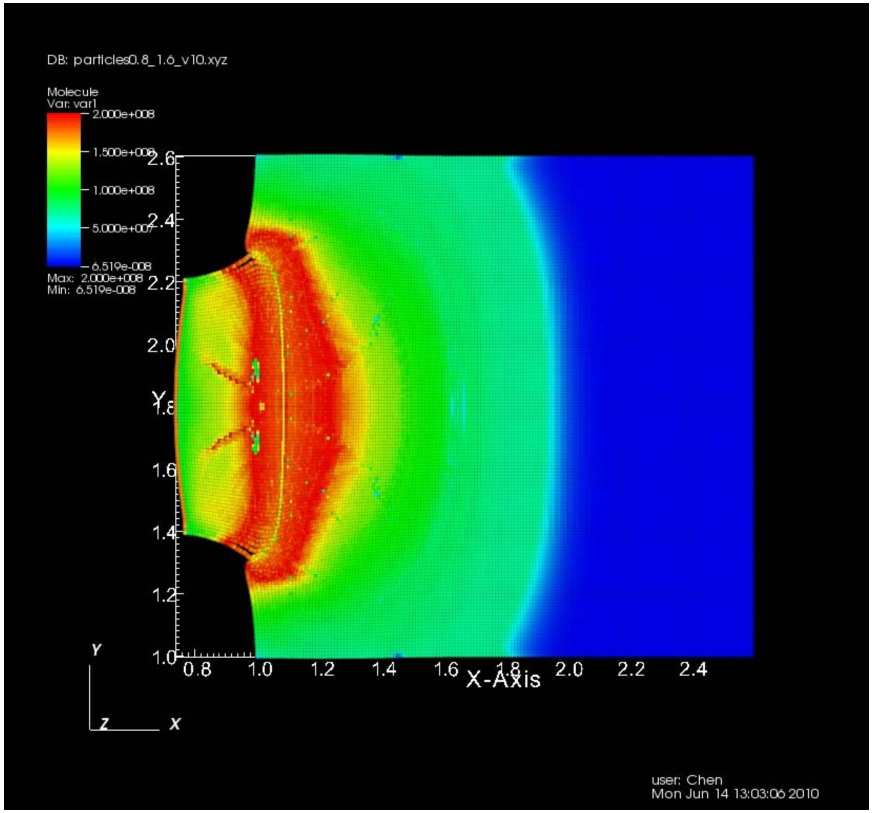


T=0.88 ms

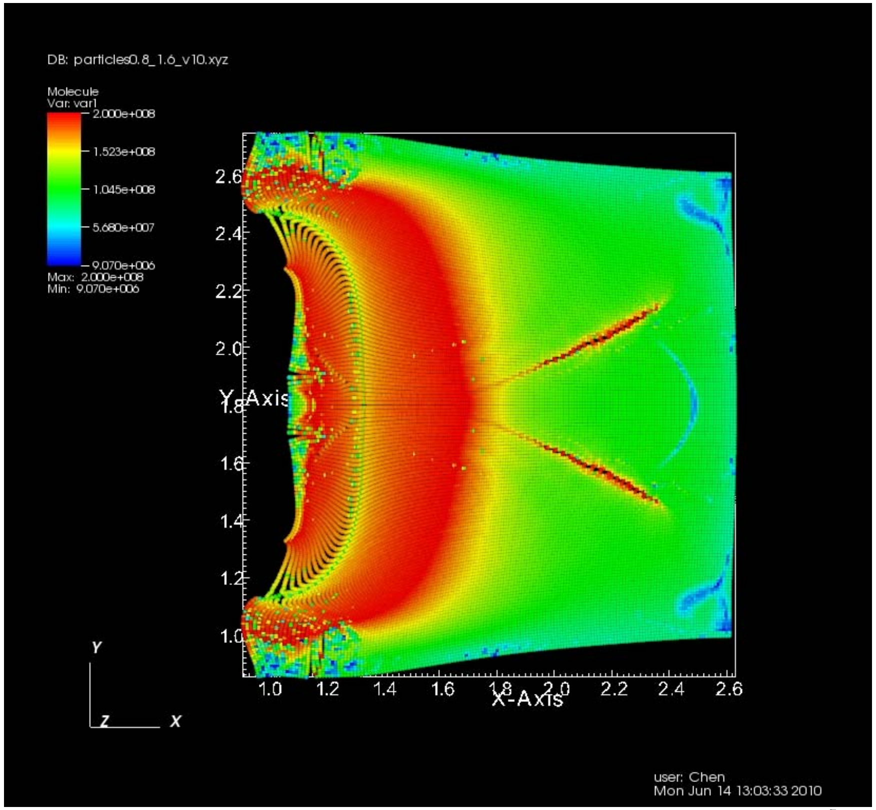
Flyer: 0.4m×0.8m; Target: 1.6m×1.6m

Impact velocity:1000m/s

Stress Distribution



T=0.18 ms

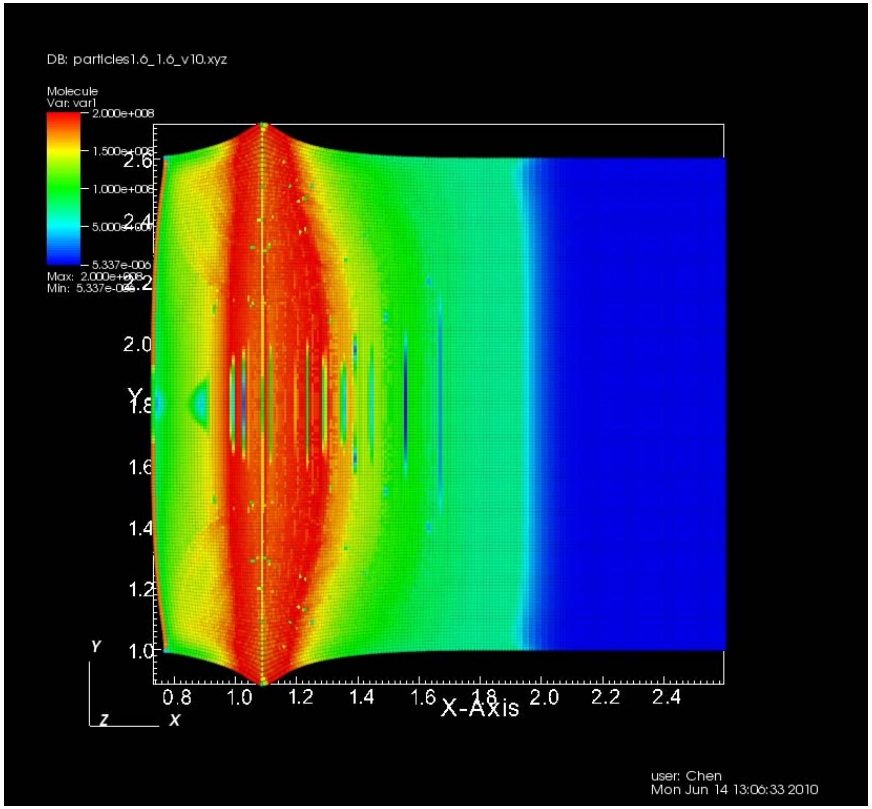


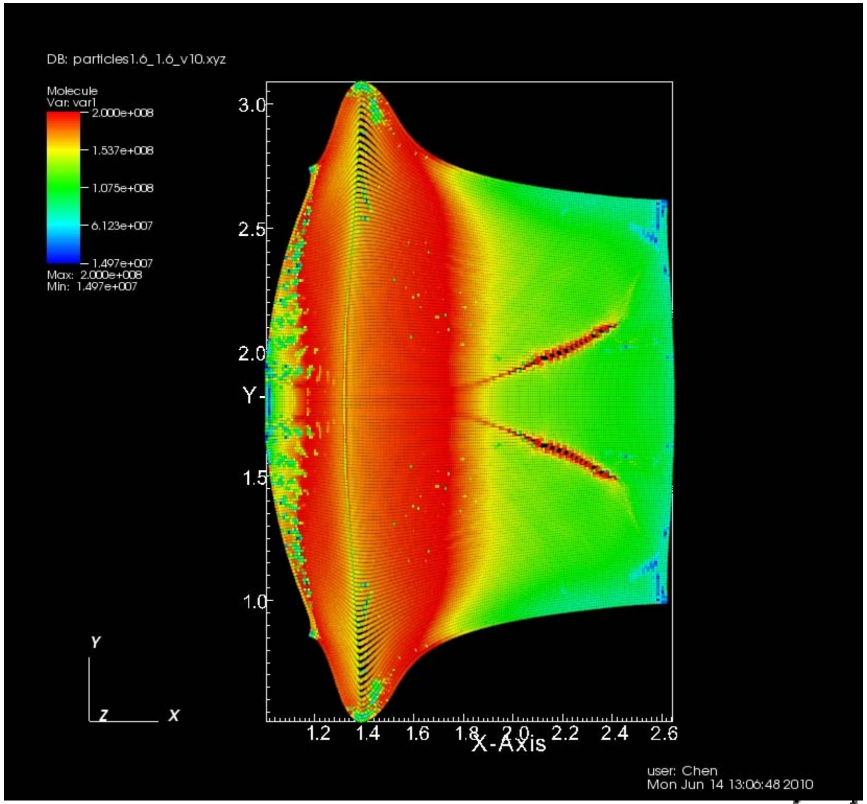
T=0.88 ms

Flyer: 0.4m×1.6m; Target: 1.6m×1.6m

Impact velocity:1000m/s

Stress Distribution





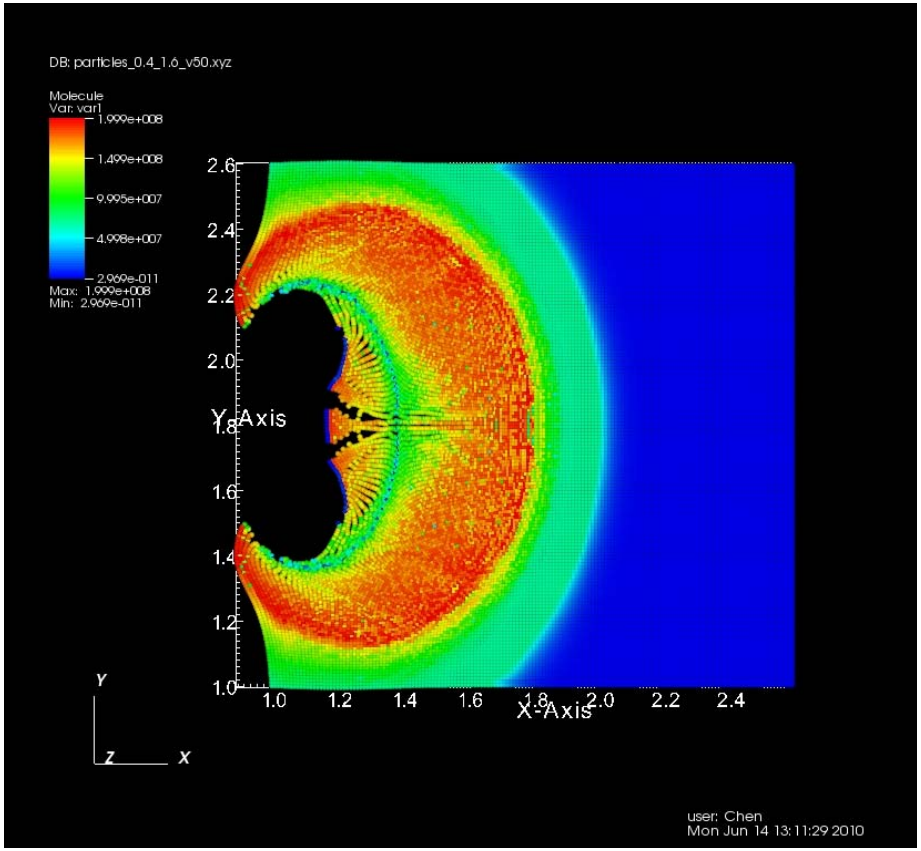
T=0.18 ms

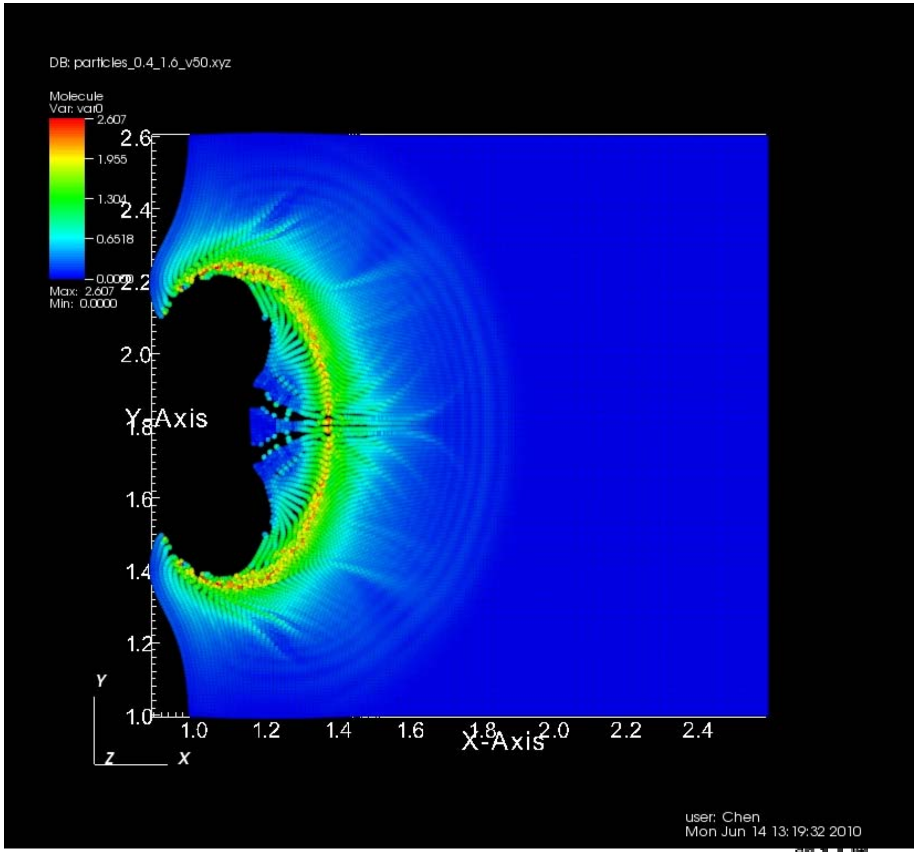
T=0.88 ms

Flyer: 0.4m×0.4m; Target: 1.6m×1.6m

Impact velocity:5000m/s

T=0.172 ms



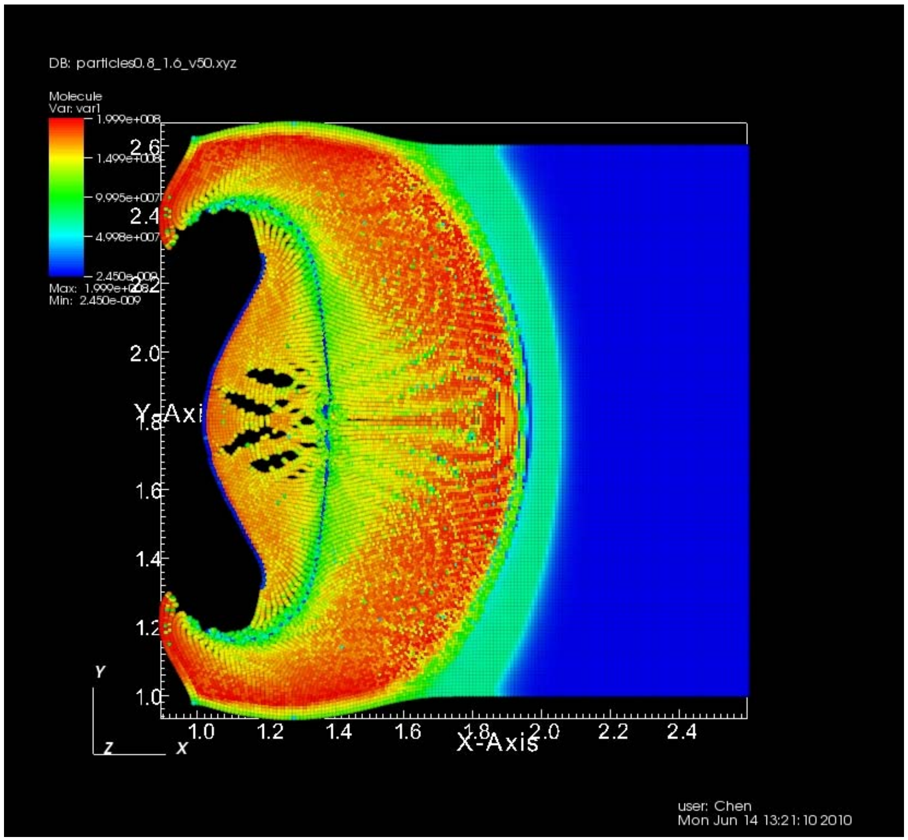


Stress Distribution **Strain Distribution**

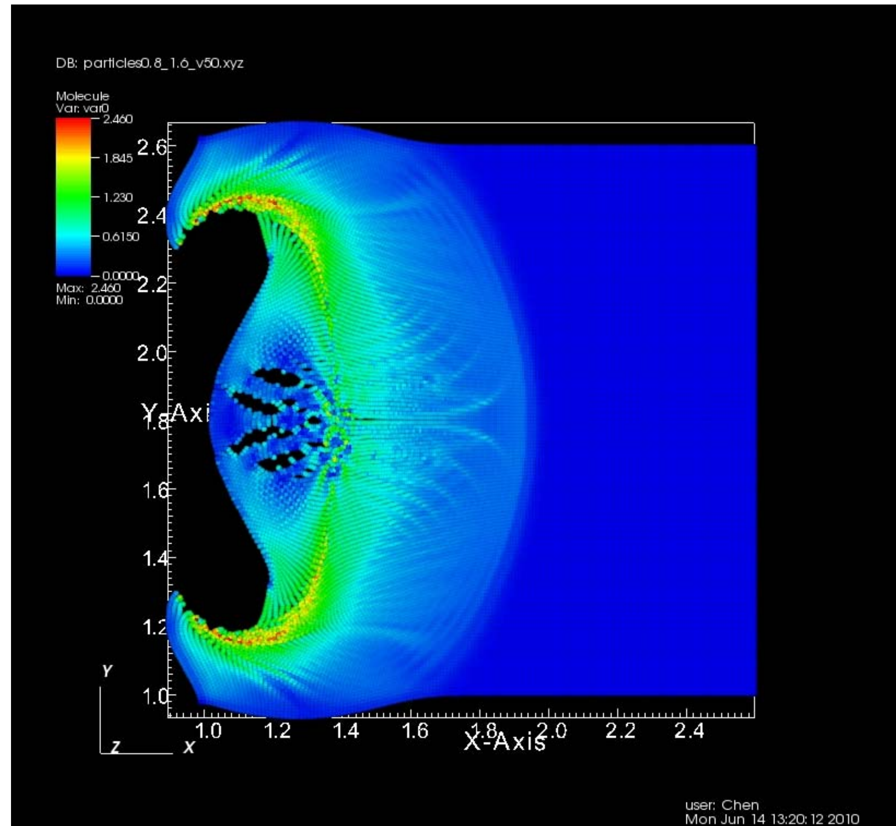
Flyer: 0.4m×0.8m; Target: 1.6m×1.6m

Impact velocity:5000m/s

T=0.172 ms



Stress Distribution

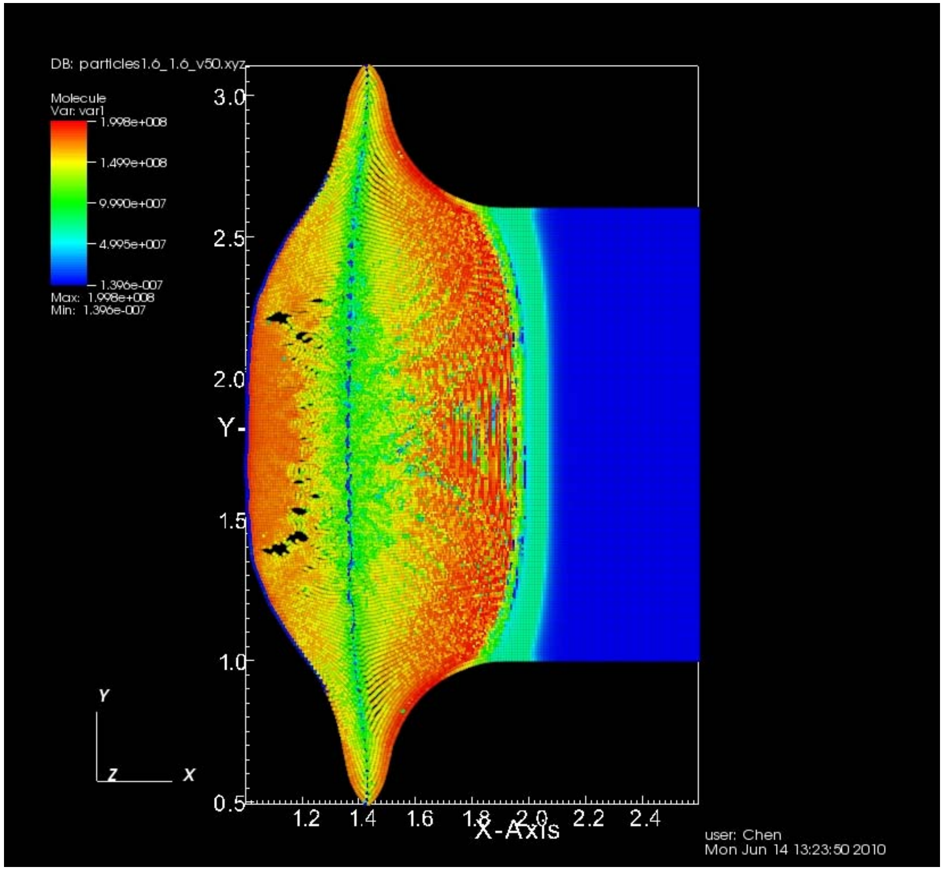


Strain Distribution

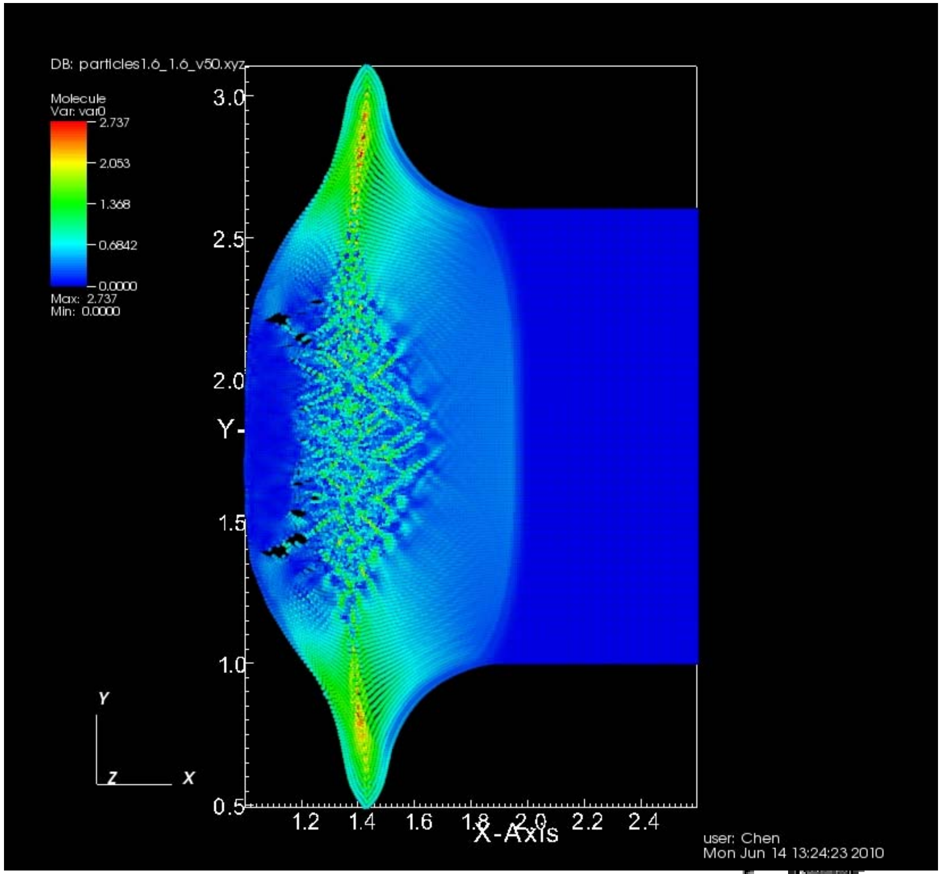
Flyer: 0.4m×1.6m; Target: 1.6m×1.6m

Impact velocity:5000m/s

T=0.172 ms



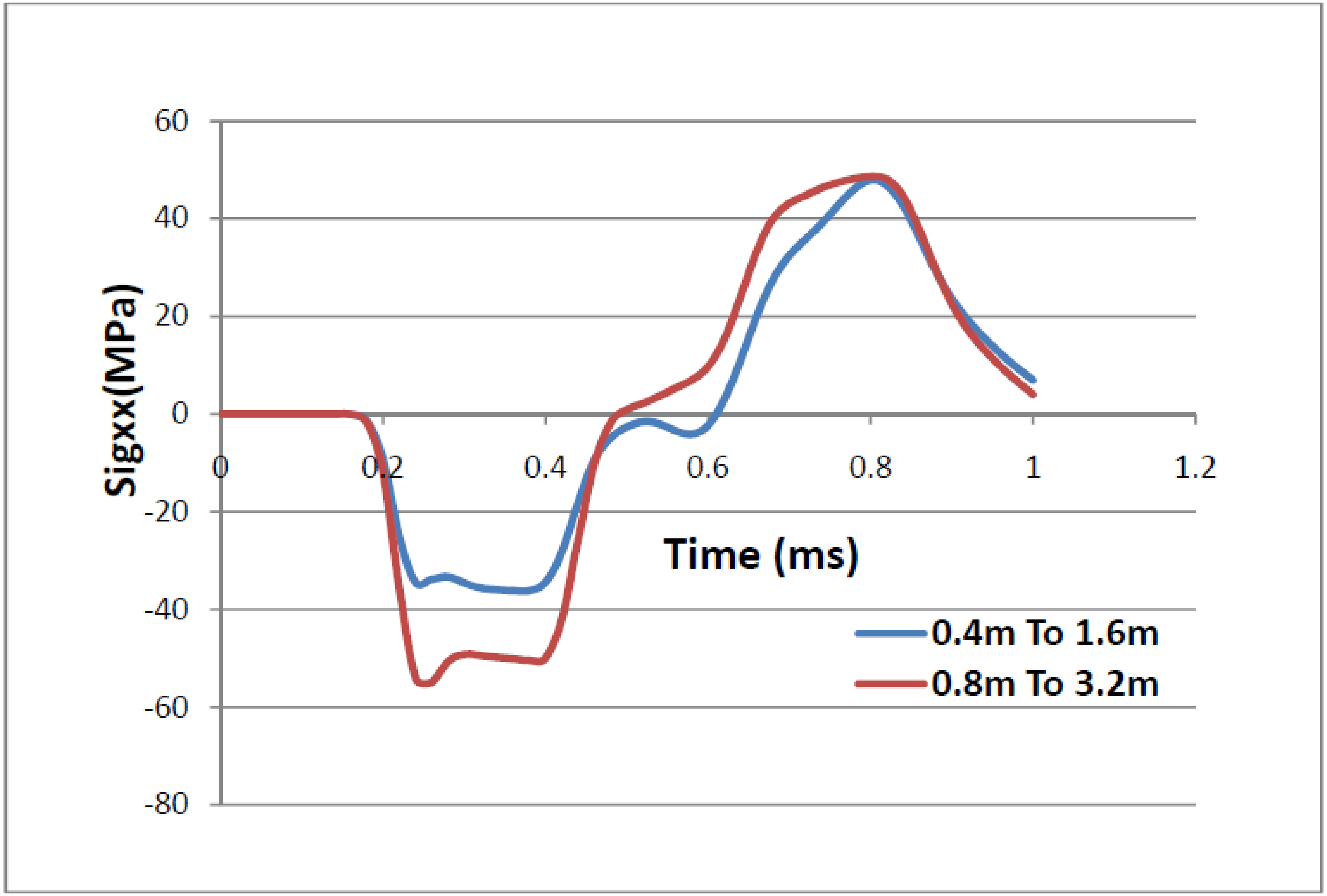
Stress Distribution



Strain Distribution

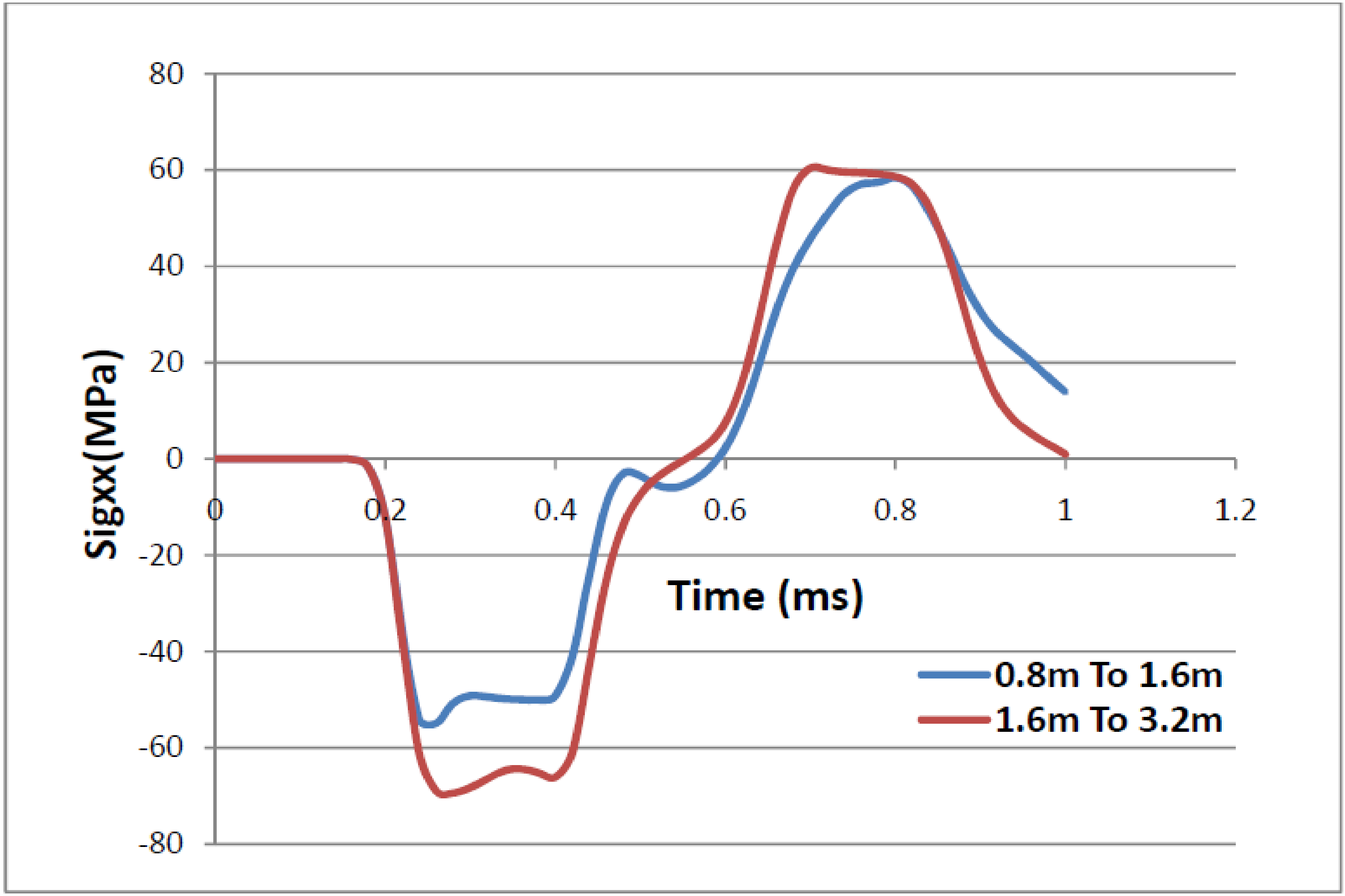
Size Effect with 1:4 Aspect Ratio

Stress histories in the middle of target
with impact velocity being 5m/s and zero Poisson's Ratio



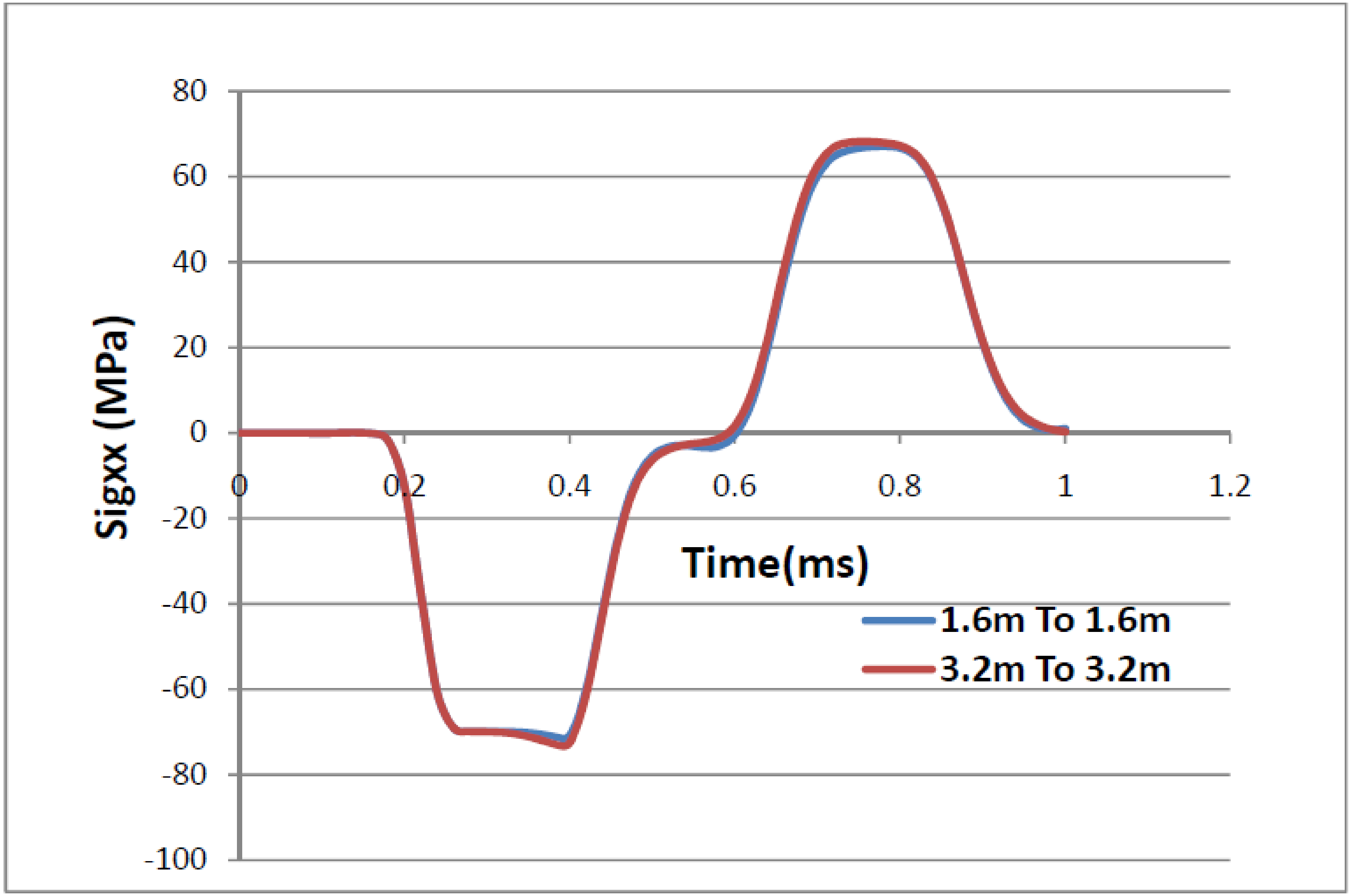
Size Effect with 1:2 Aspect Ratio

Stress histories in the middle of target
with impact velocity being 5m/s and zero Poisson's Ratio



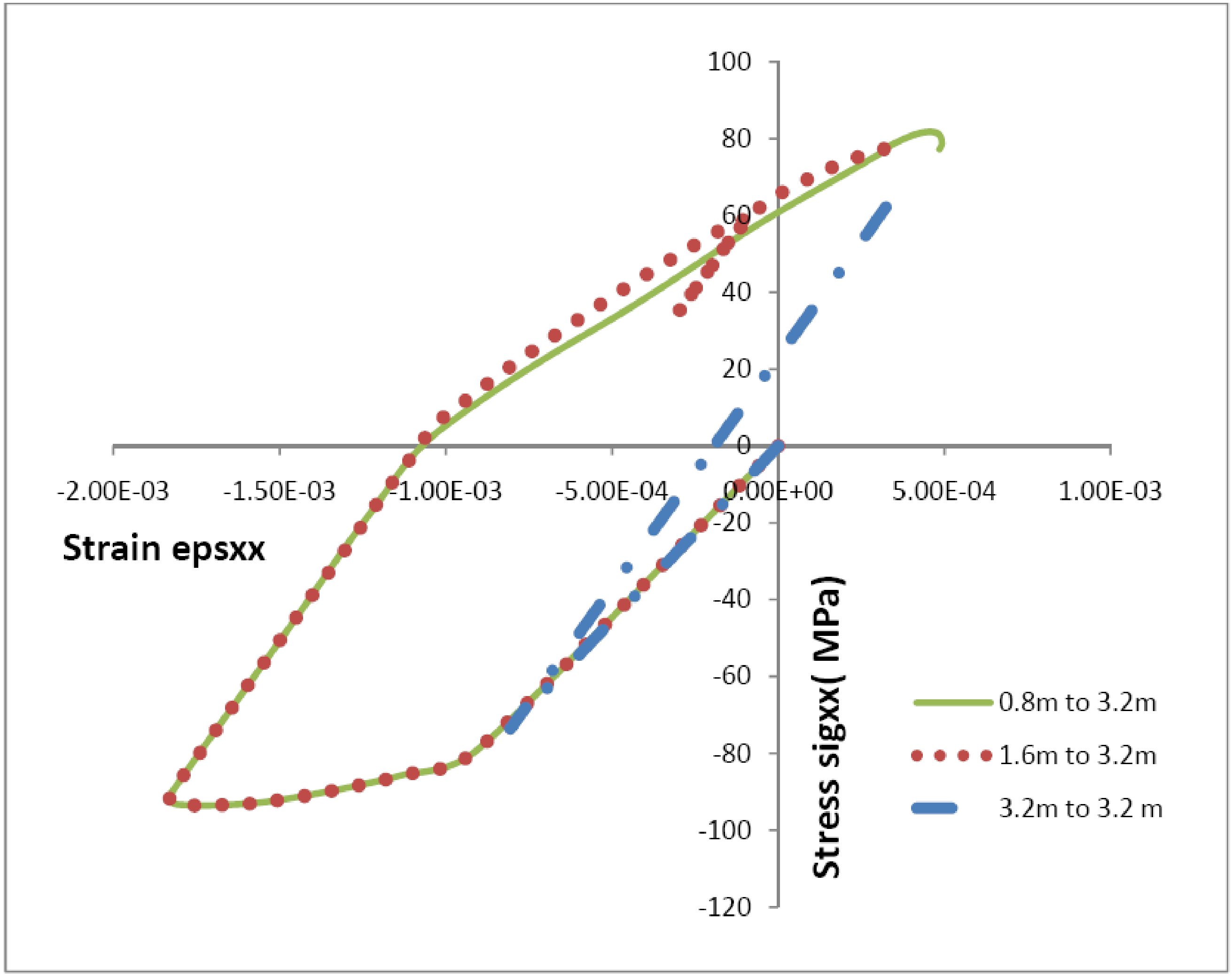
Size Effect with 1:1 Aspect Ratio

Stress histories in the middle of target
with impact velocity being 5m/s and zero Poisson's Ratio



Corresponding Stress-Strain Relations

Impact velocity: 5 m/s



2.2 Boundary Effect

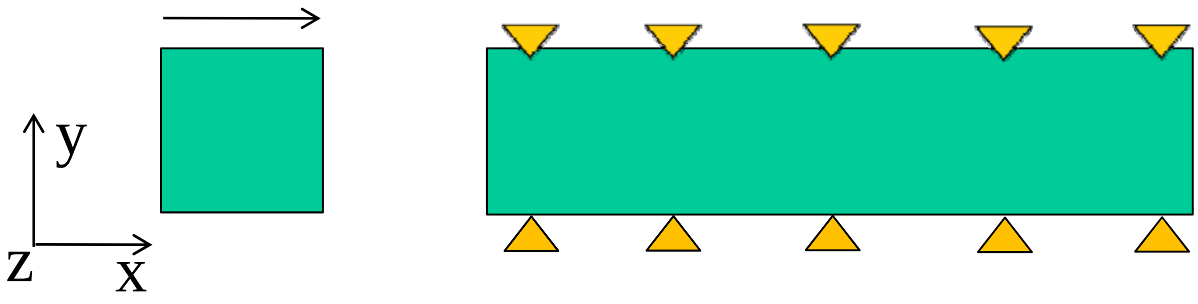
Impact velocity : 1000 m/s

Flyer: 0.4m×0.4m;

Target: 0.4*a*×1.6m;

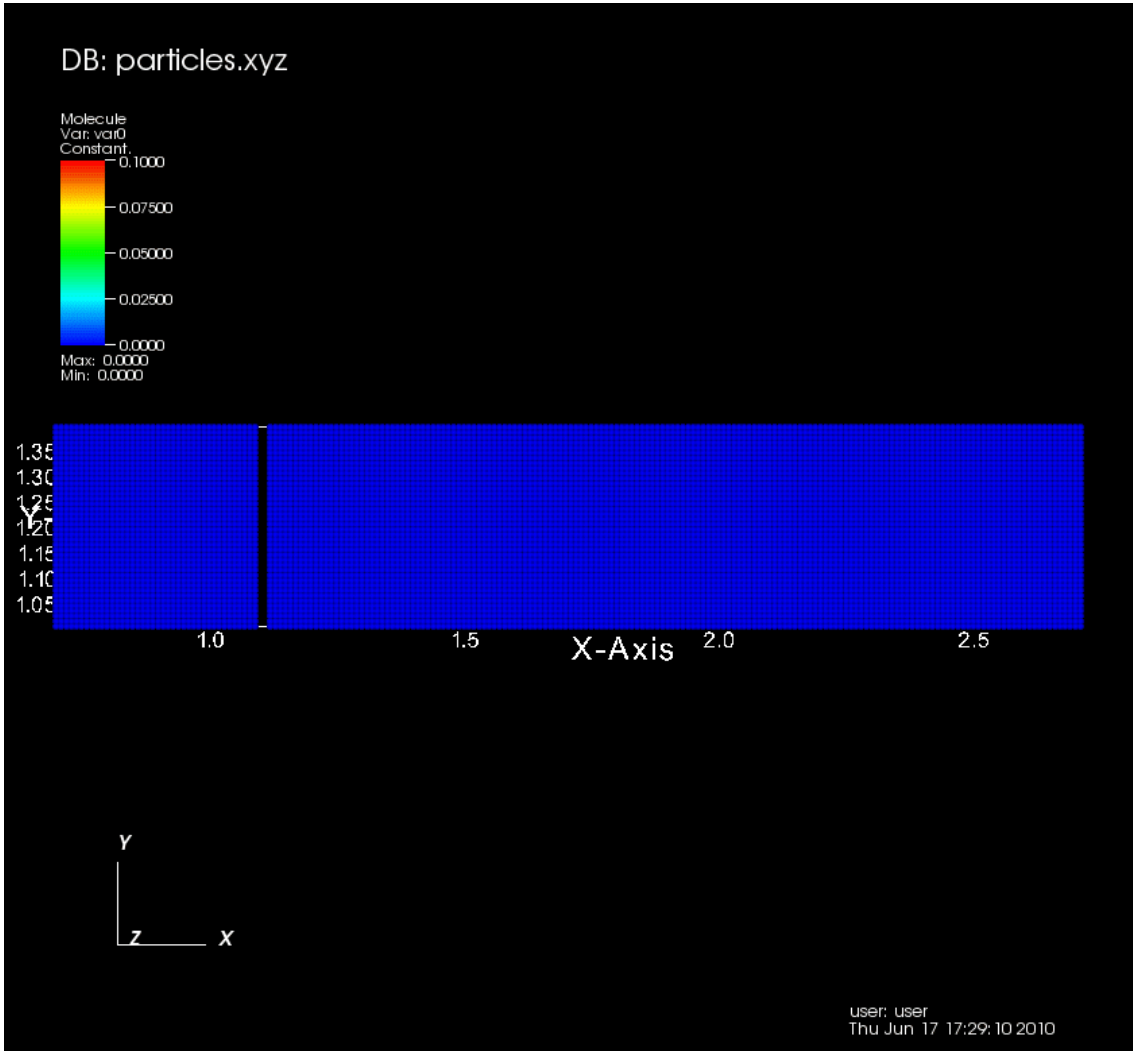
- Case1: Plan strain; X: Free; Y: Free;

- Case2: Plane strain; X :Free; Y: Fixed;



Case1: Plane strain; X-Free; Y-Free; Plastic strain evolution

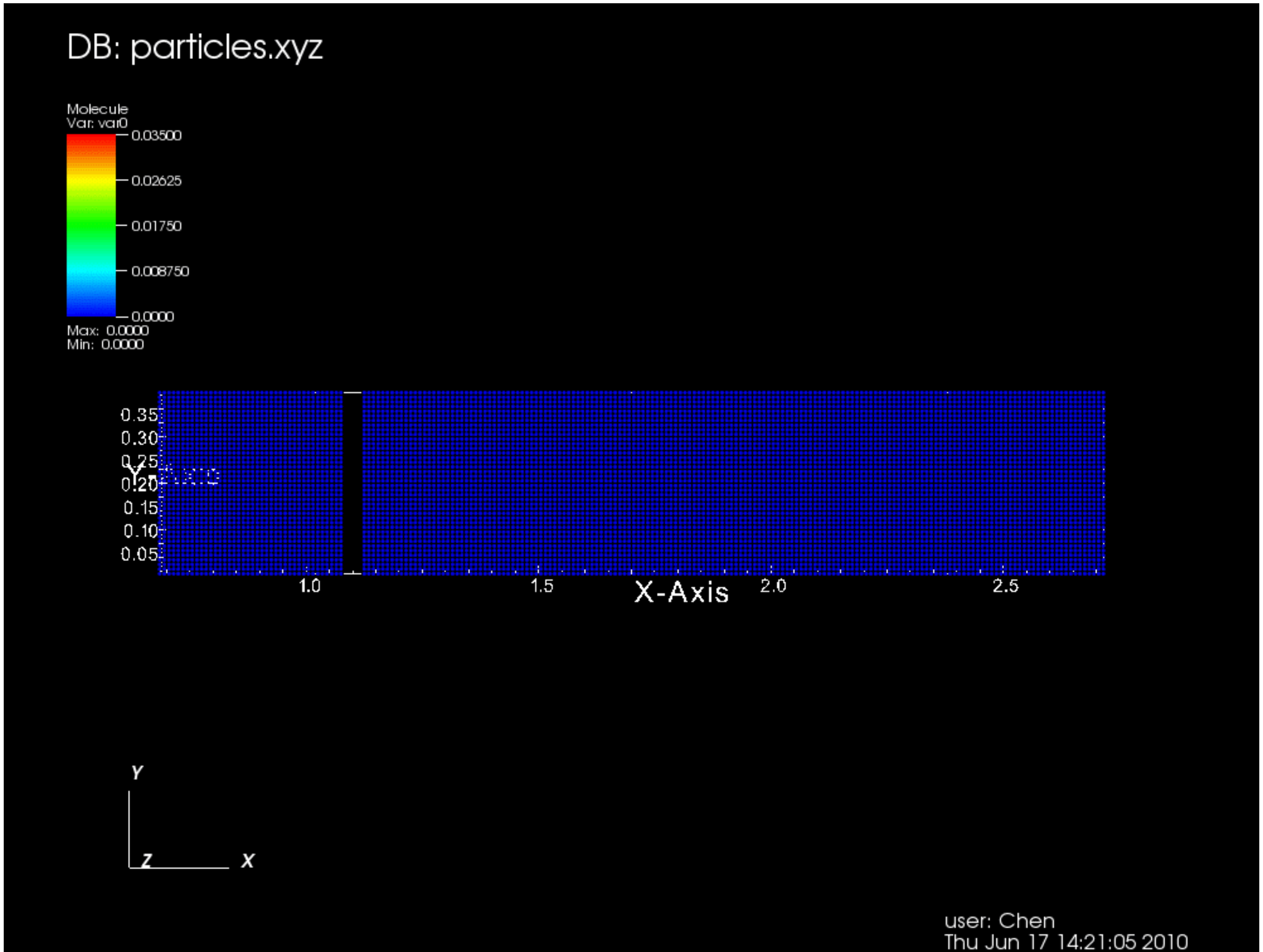
Flyer: 0.4m×0.4m;
Target: 0.4*a*×1.6m;



Case2: Plane strain; X-Free; Y-Fixed; Plastic strain evolution

Flyer: 0.4m×0.4m;

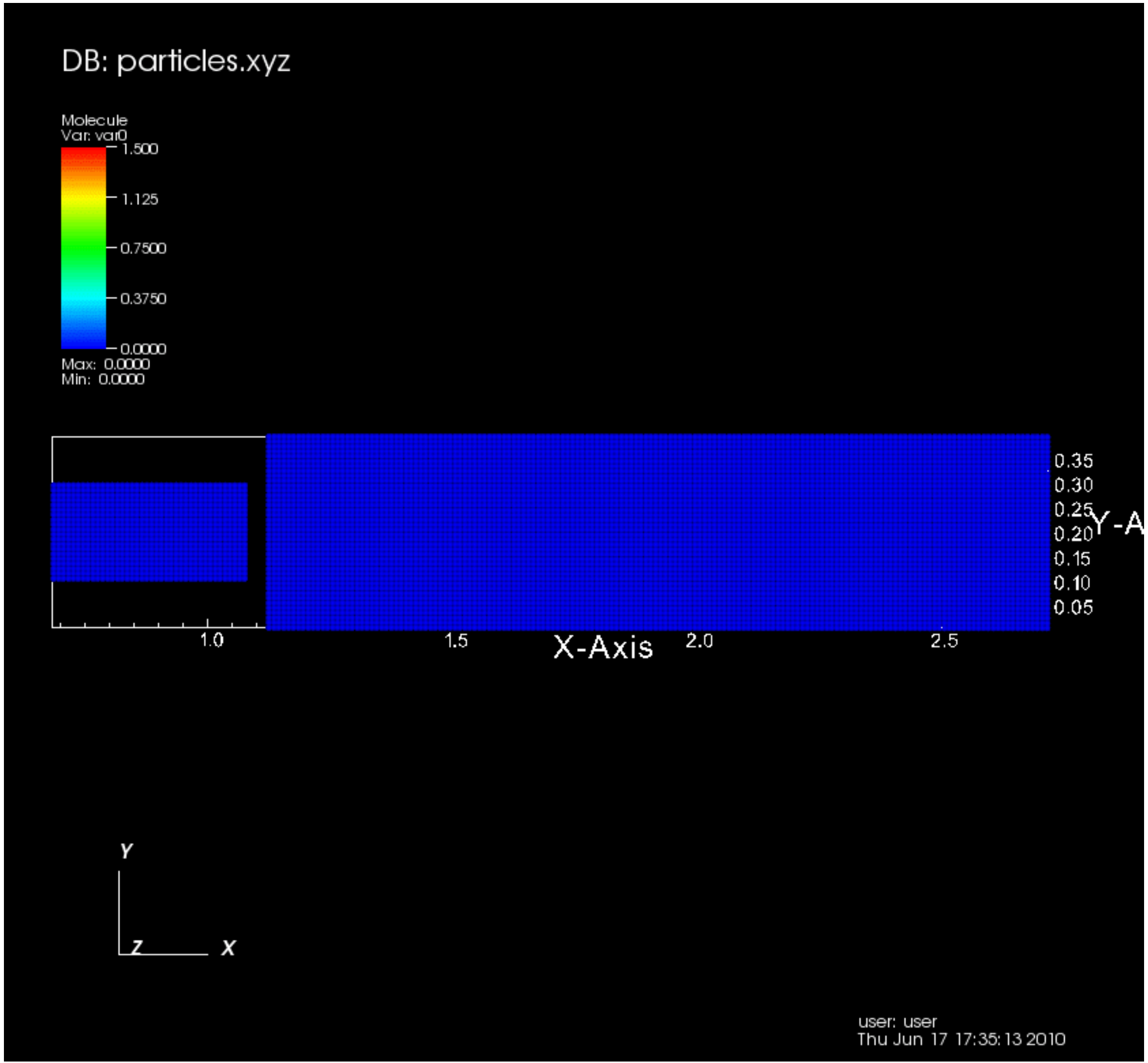
Target: 0.4*a*×1.6m;



Case2: Plan strain; X-Free; Y-Fixed; Plastic strain evolution

Flyer: 0.4m×0.2m, with the flyer size being changed

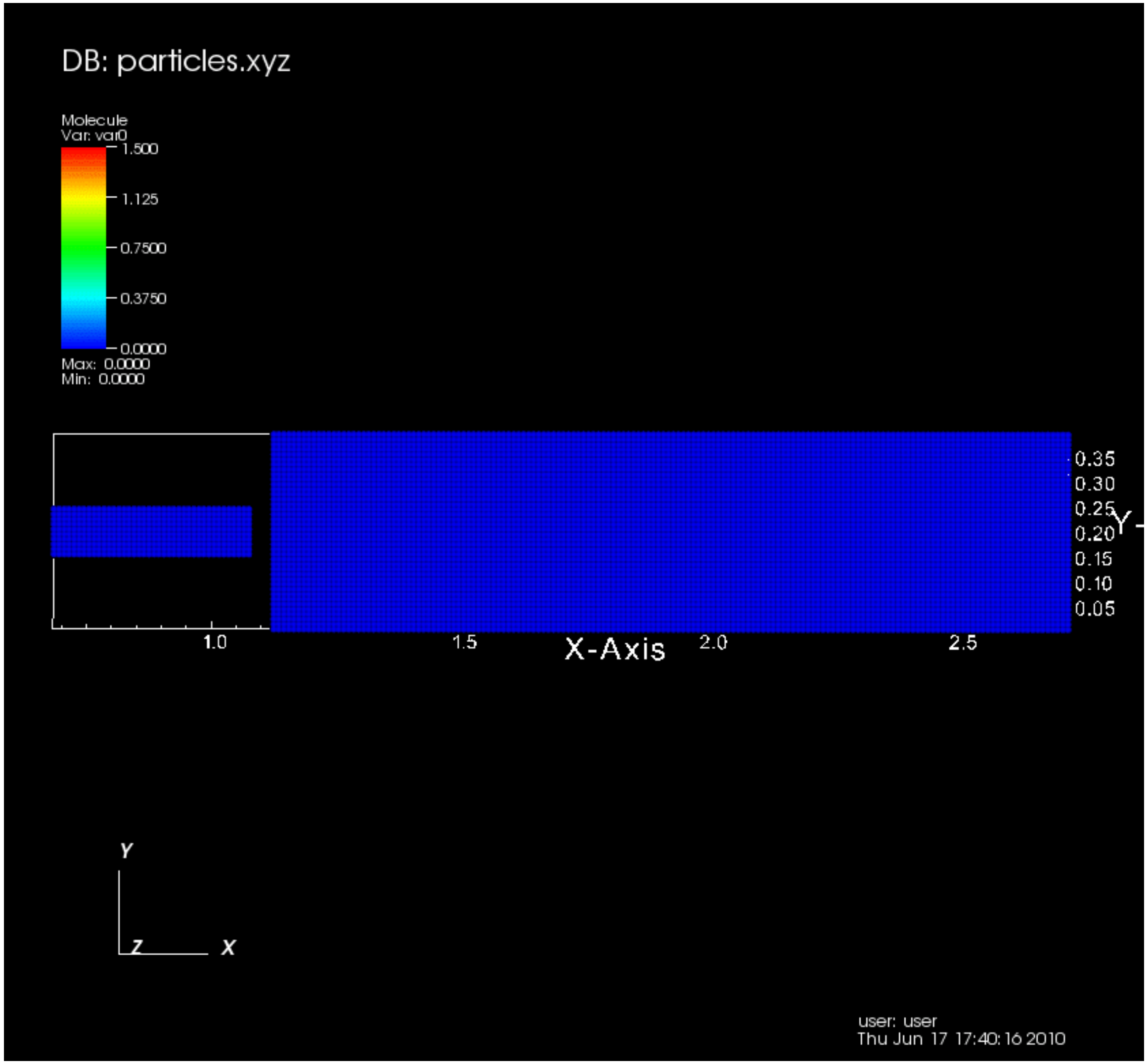
Target: 0.4*a*×1.6m;



Case2: Plan strain; X-Free; Y-Fixed; Plastic strain evolution

Flyer: 0.4m×0.1m, with the flyer size being changed

Target: 0.4*a*×1.6m;



4. Concluding Remarks and Future Tasks

- A nonlocal spatial discretization scheme appears to be necessary to effectively simulate the shock wave propagation and multi-phase interaction across different scales.
- Numerical stability and consistency must be examined to assure the convergence of the proposed nonlocal scheme.
- The impact failure evolution at both nano and continuum level exhibits the similar trend.
- The aspect ratio is more dominant than the size effect for impact problems at both nano and continuum level, which provides the way to control the rate of chemical reaction.
- The key to link the nano and continuum level information is how to formulate the rDPD potential in the proposed particle-based multi-scale approach.