



The Combination of the MPM with Other Methods for Multi-physics and/or Multi-scale Simulation

Zhen Chen

Department of Civil and Environmental Engineering

University of Missouri, Columbia, MO 65211, USA

State Key Laboratory of Structure Analysis for Industrial Equipment

Department of Engineering Mechanics,

Dalian University of Technology, Dalian 116024, P. R. China

Recent Collaborators:

Prof. T.D. Sewell, D.L. Thompson, J. Parker at University of Missouri

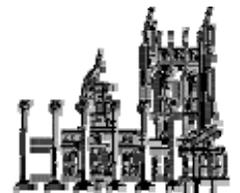
Prof. H.W. Zhang at Dalian University of Technology, China

Prof. X. Zhang at Tsinghua University, China

Prof. F. Oka at Kyoto University, Japan

Dr. X. Qiu at Metso Minerals Inc., USA

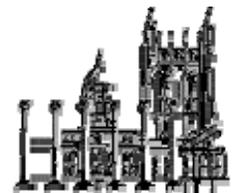
Former and Current Graduate Students





Outline

- 1. Introduction and Review**
- 2. The MPM Combined with Other Methods**
- 3. Previous Work on Energetic Composites**
- 4. Impact Responses of Nano Structures**
- 5. A Particle-Based Multi-scale Approach**
- 6. Concluding Remarks and Future Tasks**

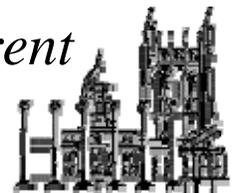




1. Introduction and Review

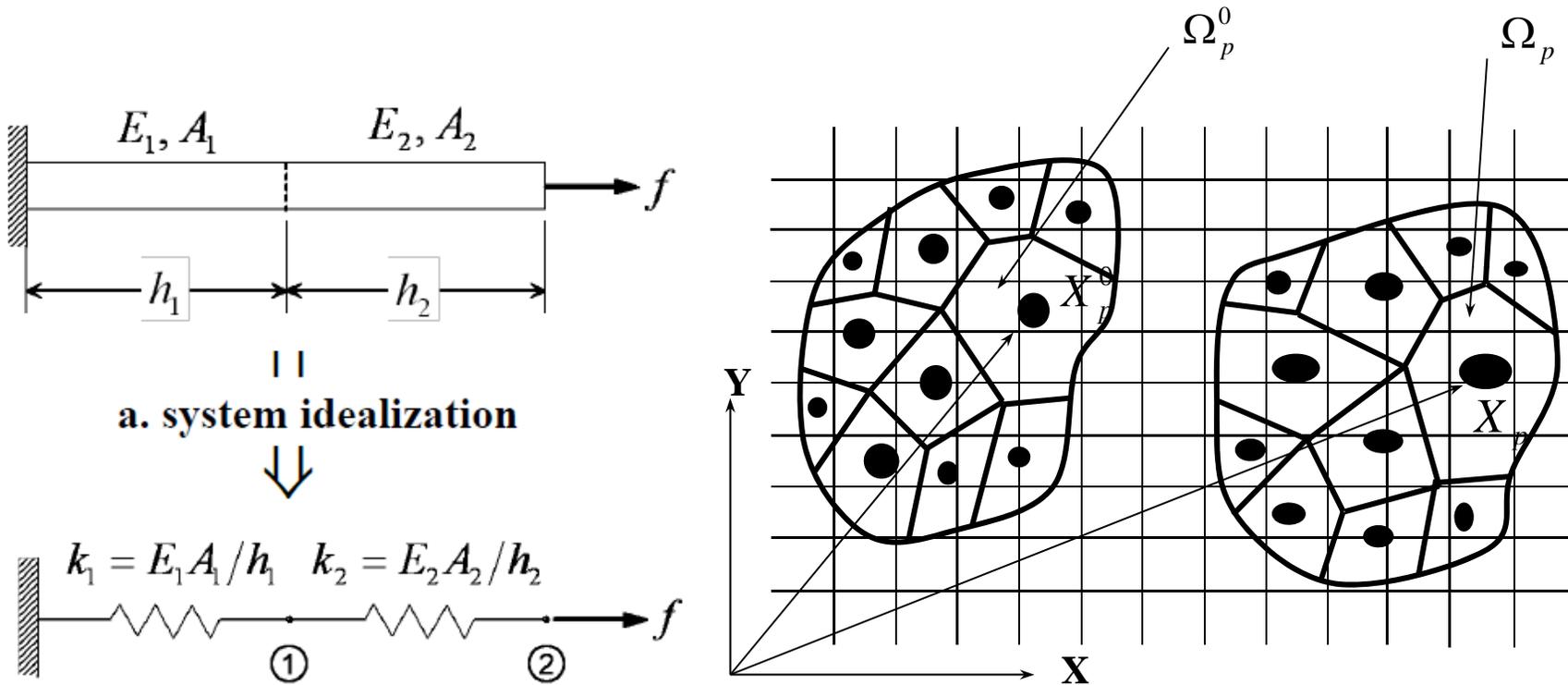
- Each spatial discretization method, whether it is mesh-based, meshfree or hybrid, has its own advantage and limitation.
- The Material Point Method (MPM) has evolved for almost twenty years, which takes advantage of both the Eulerian and Lagrangian methods while avoiding the shortcomings of each, to better simulate multi-phase interactions involving failure evolution.
- Since the MPM is based on the same weak formulation as that for the Finite Element Method (FEM), it could be easily interfaced with existing FEM codes for large-scale multi-physics simulations (Wave, Diffusion and Steady-State).
- The main limitation of the original MPM is the numerical noise caused by cell-boundary crossing of material points, which becomes more troublesome for multi-scale simulation.
- Much research has been conducted to improve the MPM. However, the space for further improvement becomes smaller!

Can we combine different kinds of numerical methods for different problems with the least computational cost?

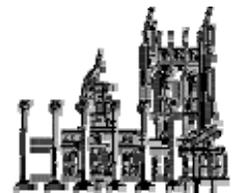




Main Features of the MPM as Compared with the FEM



$$[M] \{\ddot{u}\} + [K] \{u\} = \{f\}$$





The Improvement for Reducing Cell-Crossing Error

- Generalized Interpolation Material Point (GIMP) proposed by Bardenhagen and Kober (2004) – *Particle characteristic function to reduce the numerical noise due to cell-boundary crossing of material points.*
- Convected Particle Domain Interpolation (CPDI) proposed by Sadeghirad, Brannon and Burghardt (2011) – *Alternative grid basis functions to better track the changing particle domains for problems involving massive deformations.*
- Dual Domain Material Point (DDMP) proposed by Zhang, Ma and Giguere (2011) – *Modified gradient of the shape function for the quantities related to a gradient while leaving the other quantities unchanged from the original MPM. Two consecutive local operations replace the nonlocal one as required for the characteristic function.*





2. The MPM Combined with Other Methods

- The Combined FEM with MPM for Simulating Impact, Penetration and Blast Problems [Lian, Zhang and Liu, 2011; among others]
- The Combined FDM with MPM for Simulating Coupled Thermo-Mechanical Problems [Chen, Gan and Chen, 2008]
- The Combined FDM with MPM for Solid-Fluid Interaction Problems [Zhang, Wang and Chen, 2009; among others]
- The Combined Image-Processing with the MPM for Life Science Problems [Chen et al., 2012]
- The Combined DEM with MPM for Multi-physics in Mineral Processing [On-going project]
- The Combined GIMP with MD Method via a Hierarchical Approach for Multi-scale Simulation [Ma et al., 2005; Lu et al., 2006].

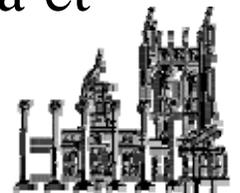
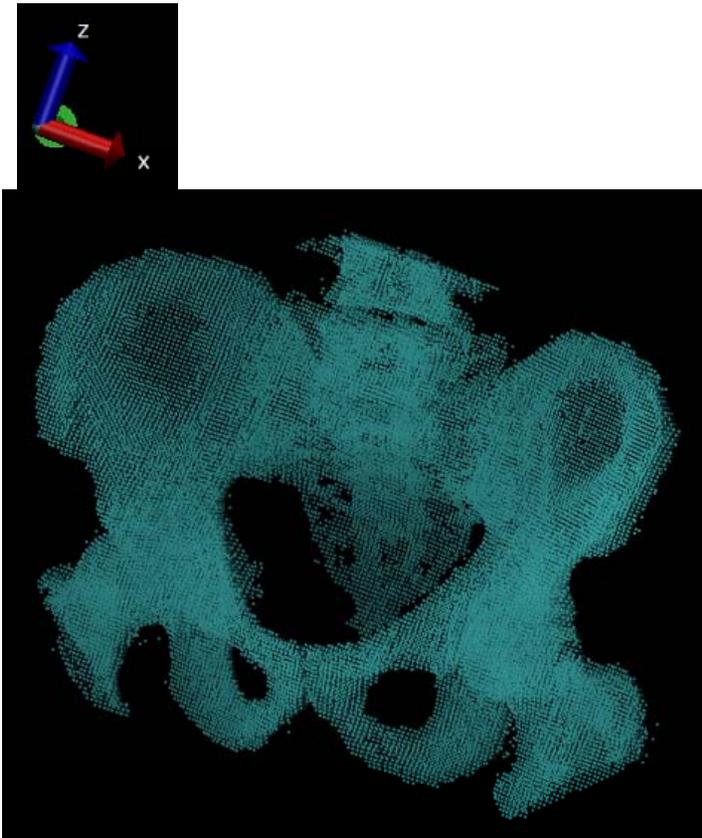
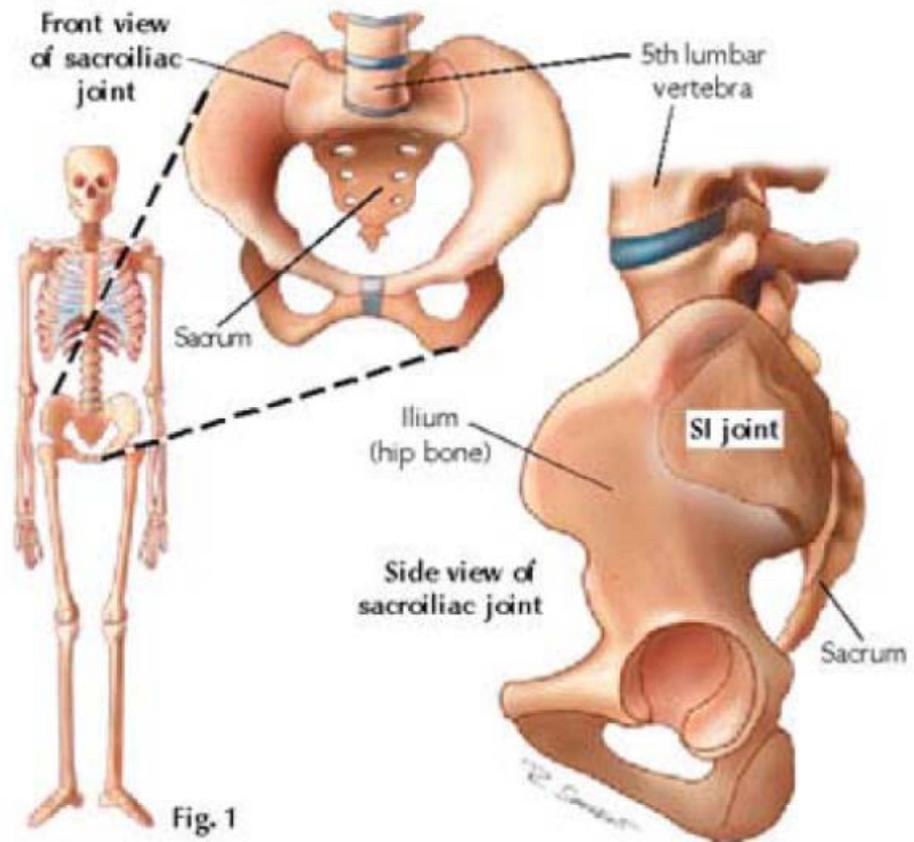




Image-Based MPM for Simulating the Impact Response

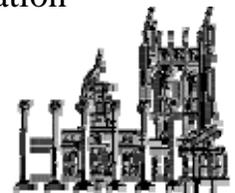


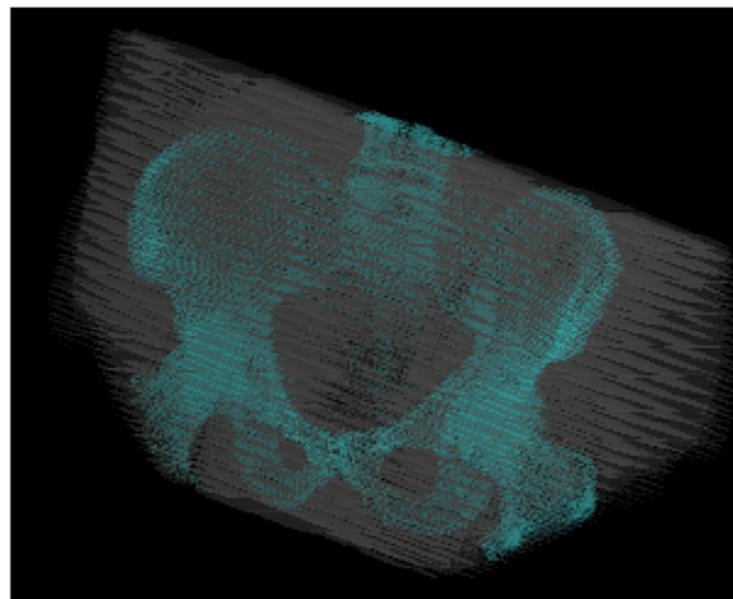
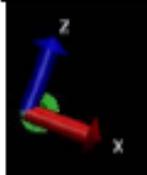
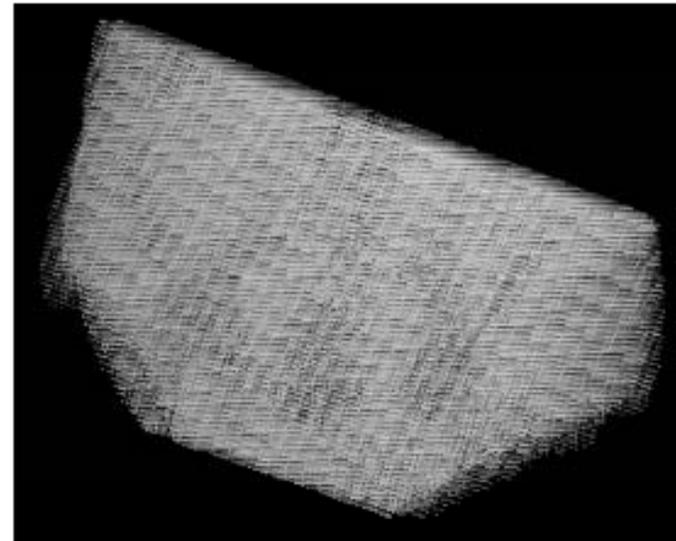
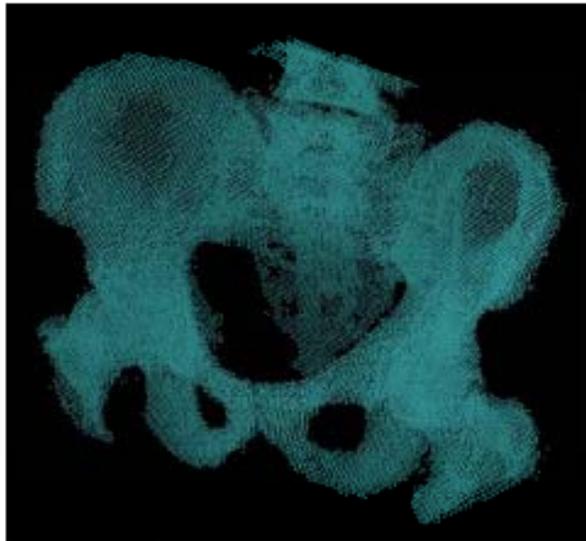
MPM model of hip bone (135053 points)



Hughston Sports Medicine Foundation

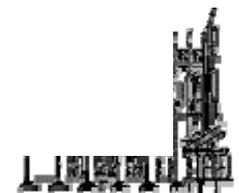
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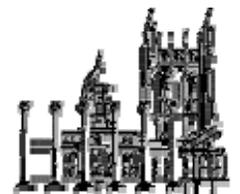
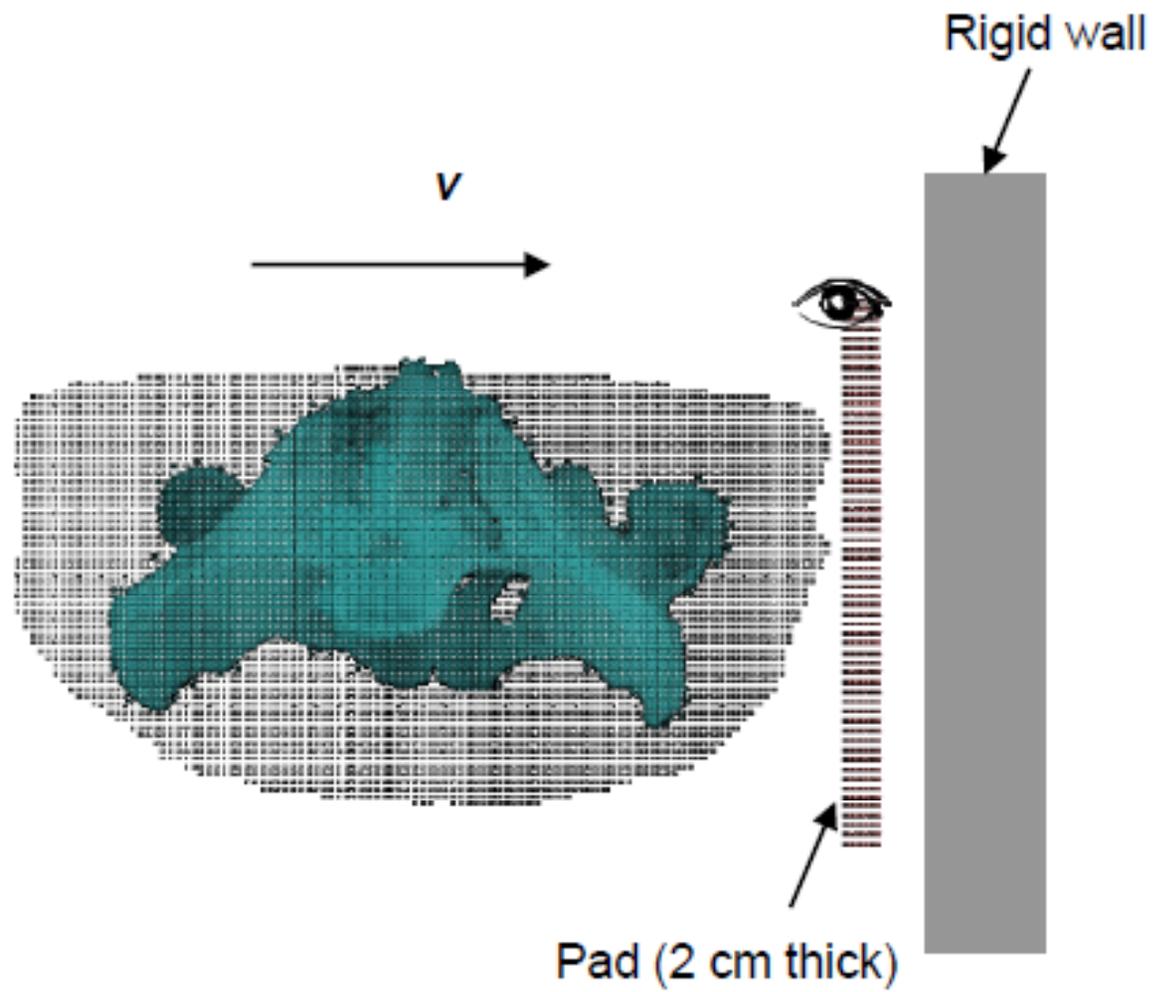


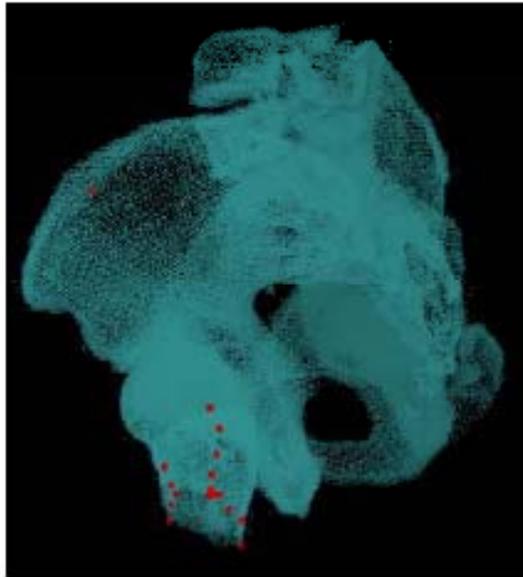


Cortical bone
Cancellous bone
Marrow

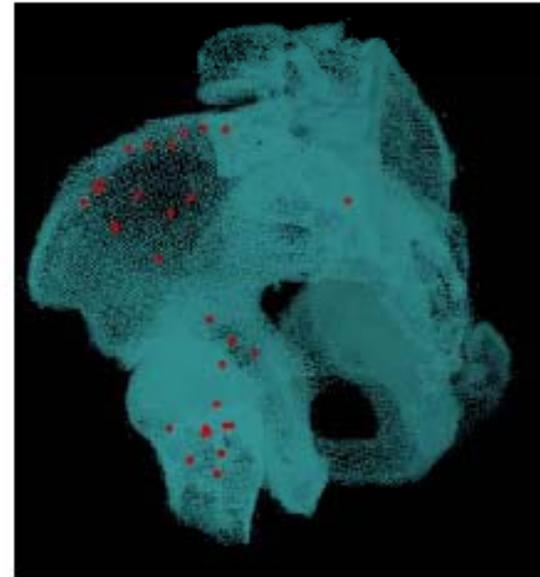
MPM model
Hip bone
(135,053 points)
Soft tissue
(217,743 points)
Total 352,796
points





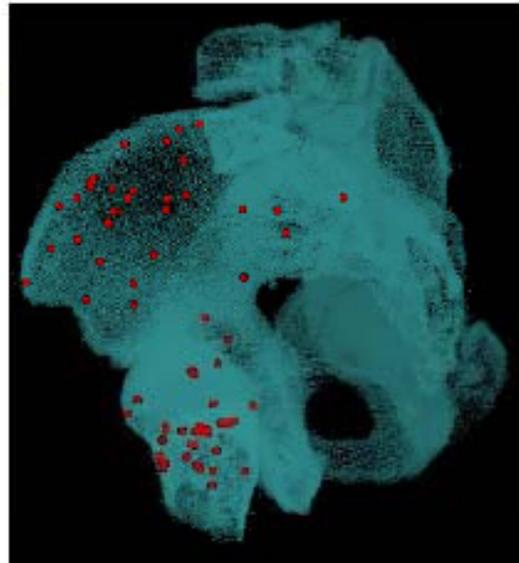


85.5 kPa

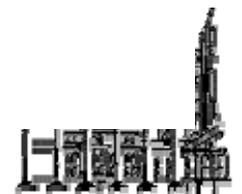


855 kPa

Pad materials with different
Young's moduluses



8 GPa

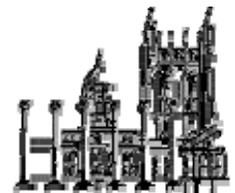




3. Previous Work on Energetic Composites

- Commonly used energetic materials are based on monomolecular 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.
- There is a lack of understanding on multi-scale interactions involved as well as physics-based modeling.

The Need for a Multi-scale Equation of State!





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

(*APL, Apperson et al., 2007*)

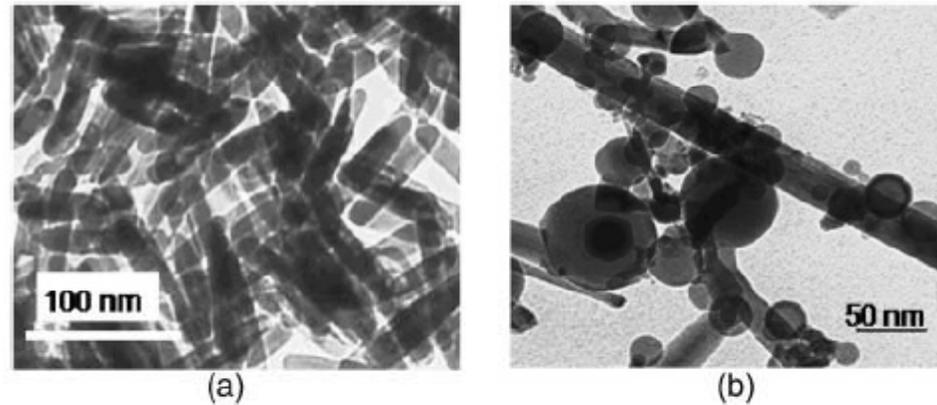
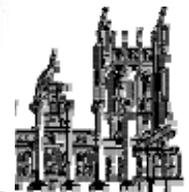
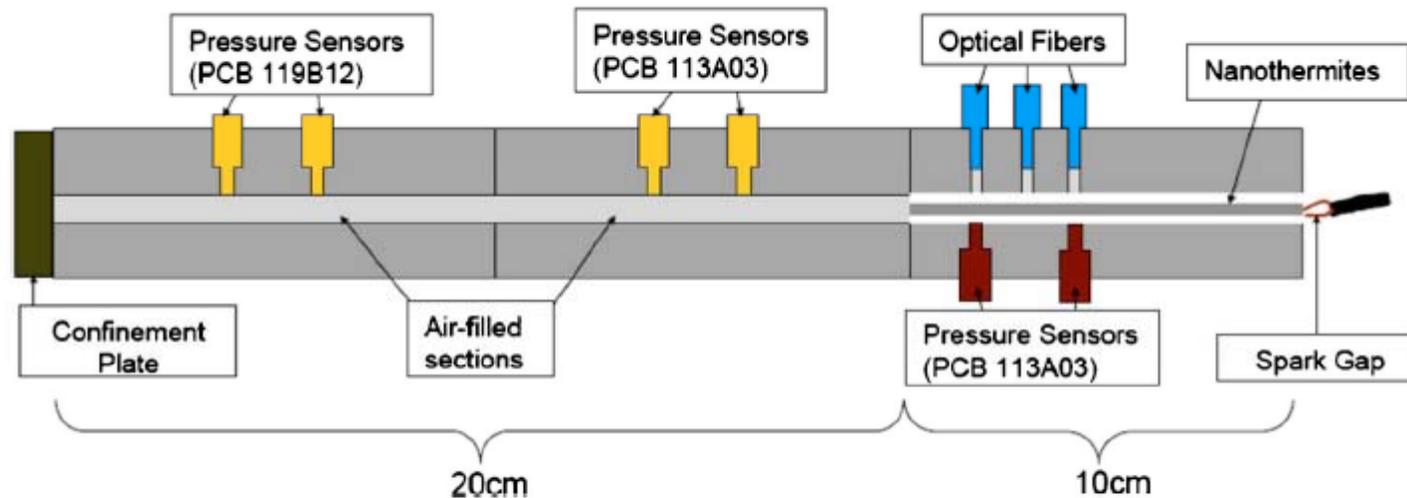


FIG. 1. TEM Images of (A) CuO nanorods and (B) self-assembled CuO nanorods/Al.





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

(*APL, Apperson et al., 2007*)

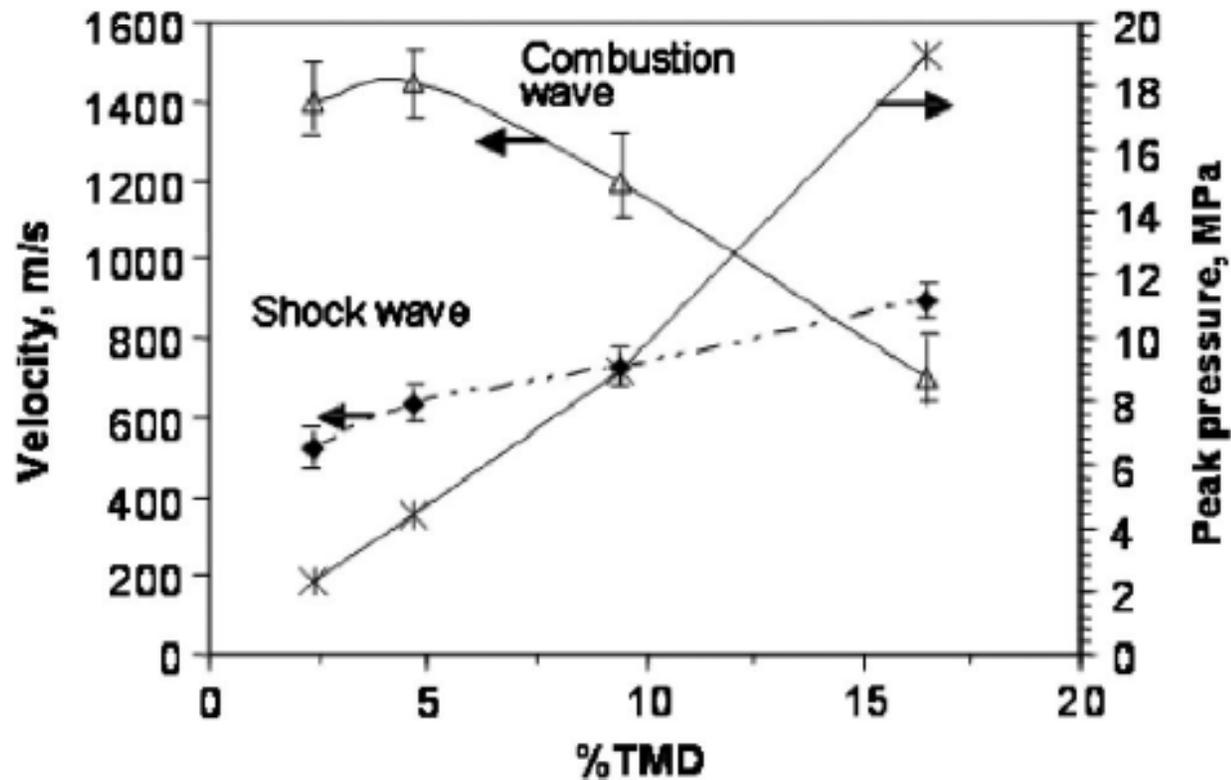
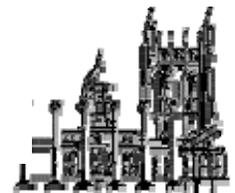


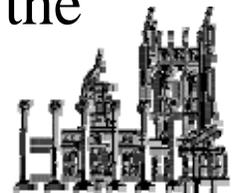
FIG. 4. Plot of combustion velocity, shock wave velocity, and peak pressure as a function of the density of physically mixed CuO/Al composite.





Continuum Modeling of Nanothermite Response (*Journal of Nanoparticle Research, Gan et al., 2010*)

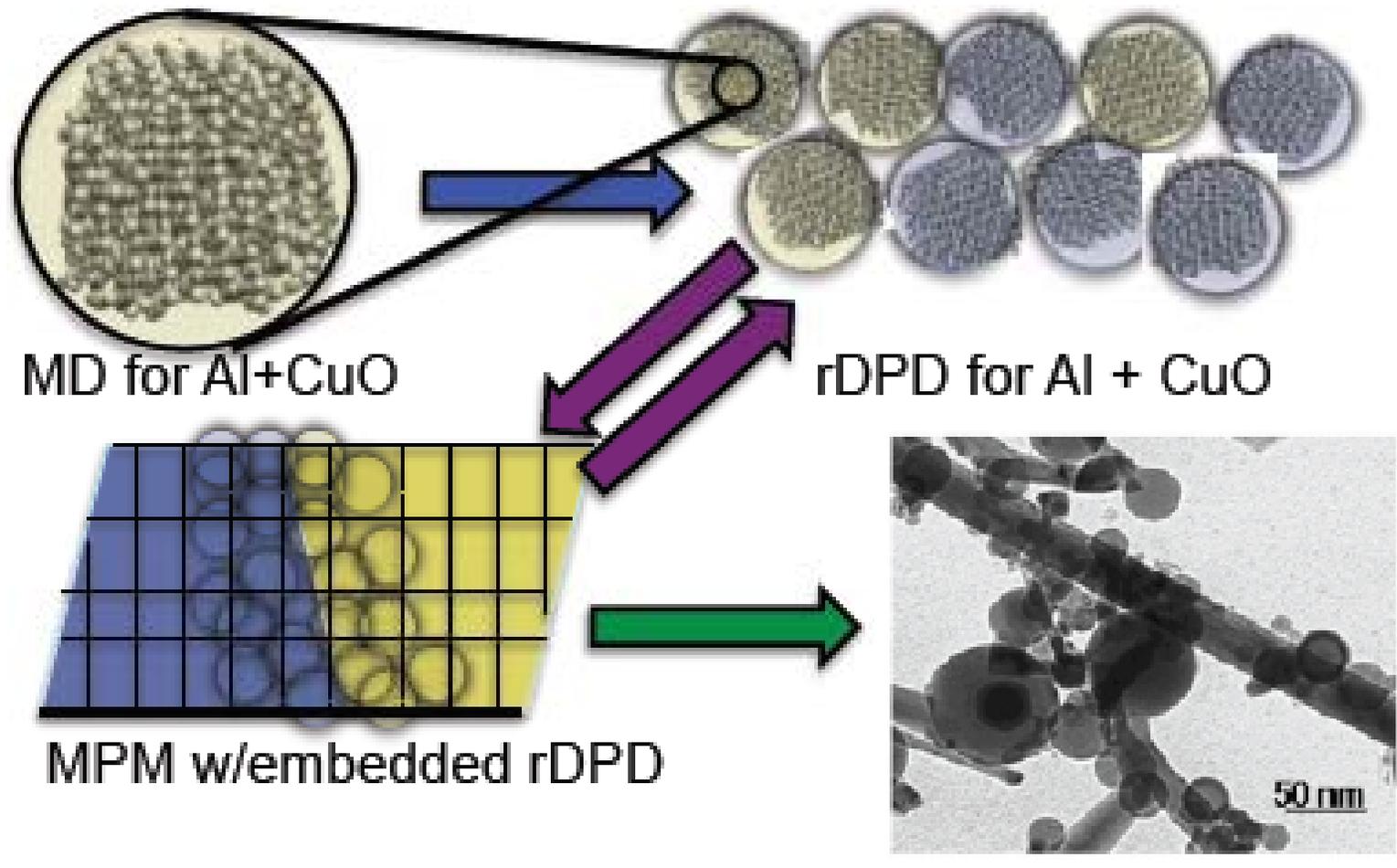
- With the assumption for the infinite reaction rate without atomistic details, an equation of state (EOS) for the detonation product of CuO/Al nanothermite composites has been developed based on the Chapman-Jouguet theory and nanothermite detonation experiment.
- The EOS has been implemented into the MPM code for coupled CFD and CSD simulation of the detonation response.
- The MPM code 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.





Particle-Based Multiscale Simulation Procedure for Predicting The Coupled Spatial-Temporal Energy-Release Properties

Hierarchical from MD to rDPD/CD)
Concurrent between rDPD/CD and MPM

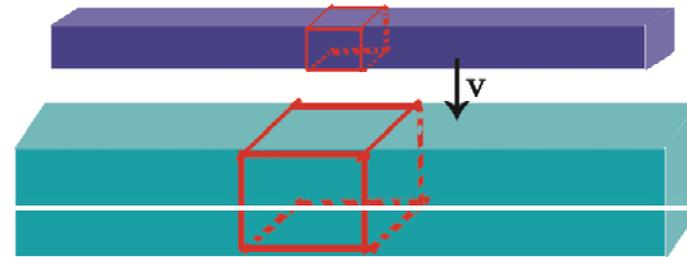
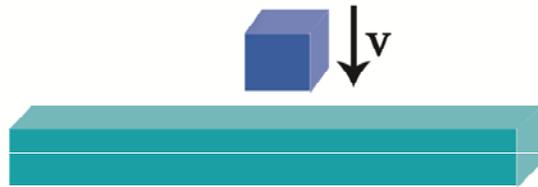




Size and Rate Effects on the Impact Response in Detonation of Nanothermite

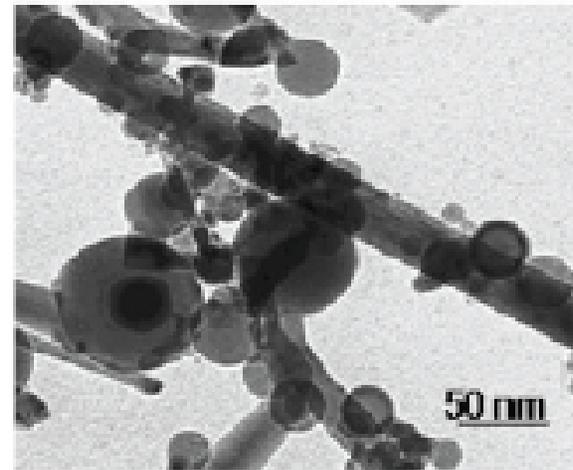
Transverse impact

(JAP, Chen et al., 2012)



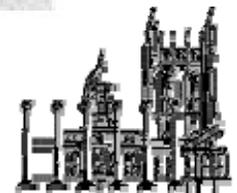
Longitudinal impact

(JPD, Jiang et al., 2012)



General Impact Modes

= Transverse impact + Longitudinal impact





4. Impact Responses of Nano Structures

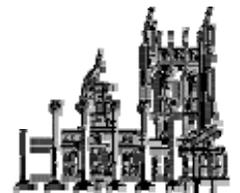
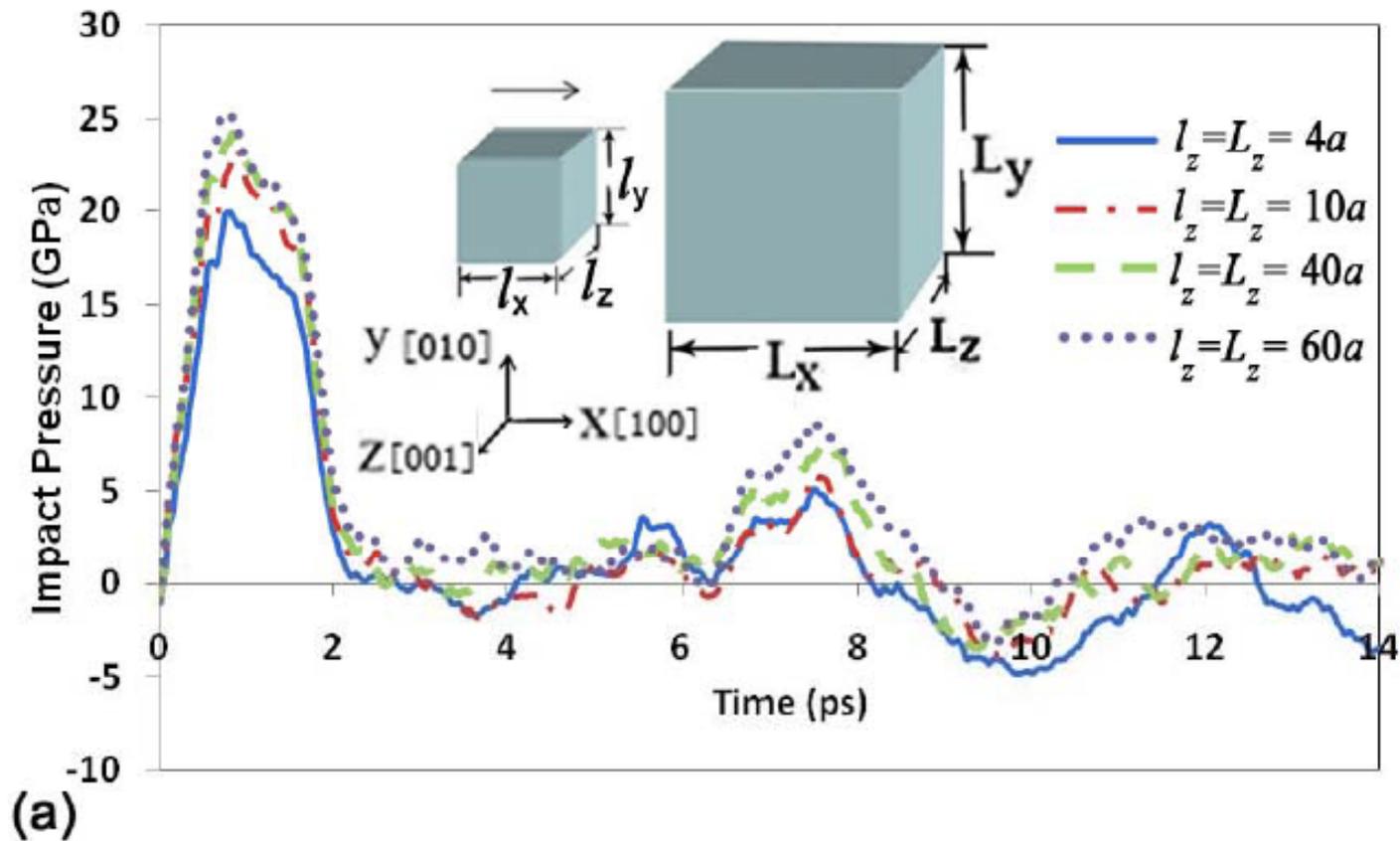
- The onset and evolution of dislocation and shear banding under impact is the key to understand the initiation of the detonation process of nanothermite composites.
- A multiscale study is being performed to investigate the link between different scales so that the multiscale Equation of State (EoS) could be formulated
- In parallel with the work on the reactive molecular potential for CuO/Al, the EAM potential is being used to understand different impact modes with single crystal structures at nanoscale.
- A comparative study between molecular and continuum level has been conducted to understand the effects of aspect ratio, size and boundary conditions on the multiscale impact responses.





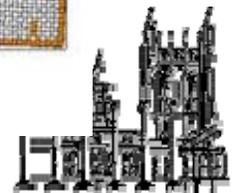
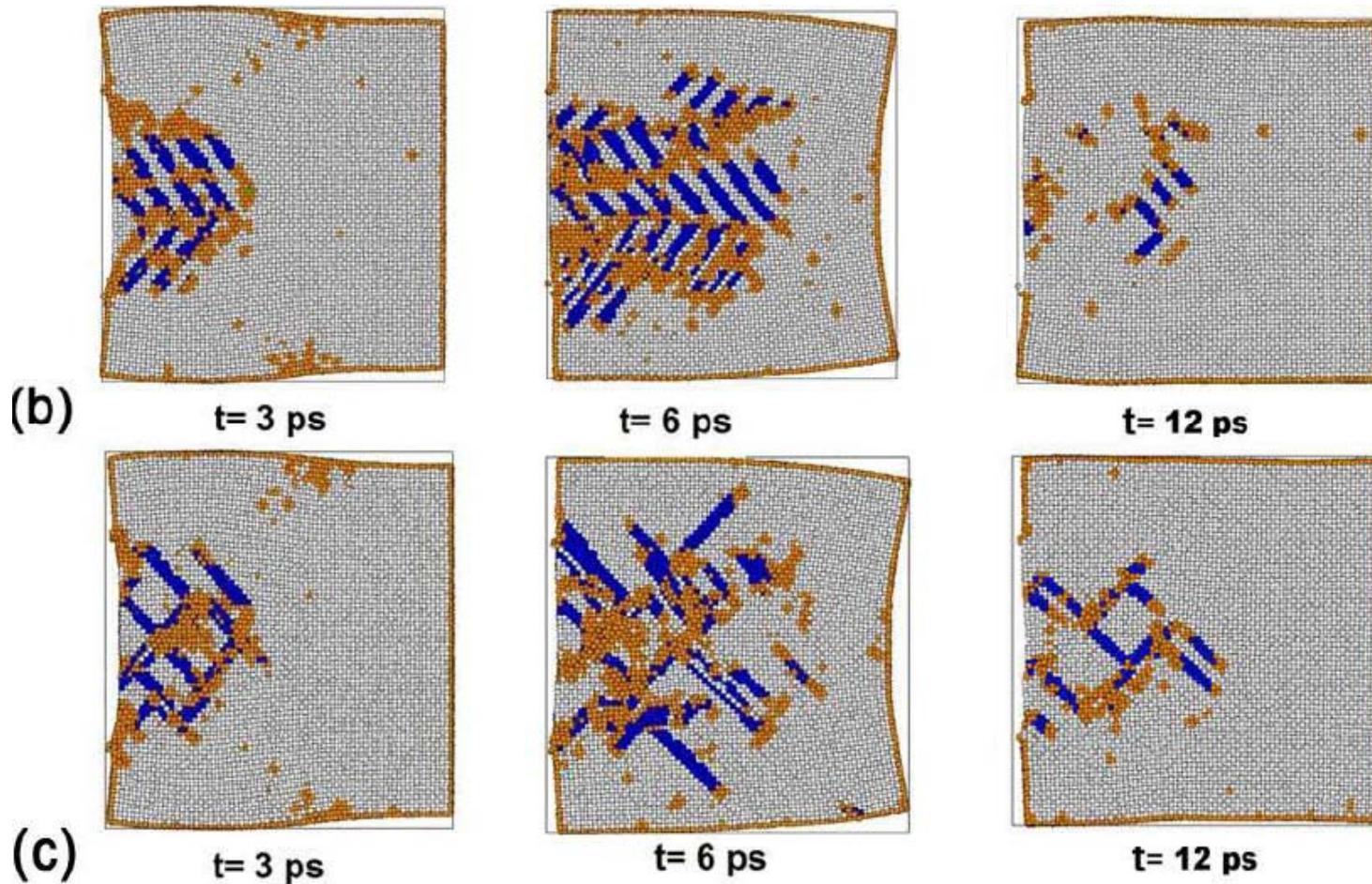
Size and Aspect Ratio Effects on the Impact Response of Copper Nanobeams

(a) The effect of sample thickness on the impact pressure for constant aspect ratio 1:2 and impact velocity 1000 m/s.





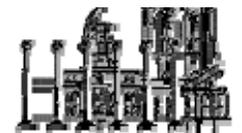
Deformation patterns of the target for sample thicknesses:
(b) $L_z = 1.452$ nm and (c) $L_z = 14.52$ nm at post-impact times.





Specification of the simulation model; $a = 0.363$ nm

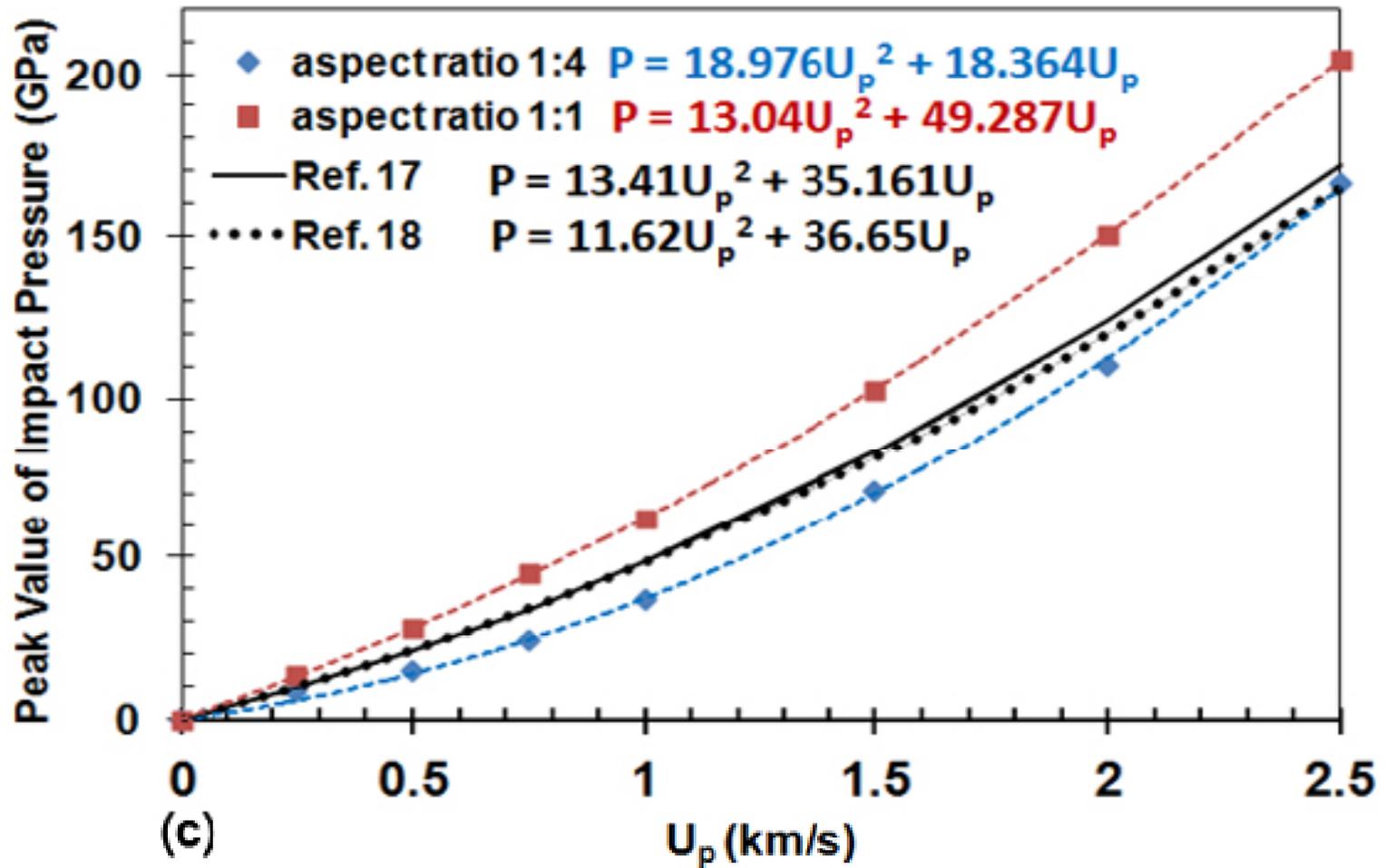
Simulation No.	Flyer size $l_x \times l_y \times l_z$	Target size $L_x \times L_y \times L_z$	Impact velocity (m/s)	Aspect ratio (l_y/L_y)
1	$10a \times 10a \times 40a$	$40a \times 40a \times 40a$	500	1:4
2	$10a \times 10a \times 40a$	$40a \times 40a \times 40a$	1000	1:4
3	$10a \times 10a \times 40a$	$40a \times 40a \times 40a$	1500	1:4
4	$10a \times 10a \times 40a$	$40a \times 40a \times 40a$	2000	1:4
5	$10a \times 10a \times 40a$	$40a \times 40a \times 40a$	3000	1:4
6	$10a \times 10a \times 40a$	$40a \times 40a \times 40a$	4000	1:4
7	$10a \times 10a \times 40a$	$40a \times 40a \times 40a$	5000	1:4
8	$10a \times 20a \times 40a$	$40a \times 40a \times 40a$	1000	1:2
9	$10a \times 40a \times 40a$	$40a \times 40a \times 40a$	500	1:1
10	$10a \times 40a \times 40a$	$40a \times 40a \times 40a$	1000	1:1
11	$10a \times 40a \times 40a$	$40a \times 40a \times 40a$	1500	1:1
12	$10a \times 40a \times 40a$	$40a \times 40a \times 40a$	2000	1:1
13	$10a \times 40a \times 40a$	$40a \times 40a \times 40a$	3000	1:1
14	$10a \times 40a \times 40a$	$40a \times 40a \times 40a$	4000	1:1
15	$10a \times 40a \times 40a$	$40a \times 40a \times 40a$	5000	1:1
16	$10a \times 20a \times 40a$	$40a \times 80a \times 40a$	1000	1:4
17	$10a \times 10a \times 40a$	$40a \times 80a \times 40a$	1000	1:8





Size-Dependent Equation of State

(*Journal of Applied Physics*, Chen et al., 2012)





Preliminary Results on the Transition from the “Inverse Hall-Petch” to classical Hall-Petch Effect

(AMS, Chen et al., 2012)

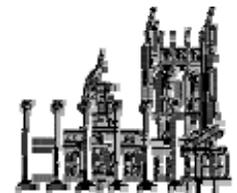
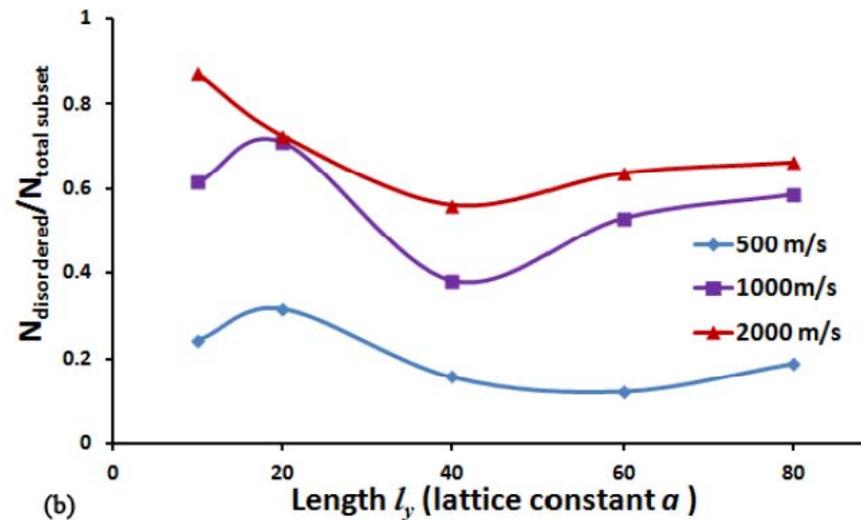
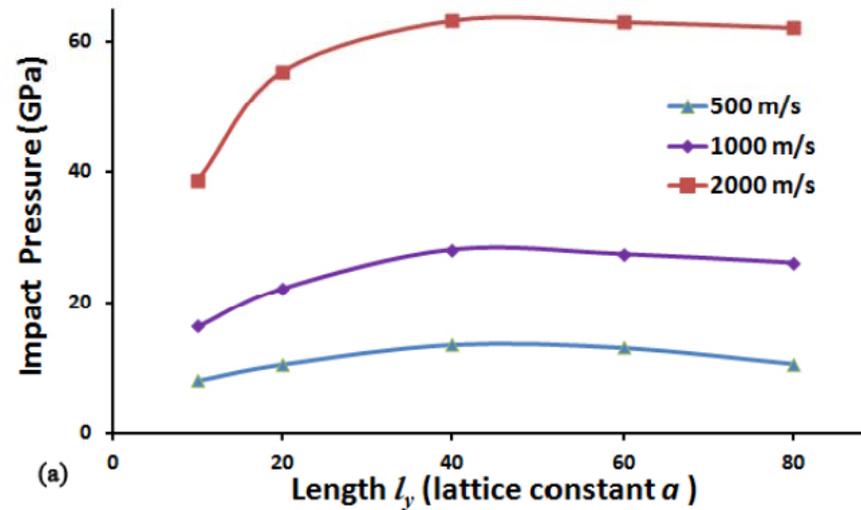




Fig. 3. Time histories of the impact pressure and number densities of target atoms in hcp crystal structures for simulations 2, 8, and 10 with different aspect ratios.

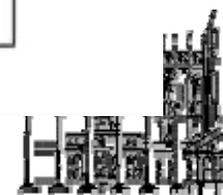
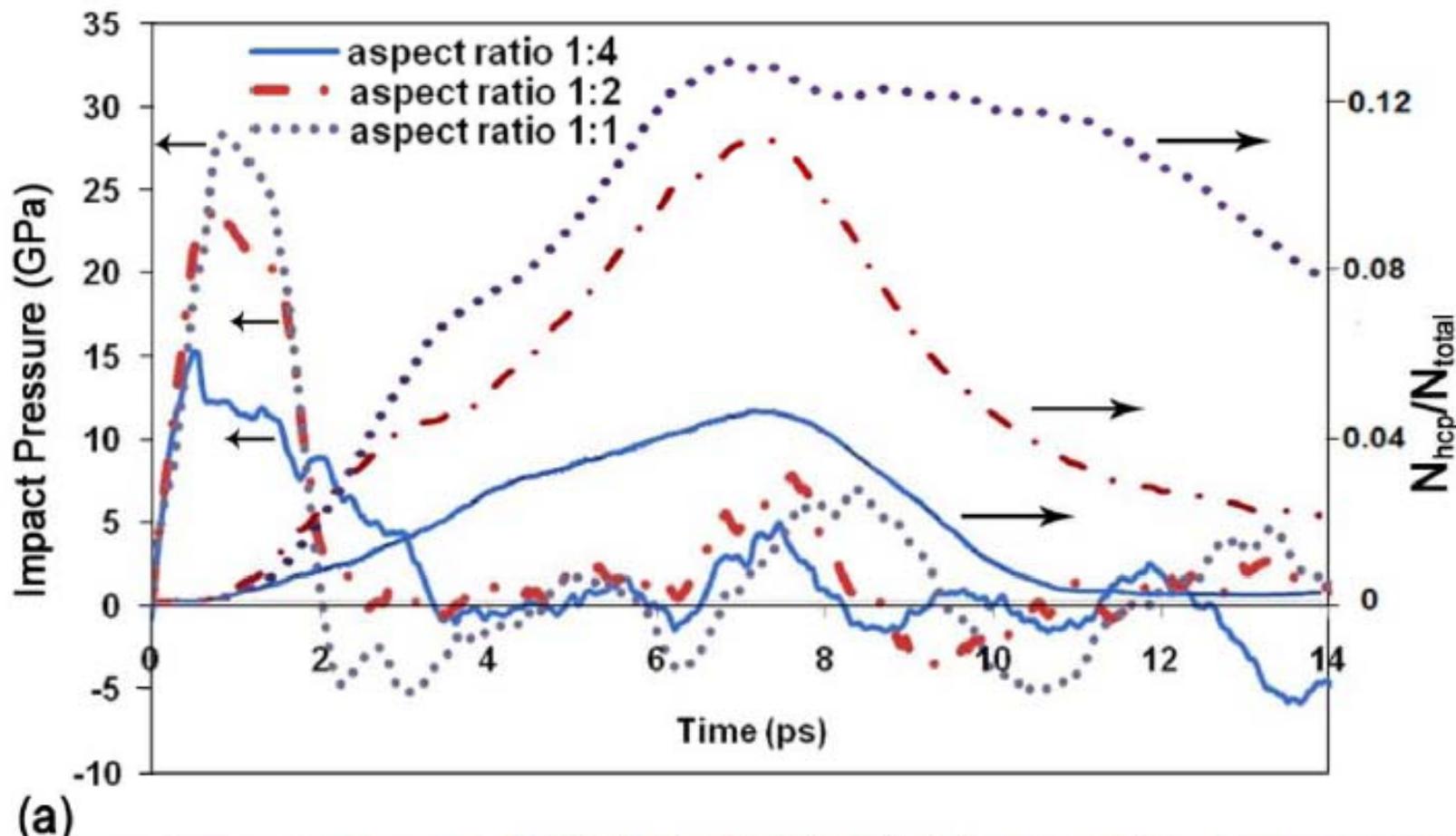




Fig. 5 Target deformation patterns with time in (a) simulation 2 and (b) simulation 8, respectively.

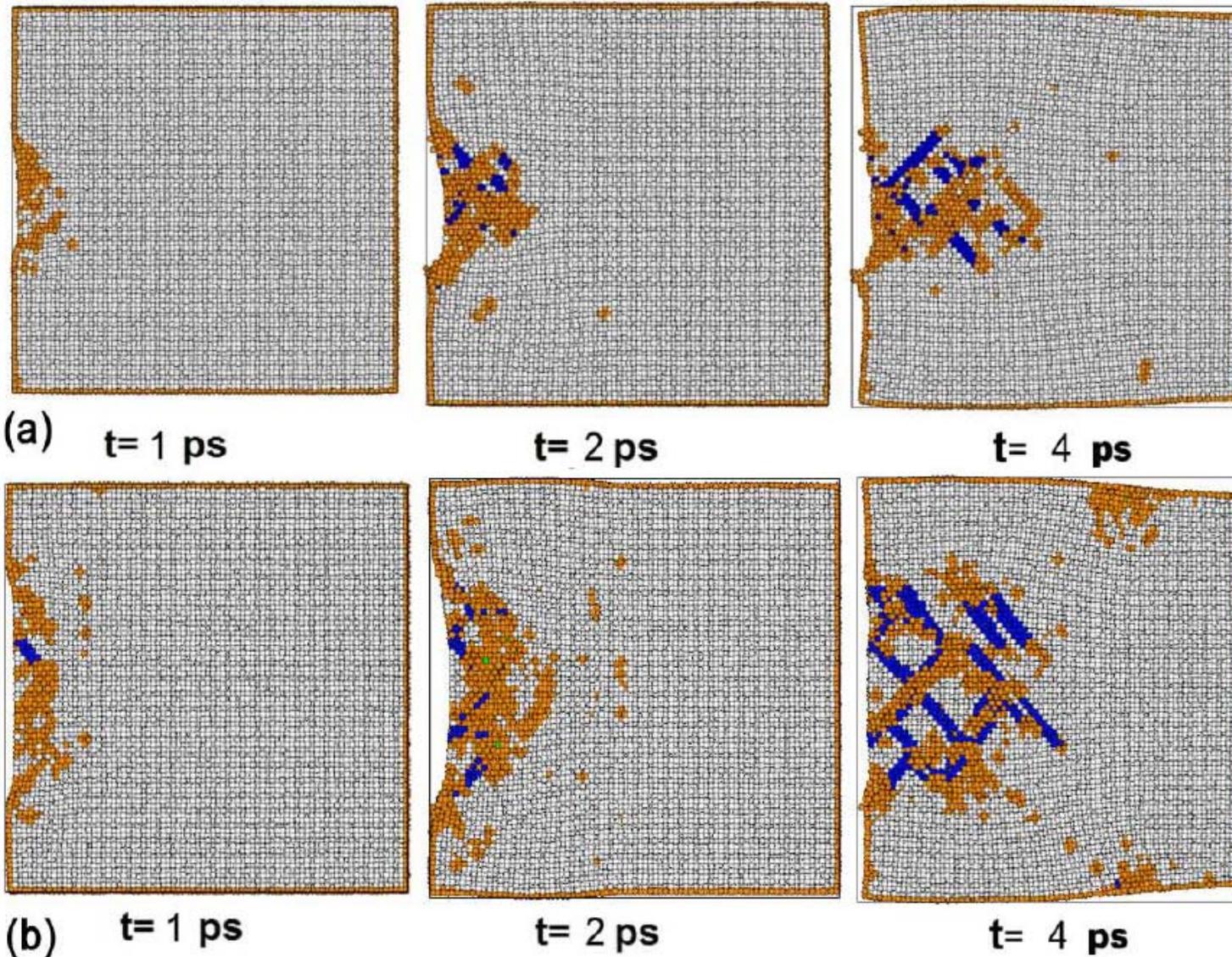
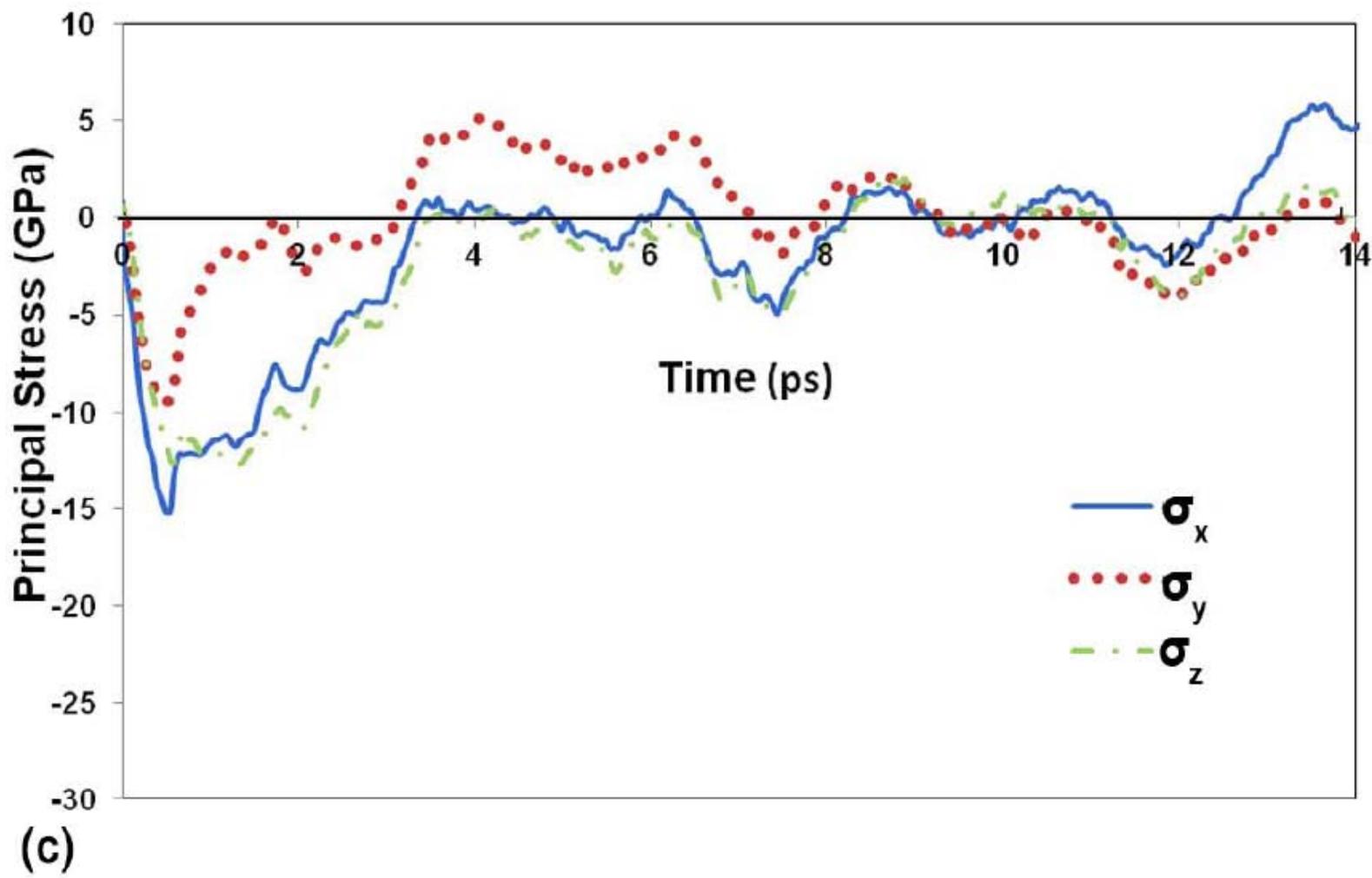




Fig. 5 (c) Time histories of the principal stresses in the target (simulation 2).



(c)

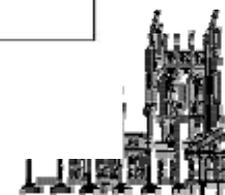




Fig. 5 (d) Time histories of the principal stresses in the target (simulation 8).

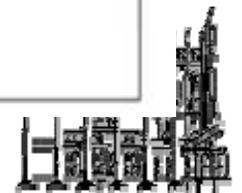
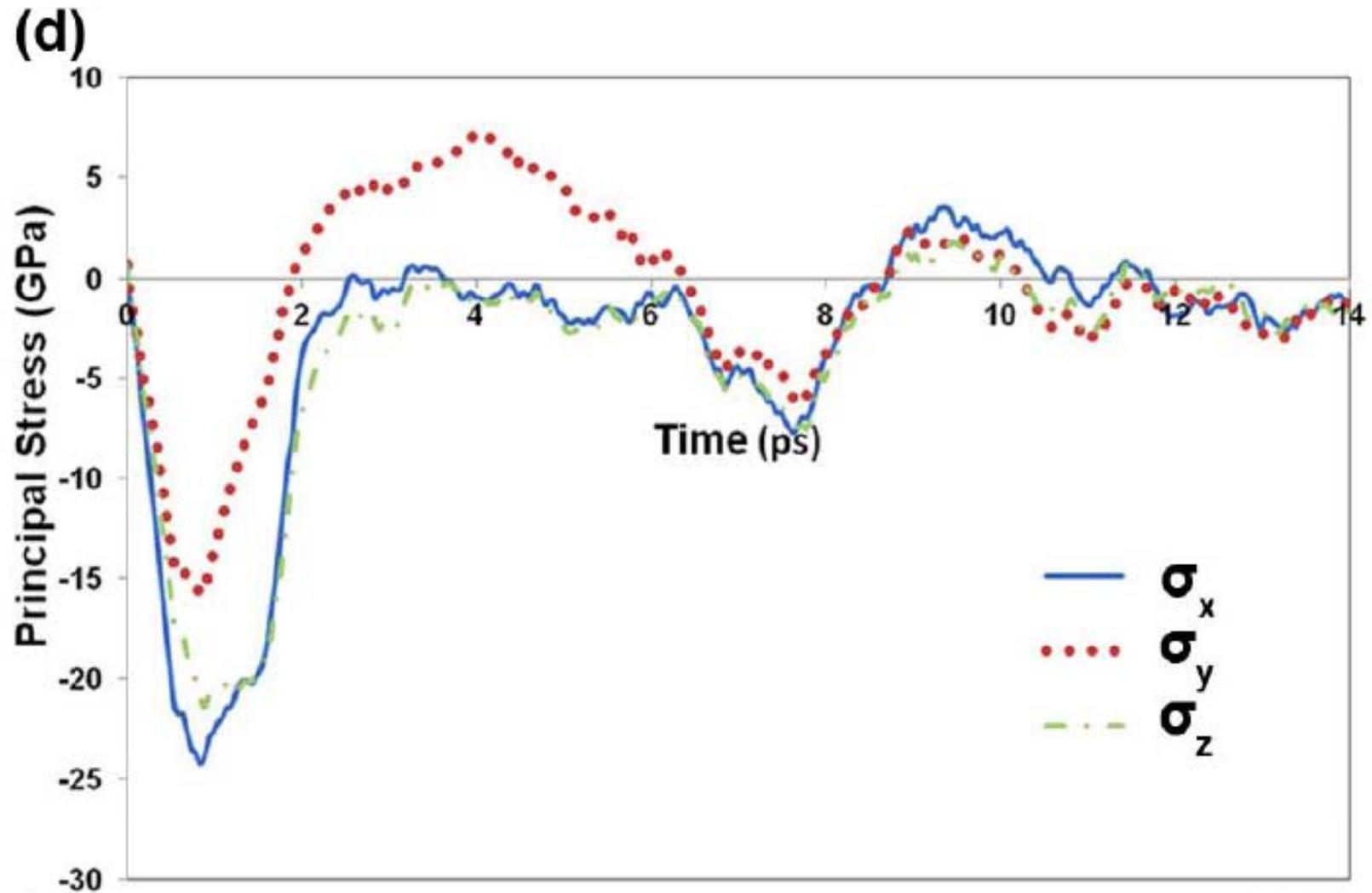
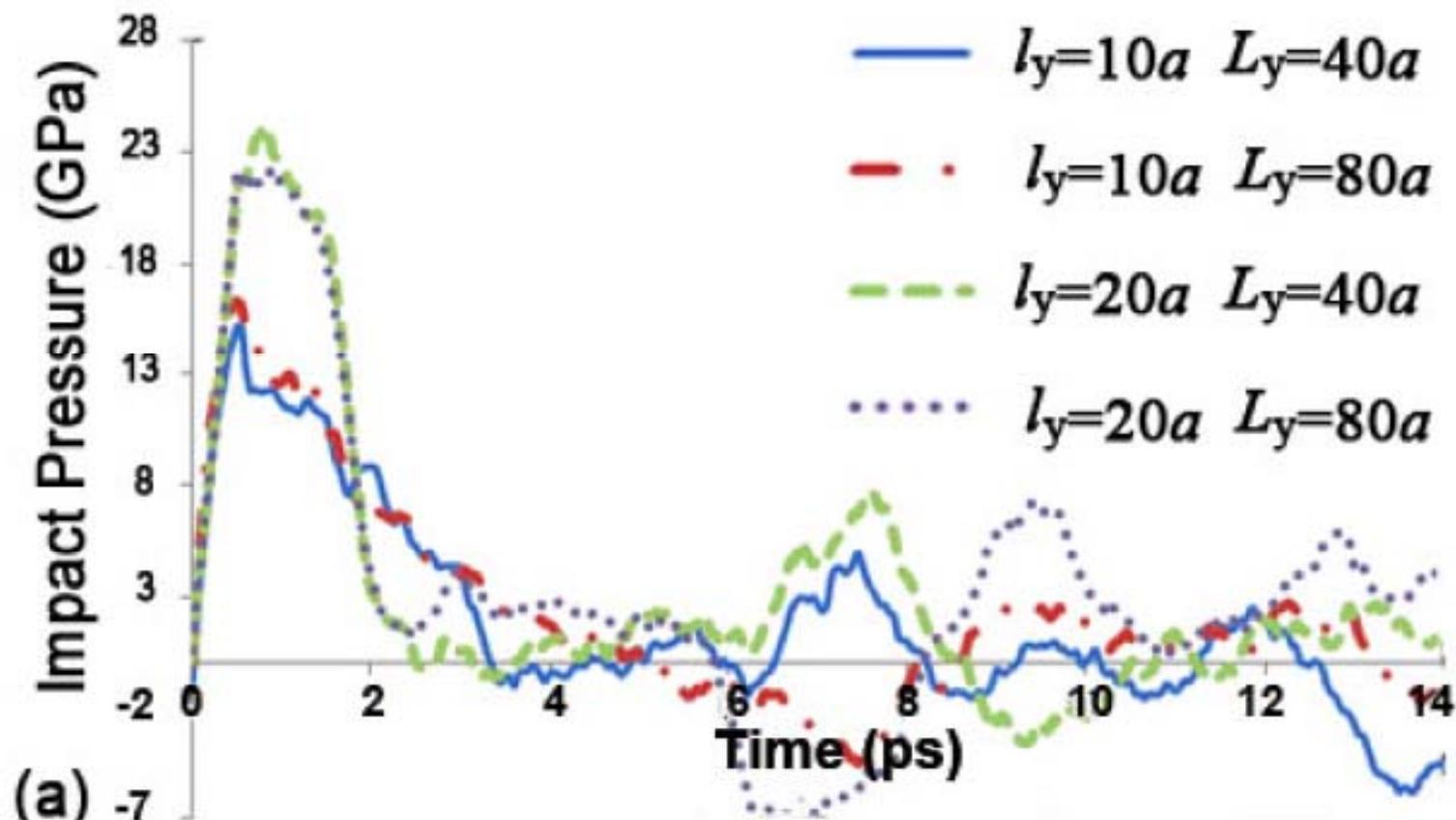
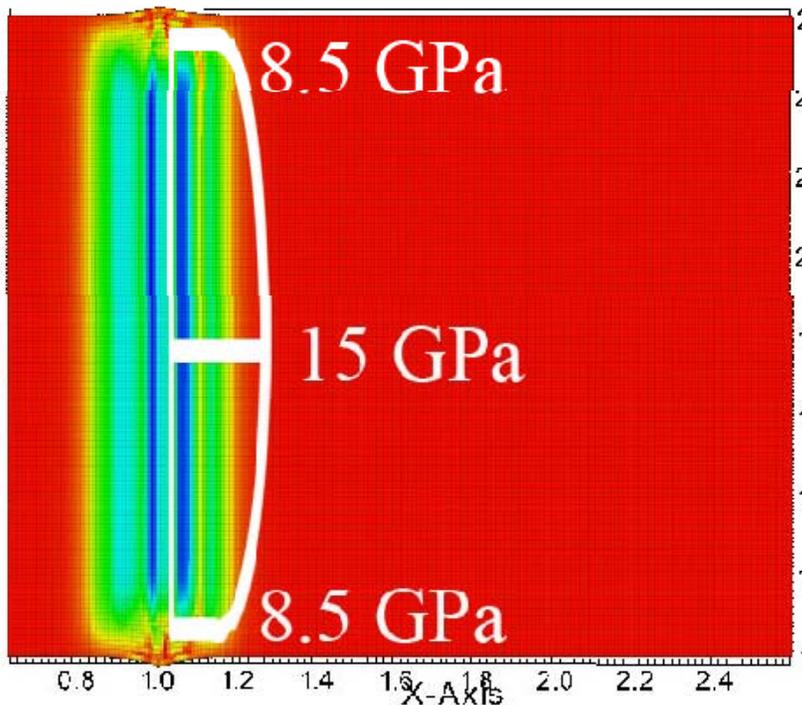
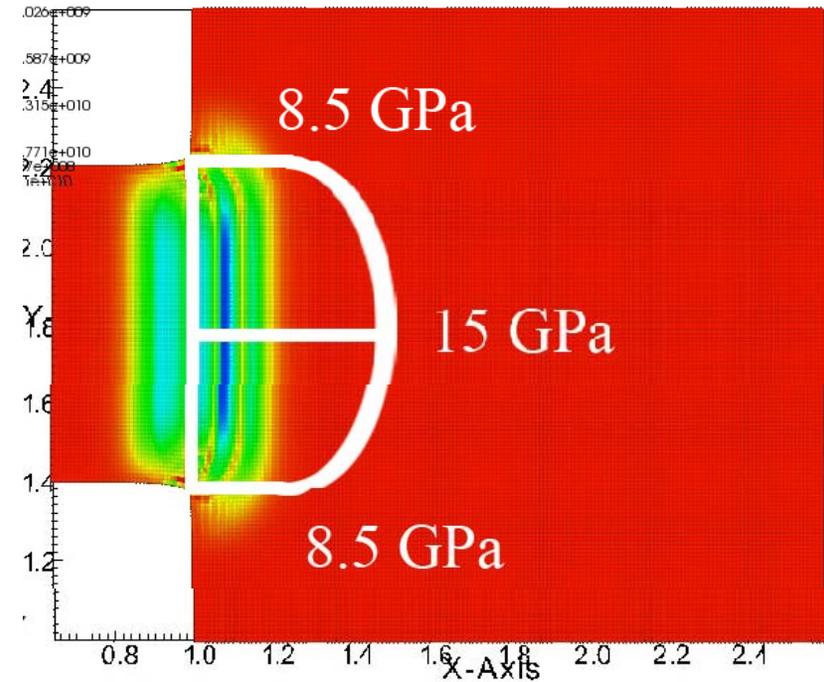
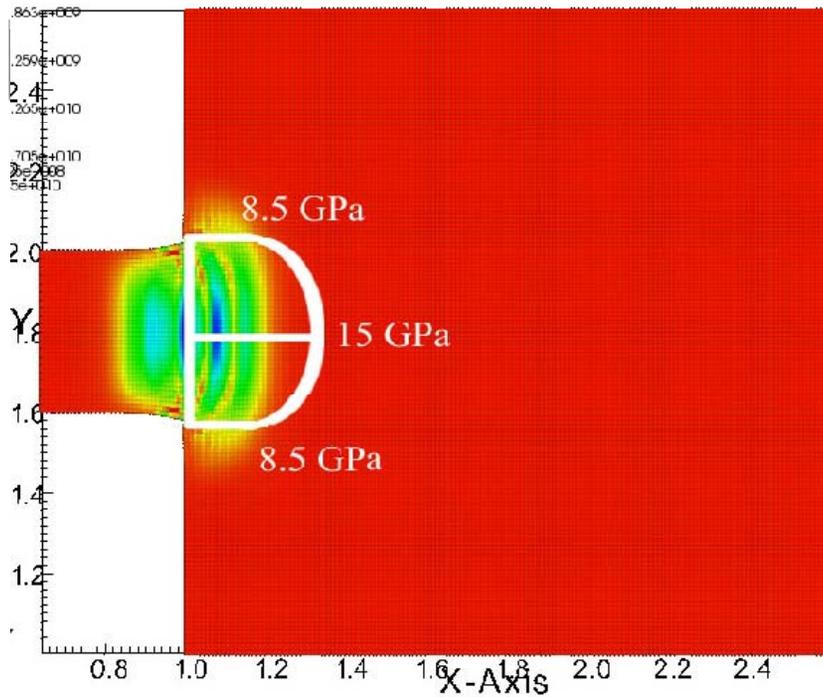


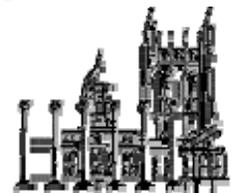


Fig. 8 Time histories of the impact pressure for simulations 2, 8, 16 and 17, respectively.





Aspect ratio effect
 simulated with a local
 constitutive model at
 continuum level





Size effect

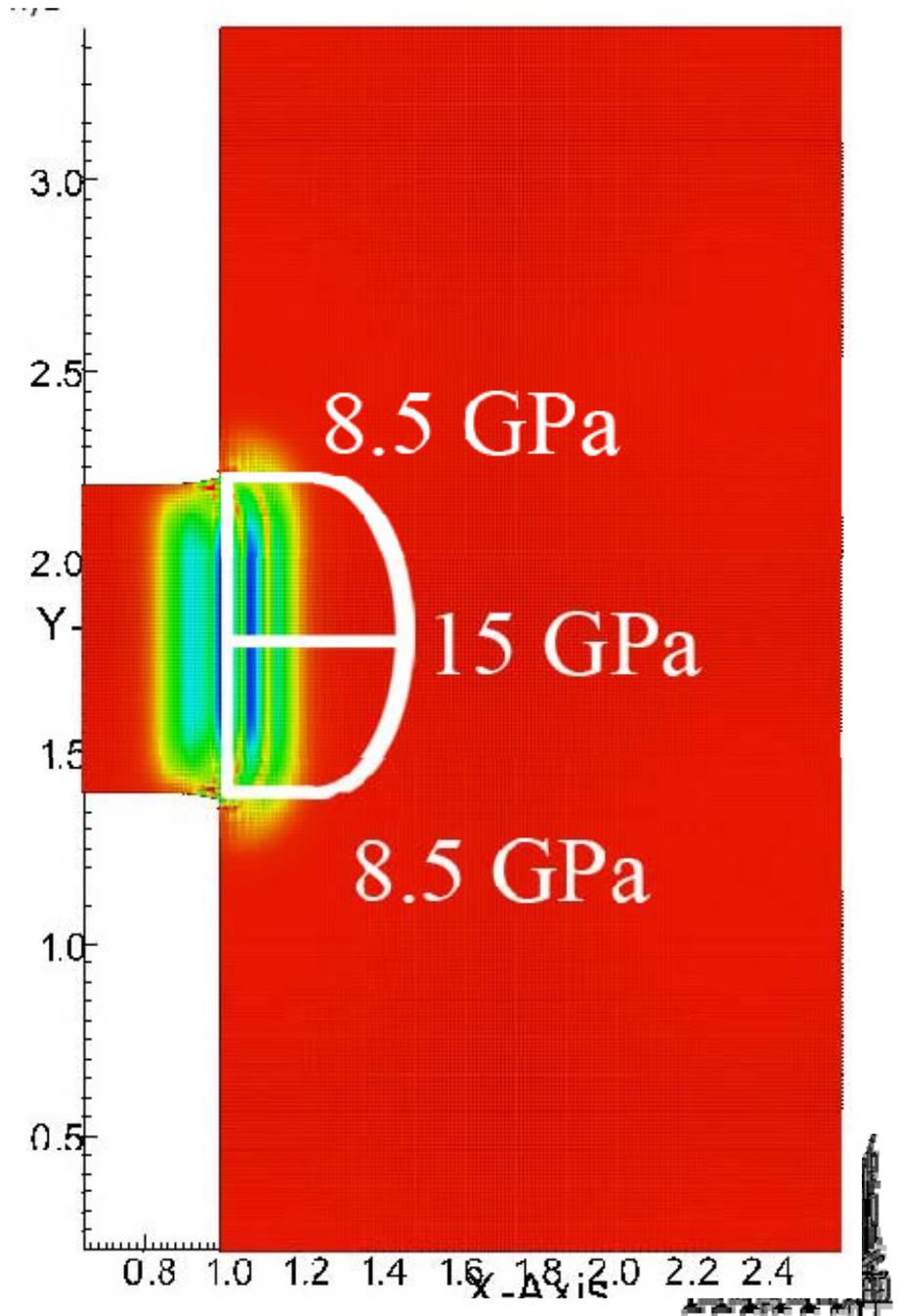
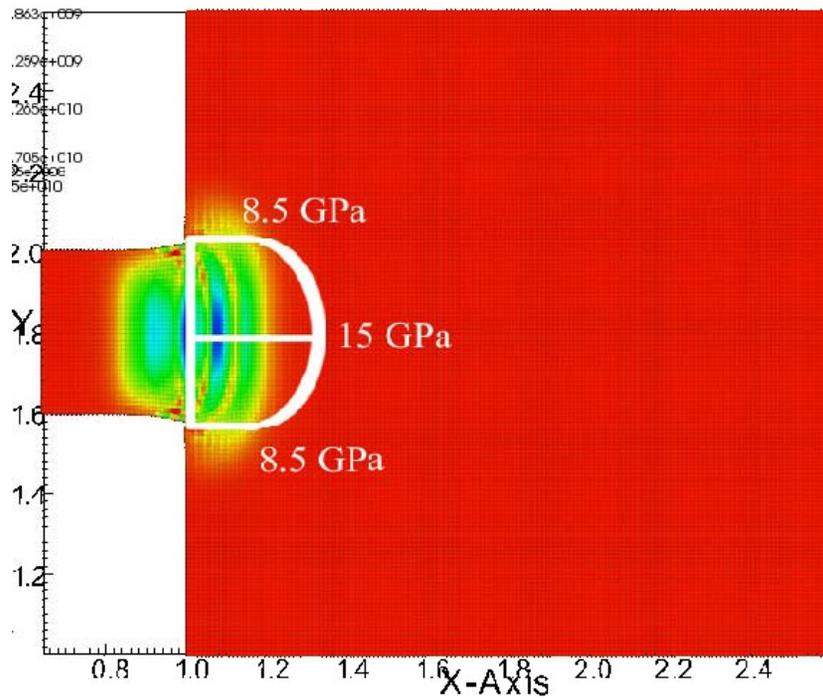
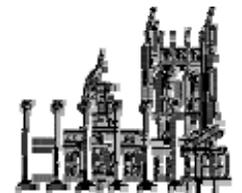
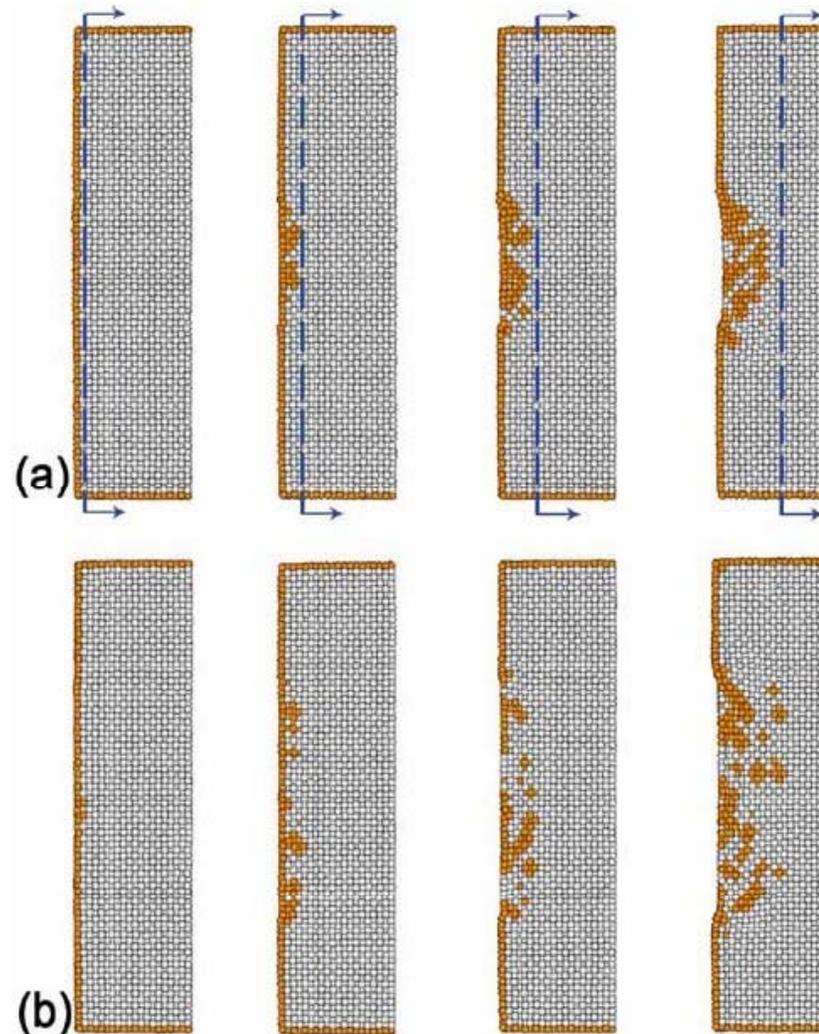




Fig. 7 Atomic configurations with time for (a) aspect ration 1:4 and (b) aspect ratio 1:2, respectively, in which only the target segments of $0 - 10a$ along the x-direction are shown.





Major Findings from the MD Simulations

- The impact response of Cu nanobeams is mainly dependent on the distance between the flyer corners, while the aspect ratio has a negligible effect.
- The evolution speed of disordered atoms diffused from the impact surface first approaches the shock wave speed, and then slows down to form dislocations.
- There might be a transition from the “inverse Hall-Petch” to the classical Hall-Petch phenomenon in single crystals as compared with that in nanocrystalline materials.
- The increase of impact velocity leads to size-dependent increases in the peak impact pressure and equivalent temperature in the target.
- The thermal gradient in the target is mainly due to the temperature difference between hcp zones and fcc atoms.



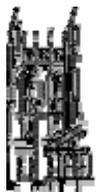
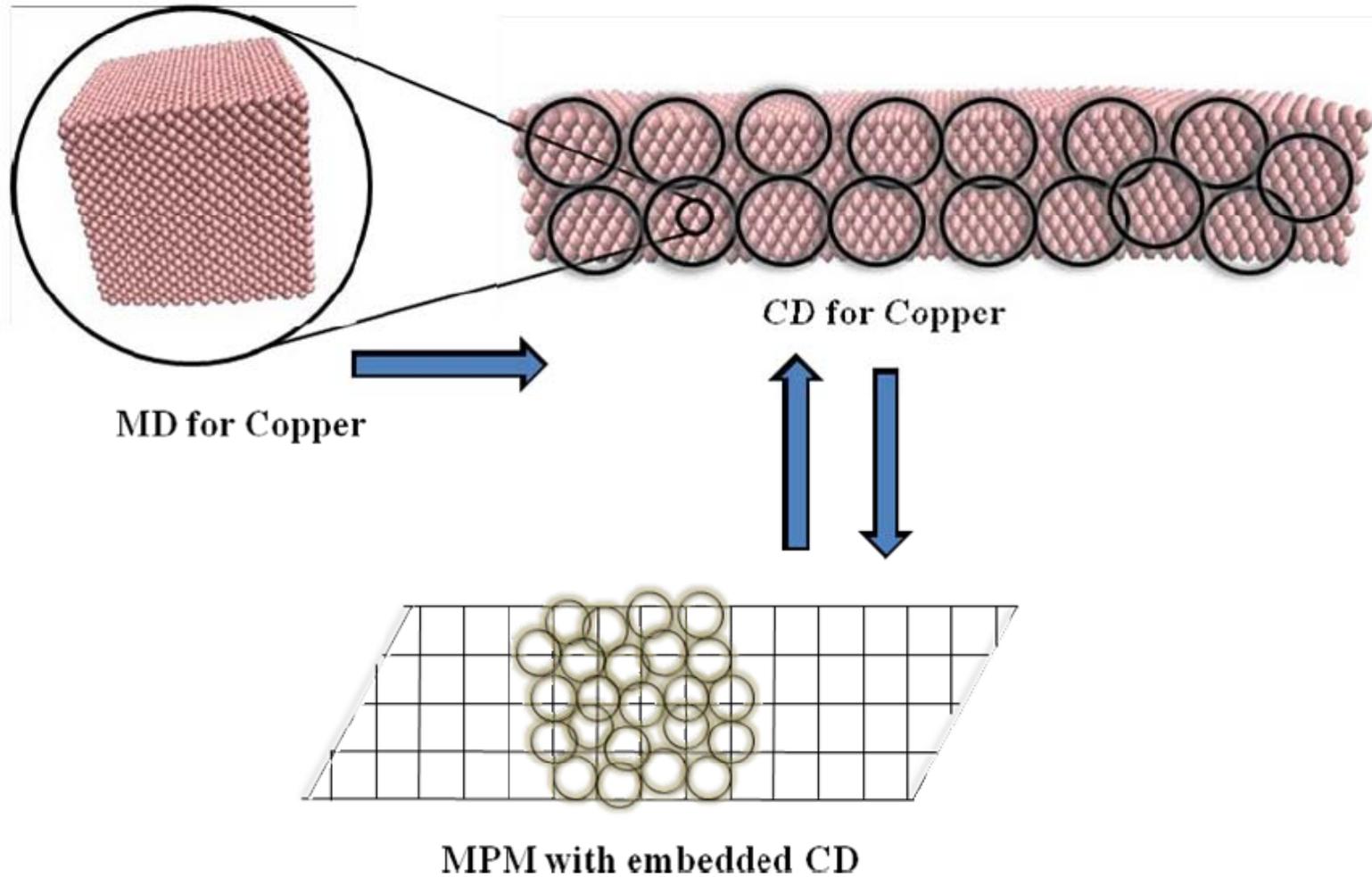


5. A Particle-Based Multiscale Approach (MMPM)

(TAML, Chen et al., 2012)

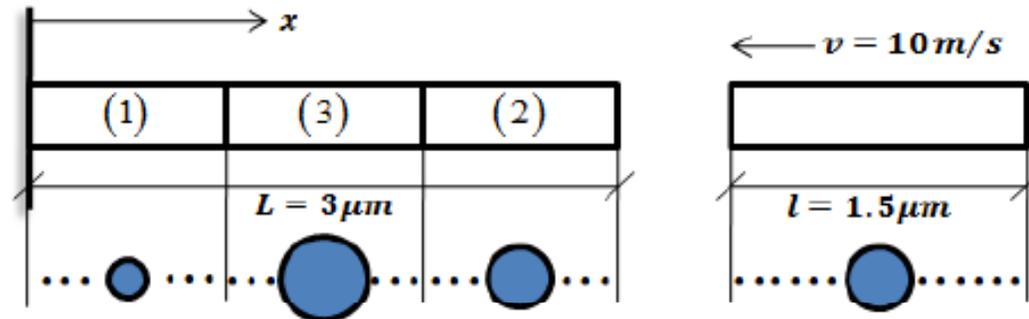
Hierarchical from MD to CD (Cluster Dynamics)

Concurrent between CD and MPM

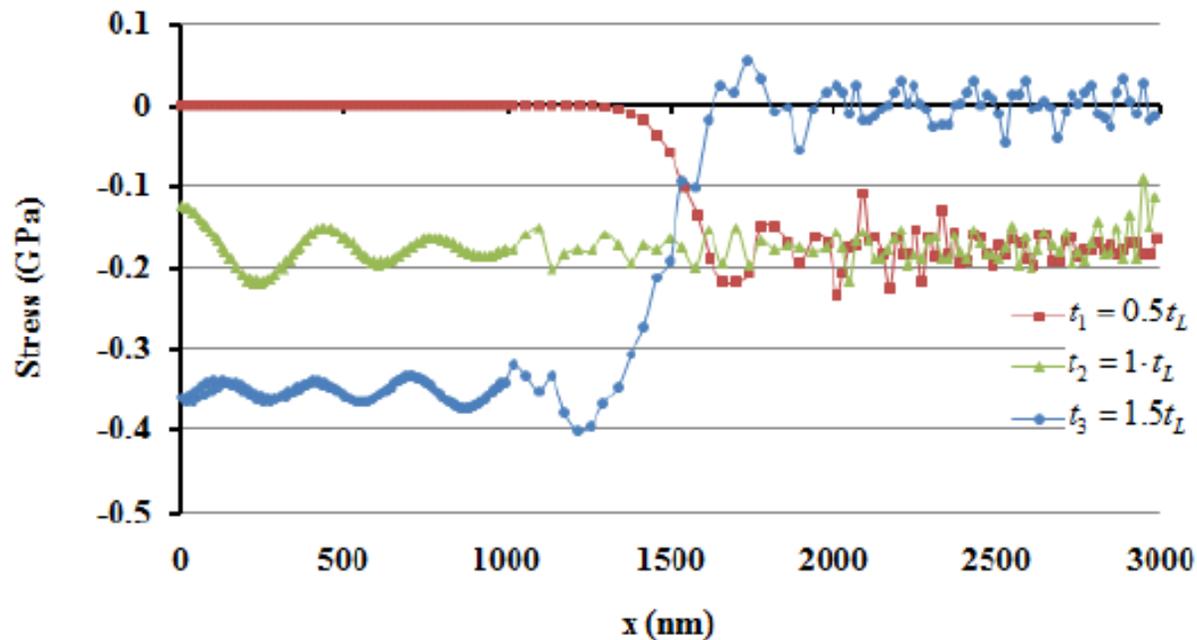




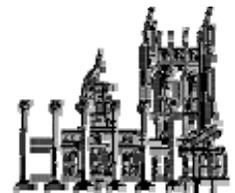
The MMPM simulation of rod-to-rod impact with the target rod consisting of clusters of different sizes.



(a) Problem geometry



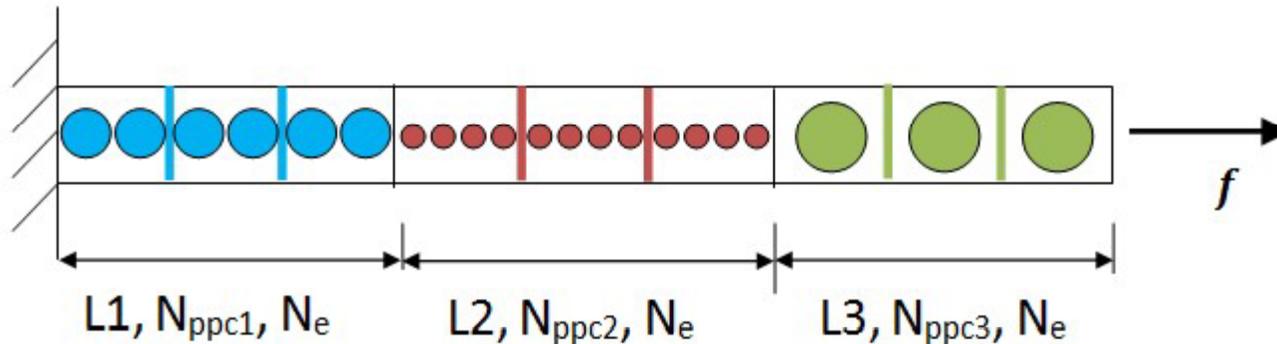
(b) Stress profile



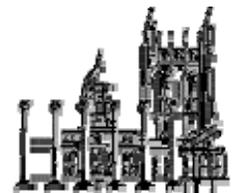


One-Dimensional Wave Propagation with MPM and DDMP

Cased I : Changing the Number of Particles per Cell (N_{ppc})

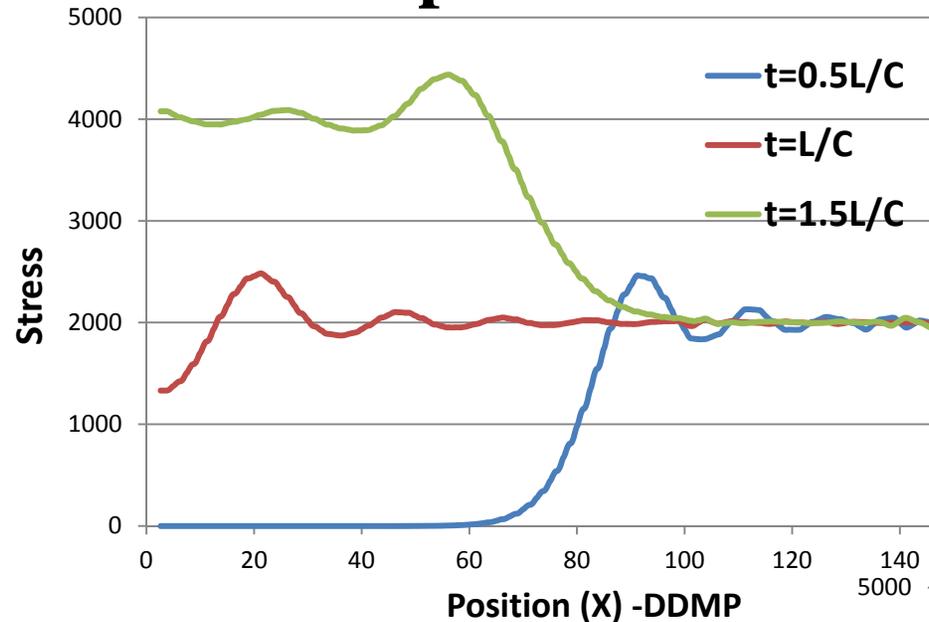


- Total length: $L=150$
- Three segments: $L_1=L_2=L_3=50$
- Number of particles per cell: $N_{ppc1}=10$, $N_{ppc2}=20$, $N_{ppc3}=4$
- Number of cells per segment: $N_e=20$
- Density: $\rho = 1$
- Young's Modulus: $E=1.0e6$
- External force: $f=2.0e3$
- Cross-section area: $A=1$



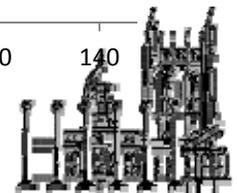
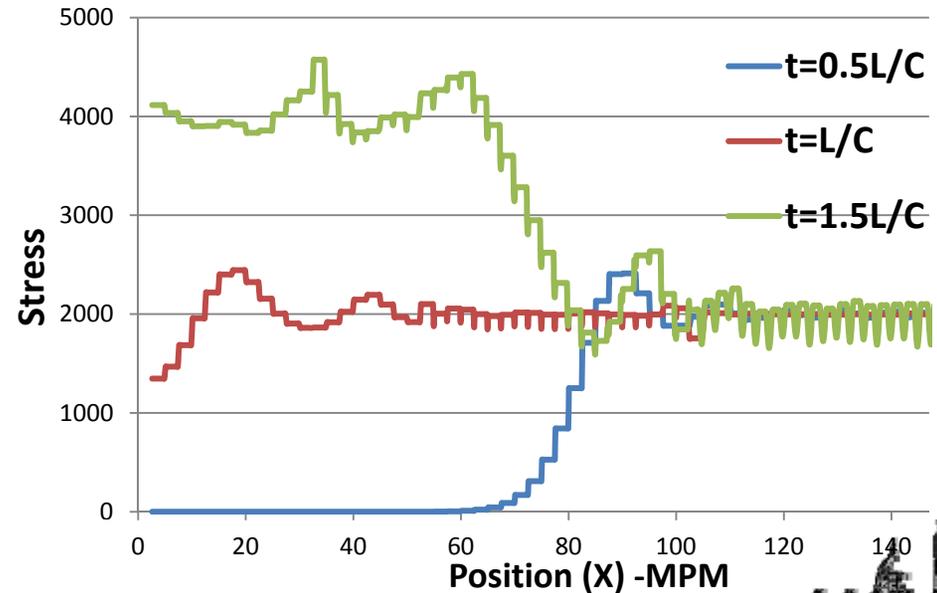


Comparison between DDMP and MPM



- With the MPM, the numerical noise becomes large if the particles cross the cell boundaries in the segment with a large number of particles per cell.

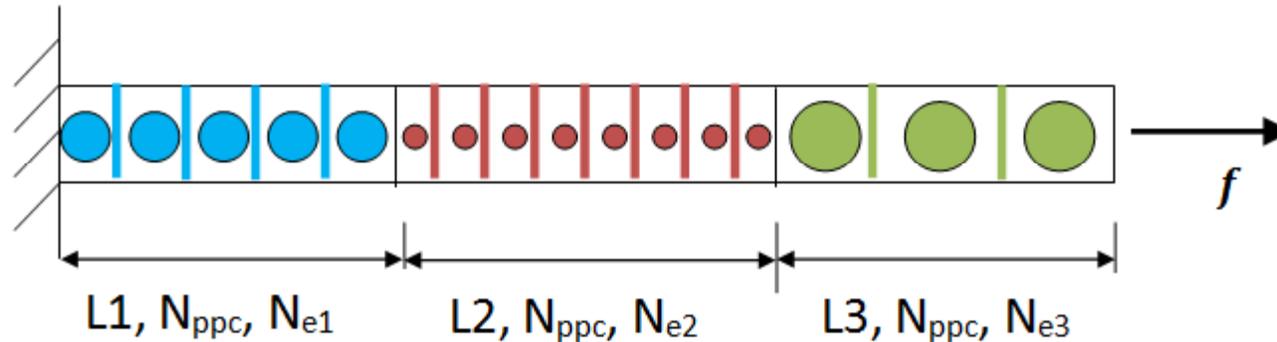
- With the DDMP, the numerical noise is small when the material particles cross the cell boundaries in the segment with a large number of particles per cell .



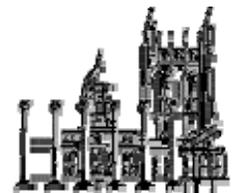


One-Dimensional Wave Propagation with MPM and DDMP

Cased II : Changing the Cell Size with Nppc Being Fixed

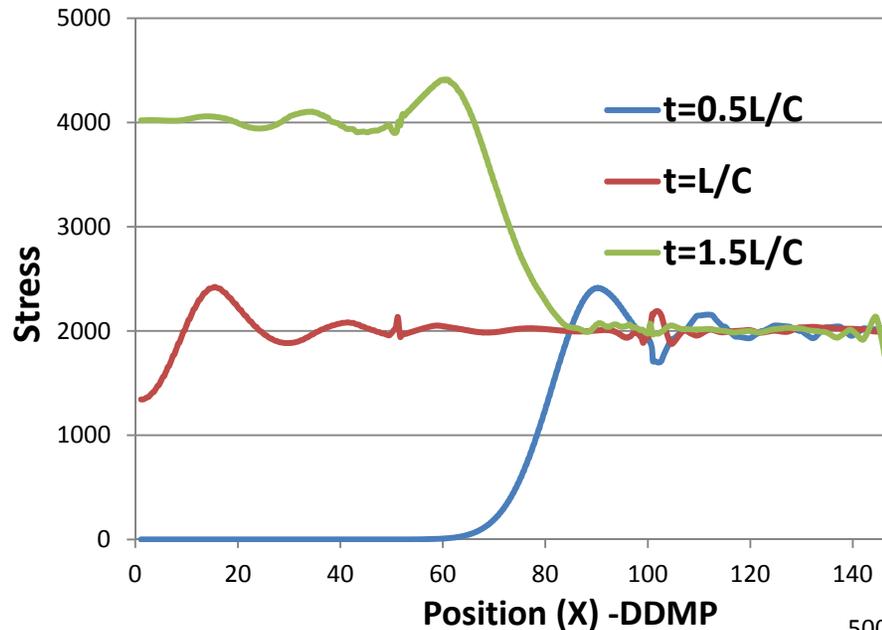


- Total length: $L=150$
- Three segments: $L1=L2=L3=50$
- Number of particles per cell: $N_{ppc}=4$
- Number of cells per segment: $N_{e1}=50, N_{e2}=100, N_{e3}=20$
- Density: $\rho = 1$
- Young's Modulus: $E=1.0e6$
- External force: $f=2.0e3$
- Cross-section area: $A=1$





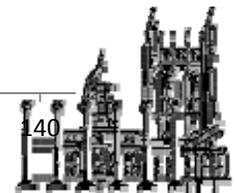
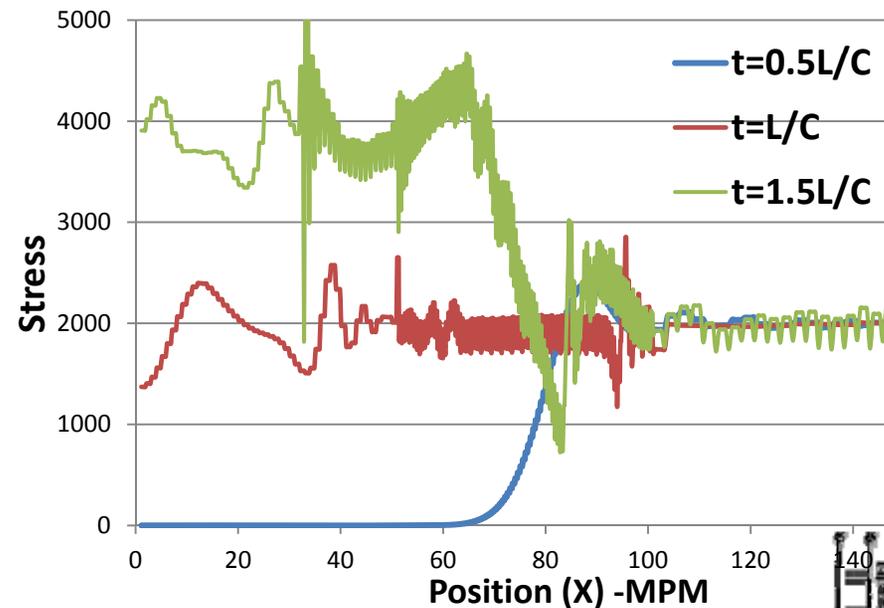
Comparison between DDMP and MPM



- With the MPM, the large numerical noise can be observed if the material particles cross the cell boundaries in the fine mesh, in addition to the stress jumps at the interface.

With the DDMP,

- Numerical noise is small when the particles cross the cell boundaries in the segment with very small cells.
- However, the stress jumps on the interface between the coarse mesh and fine mesh can be observed if the cell size difference becomes large. Further study is needed to improve the DDMP.

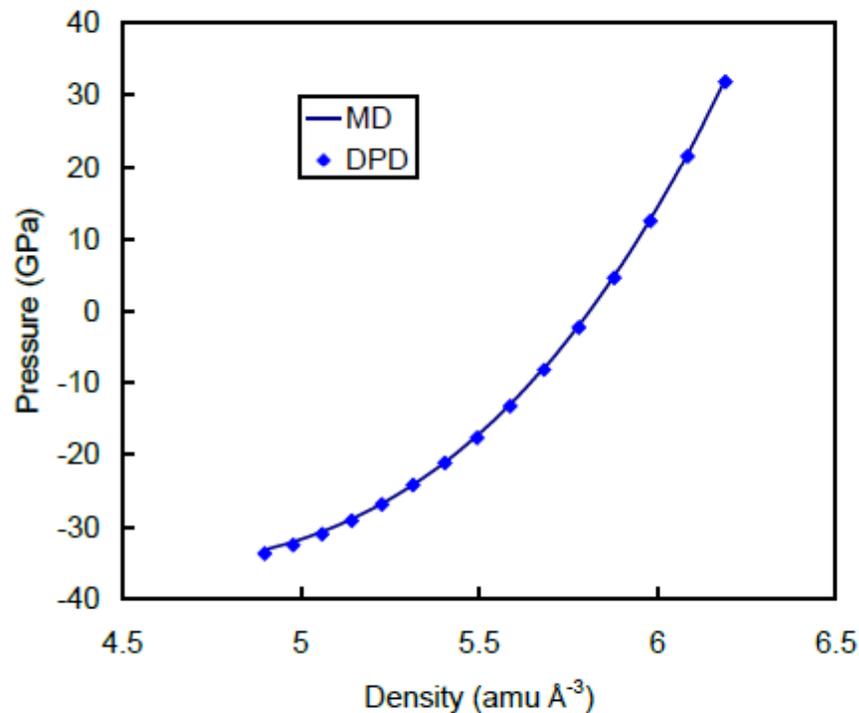




Dissipative Particle Dynamics (DPD) as an Alternative for Cluster Dynamics (CD)

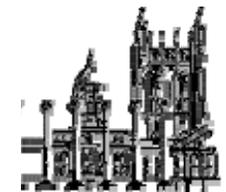
Simulation	ε (eV)	σ (Å)	Cutoff (Å)
MD	0.415	2.277	5.0
DPD	26.323	9.098	25.0

Potential parameters



Comparison of the D-P relations by the MD and DPD

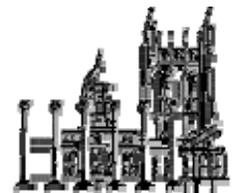
(1) The DPD results in the figure are obtained using the open source LAMMPS, (2) the DPD model size is $60a \times 60a \times 60a$, and (3) the pressure in the DPD are averaged over 20 ps.





6. Concluding Remarks and Future Tasks

1. The MPM could be combined with other numerical methods for multi-physics and multi-scale simulations in different cases with the least computational costs.
2. MD simulations have been performed to predict coupled rate and size effects at nanoscale, which provide the useful information for formulating an effective multi-scale equation of state.
3. A multi-scale simulation procedure is being developed, via hierarchical approach from MD to CD/rDPD and concurrent one between CD/rDPD and MPM, for modeling and simulating energetic composite responses, in combination with in-lab experiments.





The Deadline for Abstract Submission is March 15

Please join us in the MPM mini-symposium organized for the 2013 USNCCM to be held in July.

Our mini-symposium is entitled “MS 9.4 – The MPM and Similar Particle Methods.”

Please submit your abstract to the following website:

<http://12.usnccm.org/abstract-submission>

