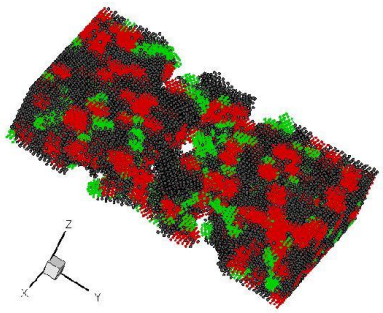
**Research Project**: Nano particle reinforced composites for critical infrastructure protection

**Research Topic**: Particle dynamic simulation

**Problem**

Multi-scale research, using particle dynamics simulation to developing continuum theory of nano-composite material systems and develop material database for nano-particle reinforced composites and other low-cost, high-strength, innovative materials, such as fly ash and polymer enhanced concrete.

**Approach**



*A 3D heteorgeous material body in tension*

The particle modeling (PM)—also called particle simulation, discrete modeling or quasi-molecular modeling—is a dynamic simulation method that typically uses a lattice of small (but not molecular level) particles, evolving according to laws of mechanics, as a discrete representation of fluids and/or solids. The method is set up so as to maintain the conservation of mass and energy and equality of Young's modulus and tensile strength of the particle system and satisfy the interaction laws between all the particles. The PM can handle a wide range of complex material systems, complicated boundary shapes and boundary conditions, dynamic free surfaces, and fracture of solids. In this project we will adopt PM for the simulation of dynamic fracture phenomena in homogeneous and heterogeneous materials. This will involve the setup of a lattice-type PM having the same functional form as the MD model (i.e., the Lennard–Jones potential), yet on centimeter length scales. In PM, the interaction force is considered only between nearest-neighbor (quasi-) particles and assumed to be of the same form as in MD. We will adopt PM for the simulation of dynamic fracture phenomena in homogeneous and heterogeneous materials, such as encountered in blasting processes.

**Findings**

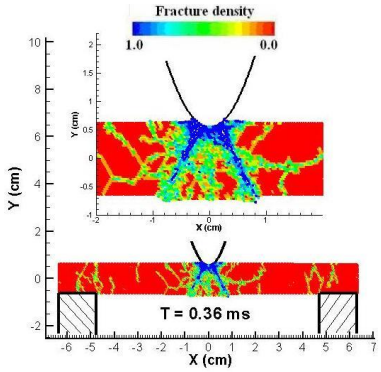
The work is in progress. However, significant accomplishment was achieved in using particle dynamics to simulate:

1- dynamic fracture of polymeric materials (e.g. nylon-6,6) and metallic materials (e.g. copper) due to impact of rigid indictor as shown in the figure.

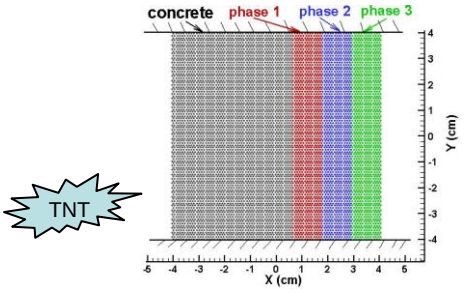
2- crack propagation and effective load-deflection curves of end notched specimens subjected to dynamic loading.

3-Dynamic fracture models under development for multi-layer CMU wall section to explore new concepts in reinforcement

Particle Dynamics codes are under evaluation to improve their accuracy and confidence.




***Impact on a 2D polymeric material body***




***Blast of retrofitted concrete wall***

**Impact**

The particle dynamics, fracture propagation simulations reported last month offer a new way to establish design requirements for nano-particle reinforcement of concrete structural components to meet severe loading (i.e. blast and seismic) demands.
A new methodology is under development, and a record of invention will be pursued through UM Office of Research once confirmatory analyses are complete.

**Researcher**: Dr. Ahmed Al-Ostaz is Associate Professor of Civil Engineering. Dr. Ge Wang is a Research Assistant Professor in the Department of Civil Engineering at University of Mississippi

(*Last update: July 2007*)