Billion-atom Multiscale Simulations of Nanosystems on a Grid

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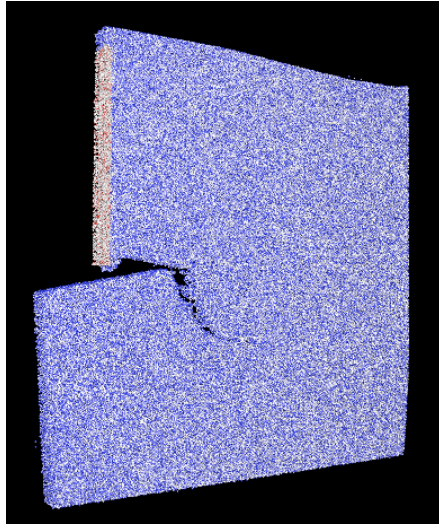
CACS USC

Outline

Research

- **Fracture in Compression; Nano-indentation; Grid Computing; Billion Atom Walkthrough**
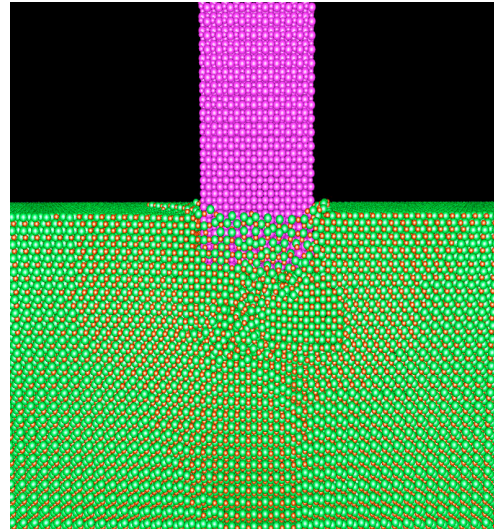
Education & Outreach

- **Computational Science Workshop for Under Represented Groups**
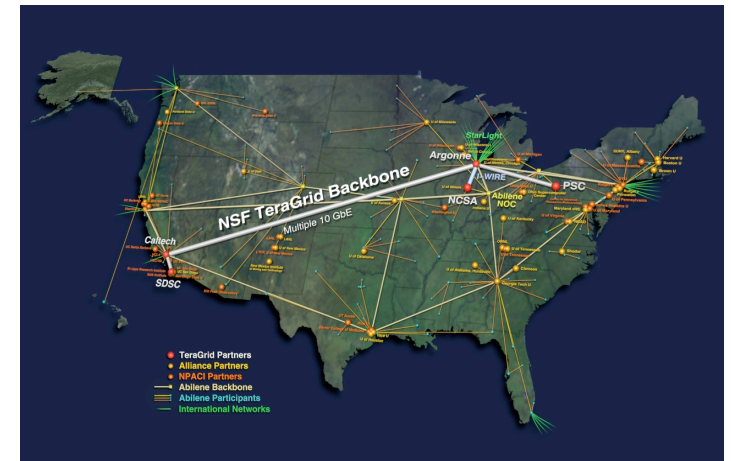
Overview of accomplishments

Compressive fracture **Nanoindentation** **Grid Computing**
USA (USC, NSF) - Japan (AIST)

- **Nucleation, growth and healing of wing cracks in silica glass under dynamic compressive loading**

- **Nanoindentation-induced dislocation emission & amorphization in silicon carbide**

- **GRID Computing: Environmentally assisted fracture in silicon using divide & conquer strategy**

Education & Outreach

- **Dual Degree Program: PhD (Science or Eng) + MS (CS)**
  - > MS with specialization in Cybersecurity
  - > MS with specialization in High Performance Computing & Simulations

- **Reaching out to underrepresented groups through hands-on computational science workshops**
  - > 21 students and 11 faculty mentors from minority institutions form 12 states (CA, GA, IL, LA, MD, MT, OH, SC, TX, USVI, VA)
  - > Students with varying backgrounds—freshmen through seniors Applied physics, biology, chemistry, computer science, mathematics, physics, computer engineering, mechanical engineering and school of pharmacy

- **Hands-on experience in parallel computing**
  - > Assembly of PCs nodes from off-the-shelf components, Scientific and simulation Software Scientific and simulation softwar, Connecting them to a Gigabit switch Algorithmic and simulation exercises in a tutorial setting

Participants from U Texas, Pan-American (Hispanic minority institution) and Norfolk State University (African American minority institution) subsequently built their own clusters.
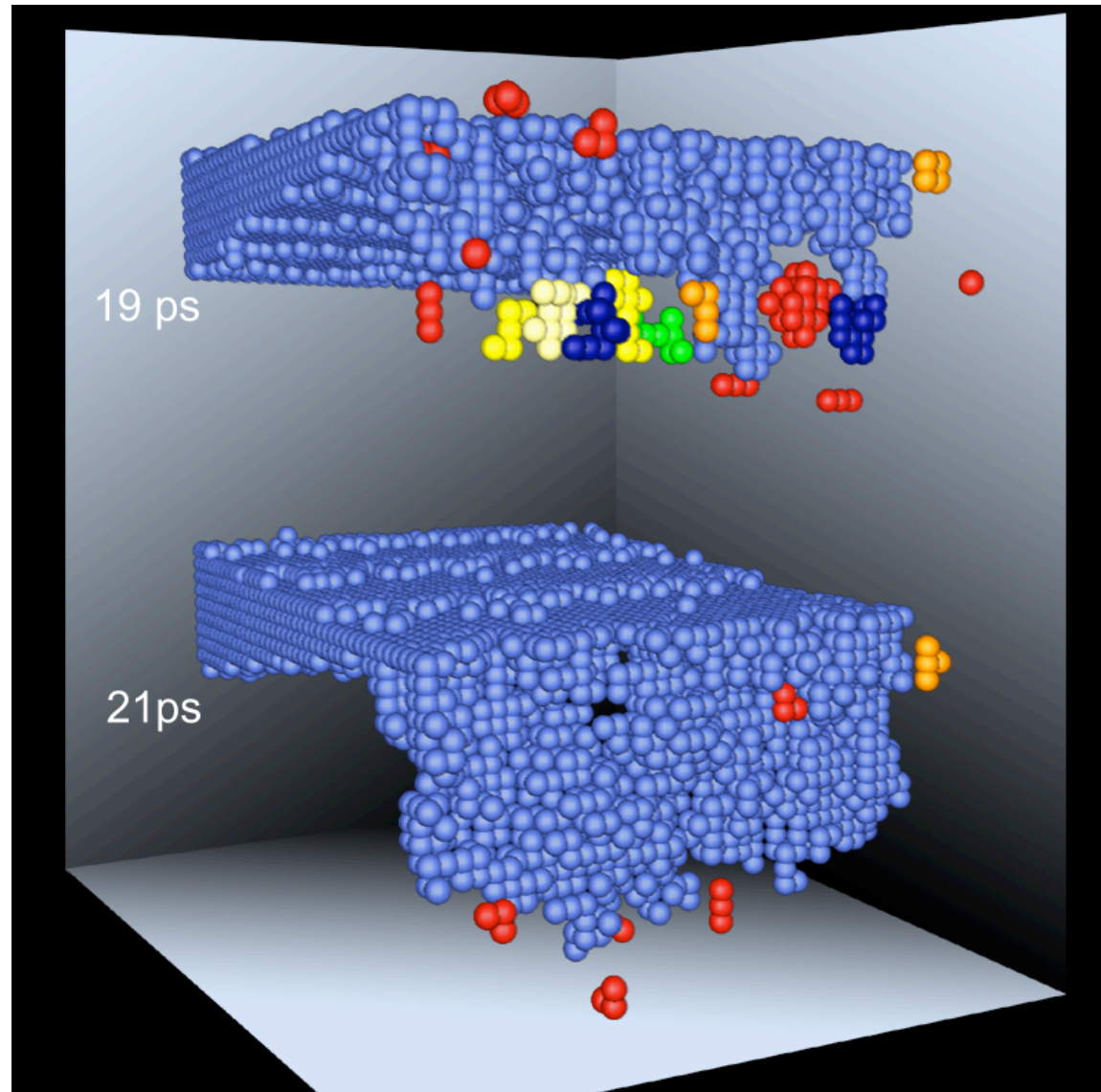
Research

Wing crack dynamics in confined silica glass
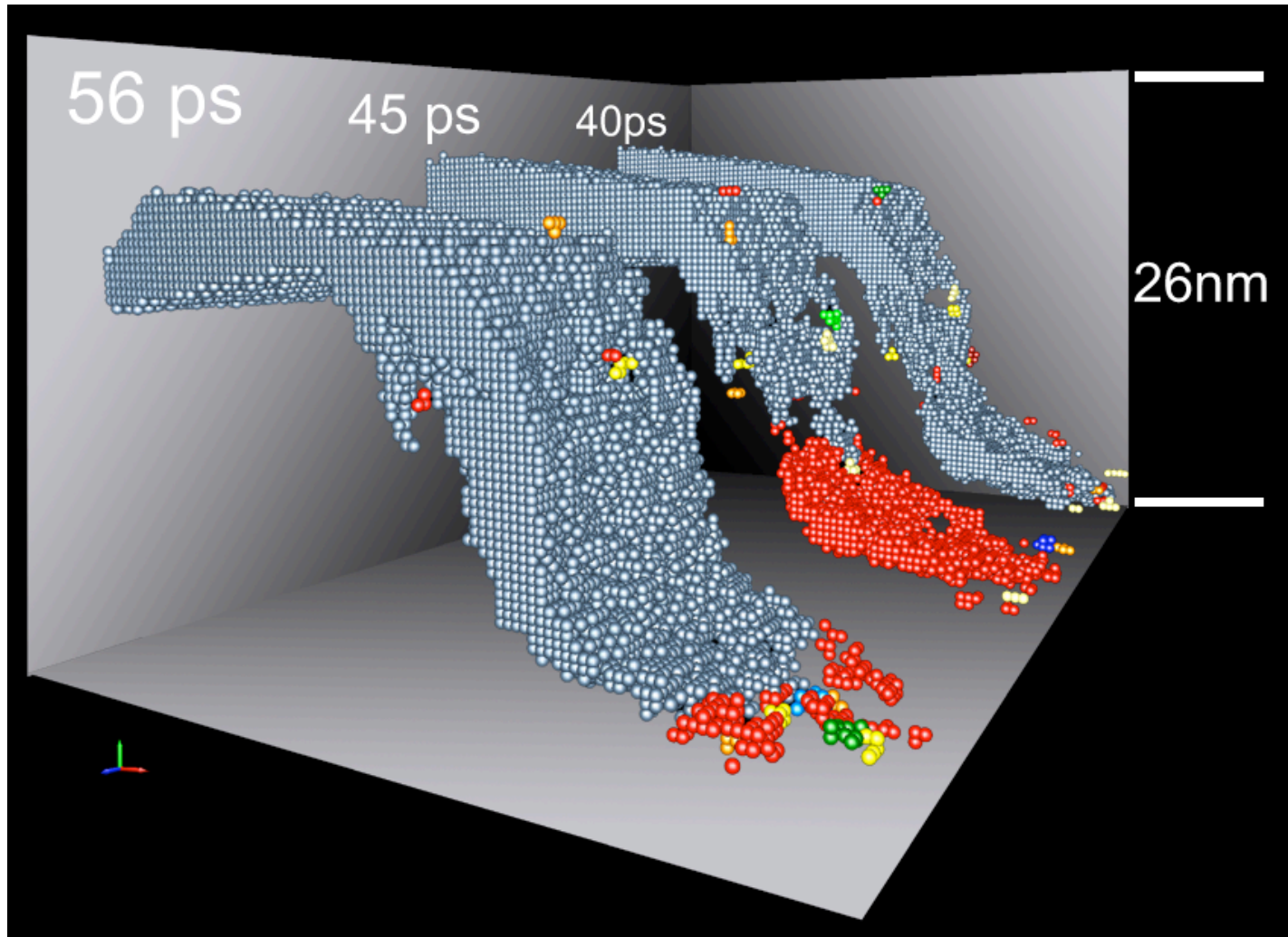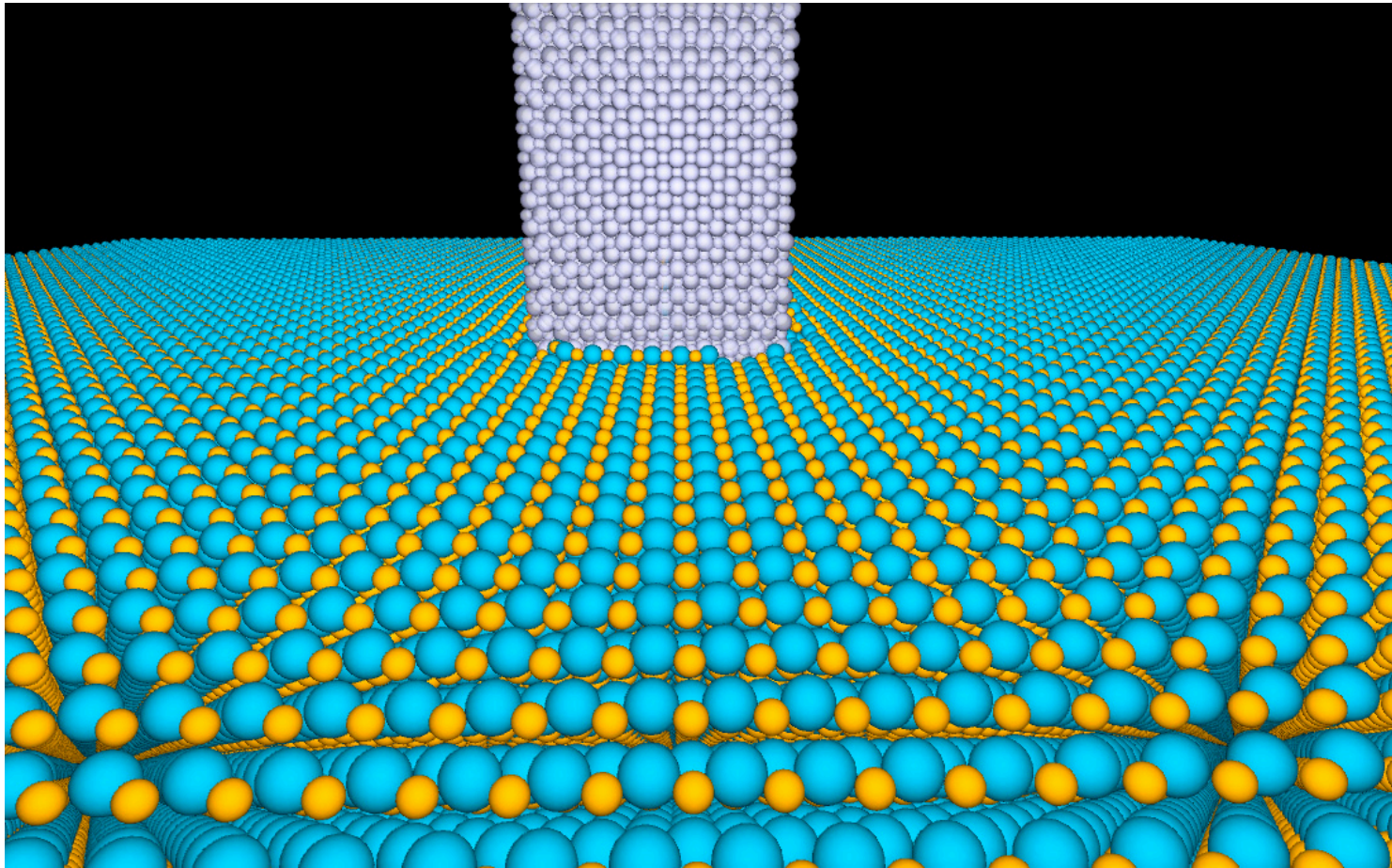
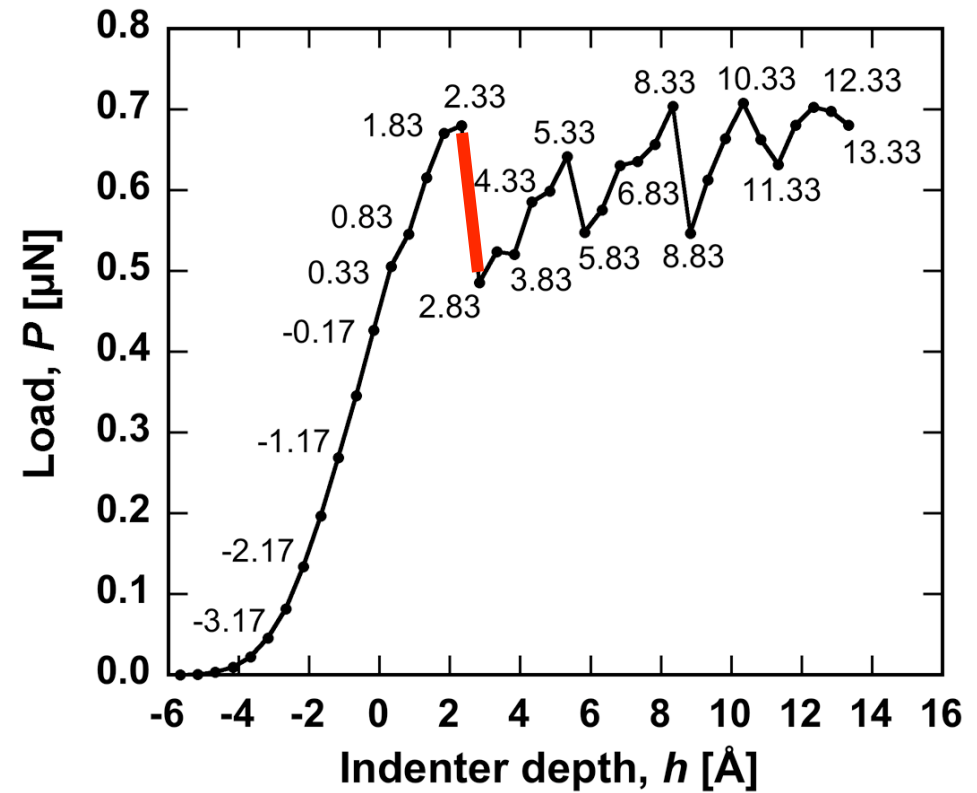## Impact speed = 150 m/s
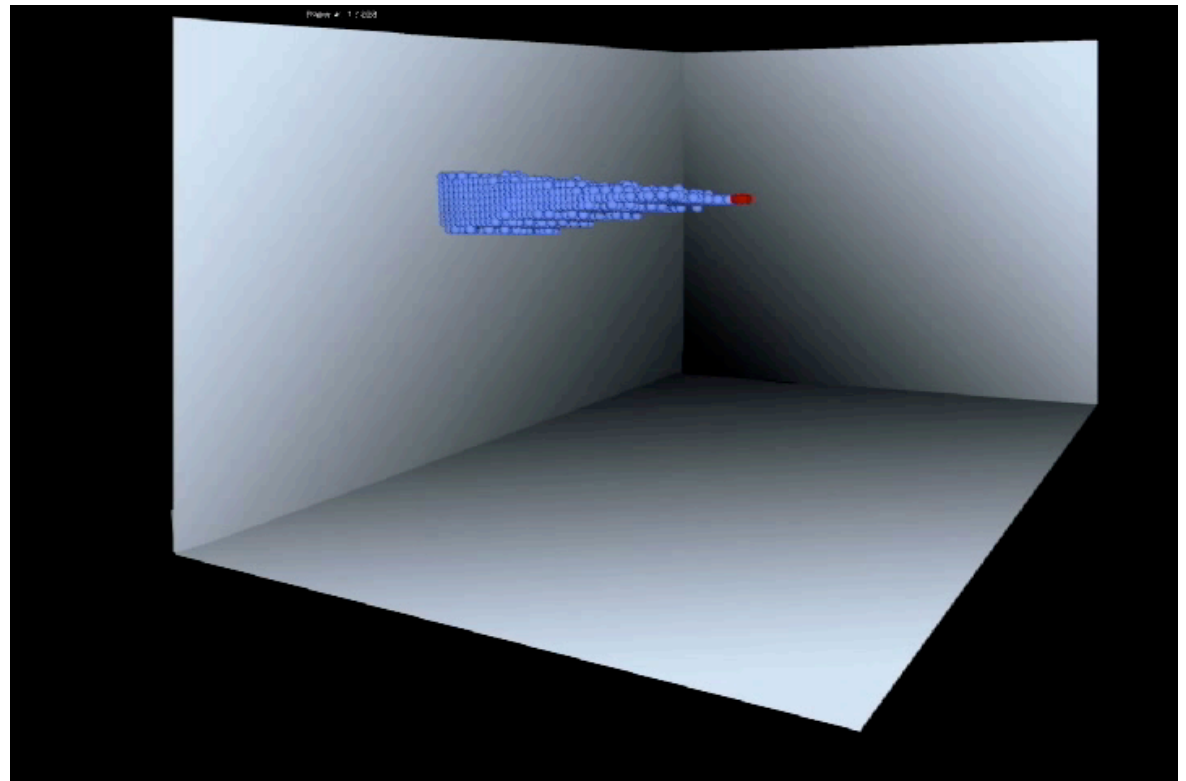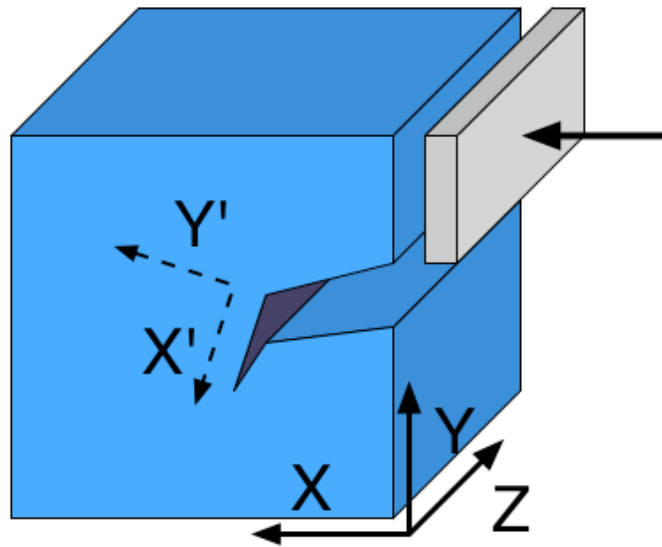
Wing Crack Growth
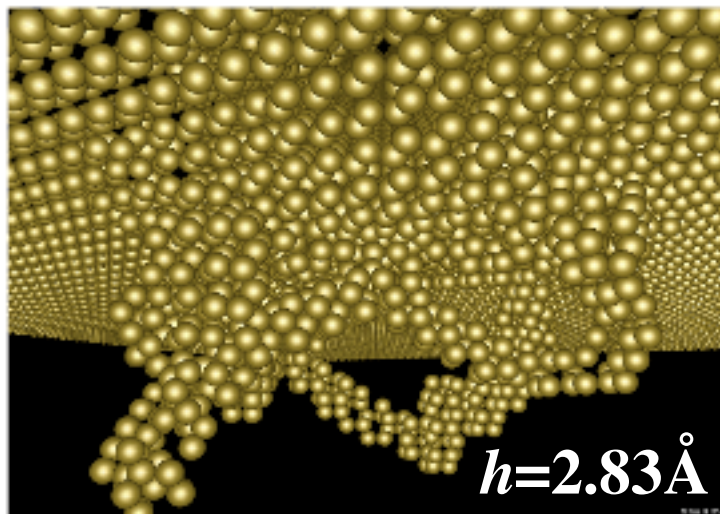
Wing Crack Healing
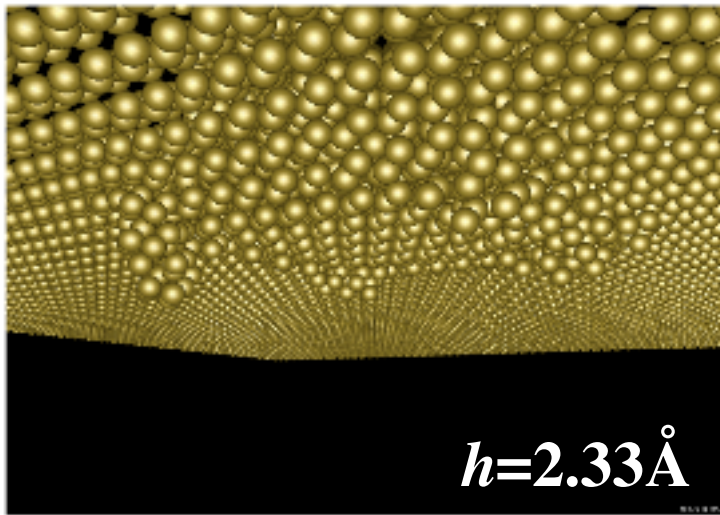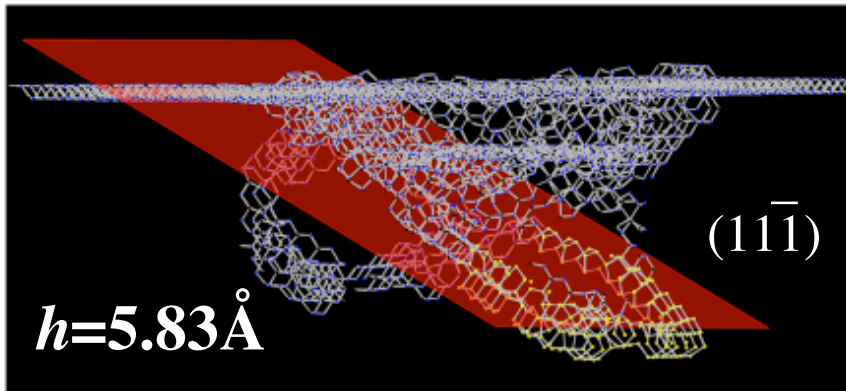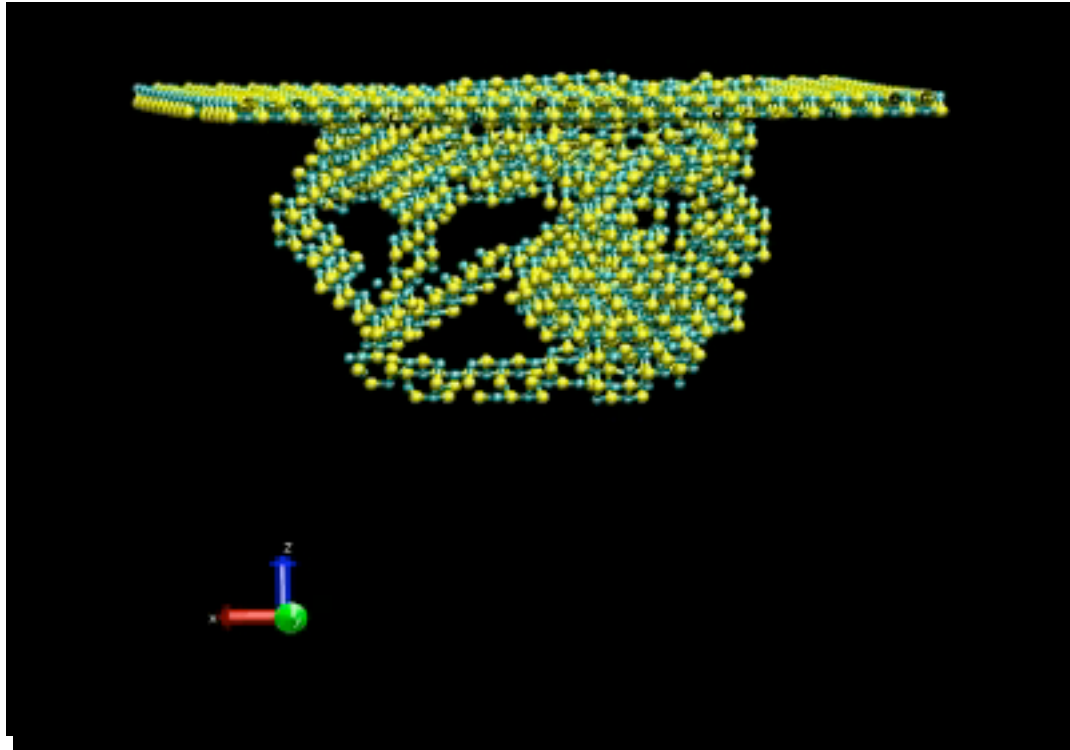
Impact Speed = 375 m/s

Nanoindentation in Silicon Carbide

Nanoindentation yields important information about elastic and plastic deformations

Dislocation Analysis Using n-fold Rings
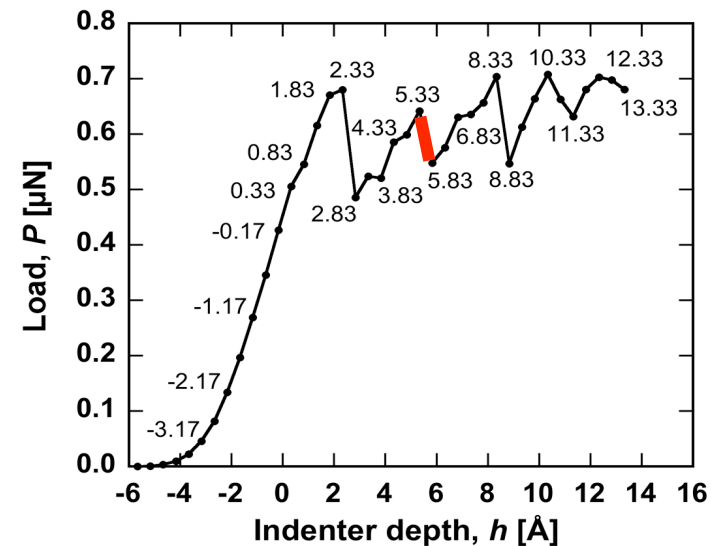

h=2.33Å

h=2.83Å

- **Outburst of dislocation loops at the first load drop**

Dislocation Analysis Using n-fold Rings

- **Dislocation loops begin to coalesce at h = 5.83Å**

- **Before the load drop:** h = 5.33Å: (111), (11$\bar{1}$)
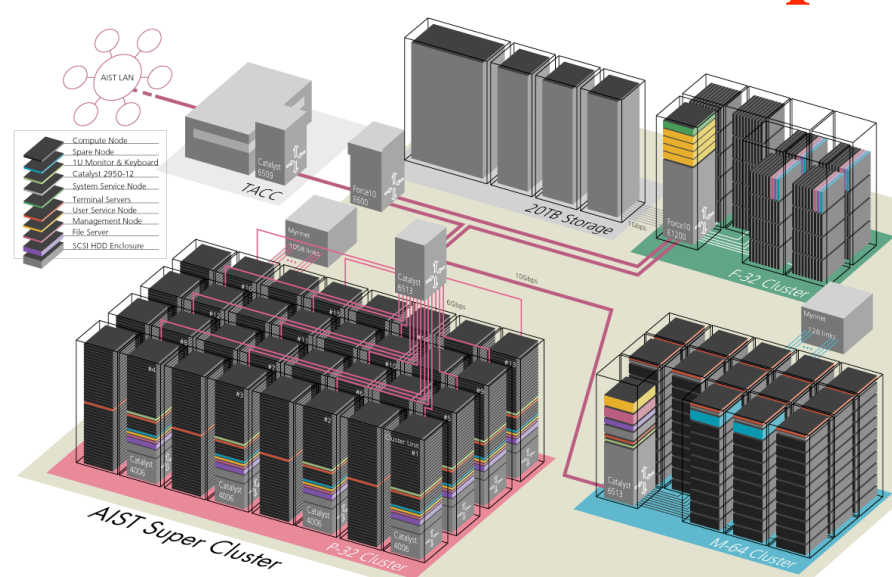

(11$\bar{1}$)

h=5.83Å

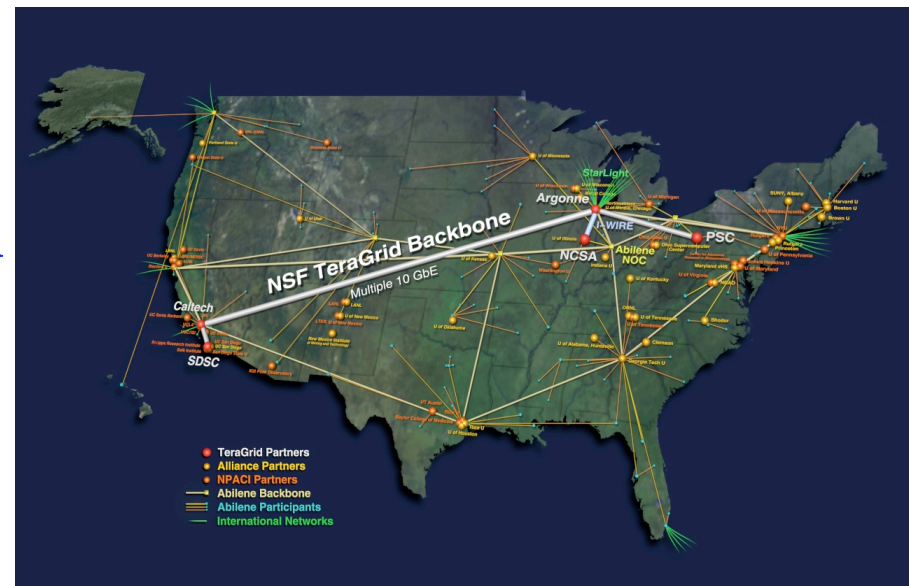- **After the load drop:** h = 5.83Å: (11$\bar{1}$)

Large-scale Simulations Using GRID

Massively parallel machines in Japan
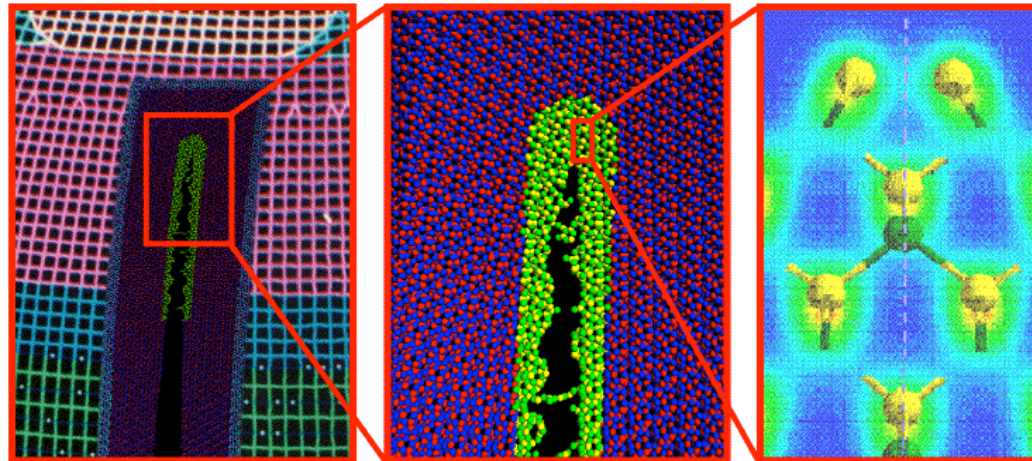
2000 AMD Opteron Supercluster

Grid of globally distributed supercomputers

Quantum-to-Atomistic-to-Continuum Simulations
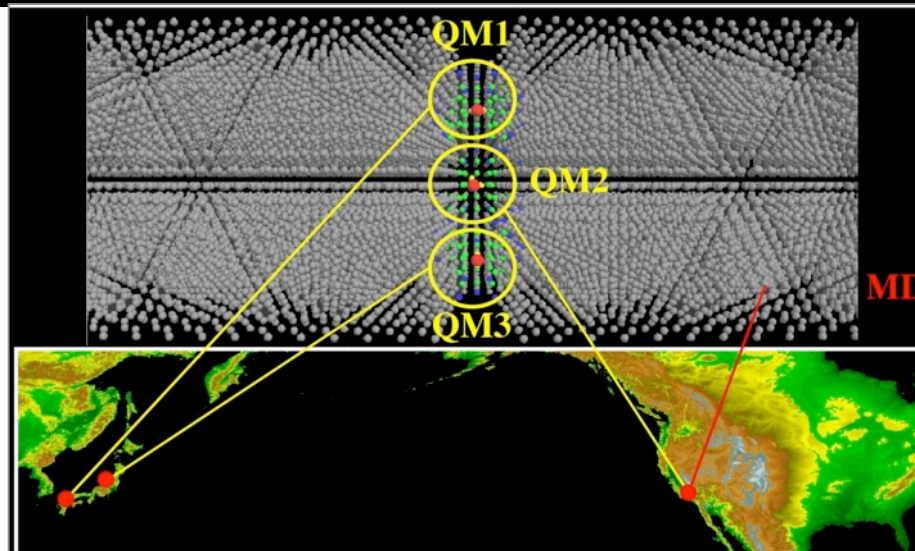# Global Collaborative Simulations on GRID

Finite Element
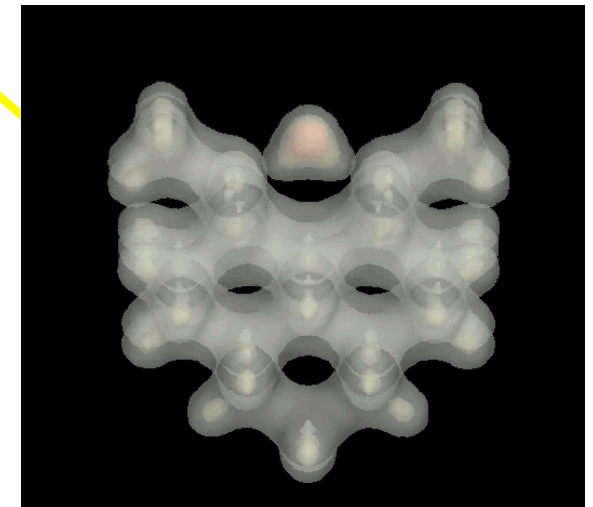
Molecular Dynamics

Density Functional

QM1
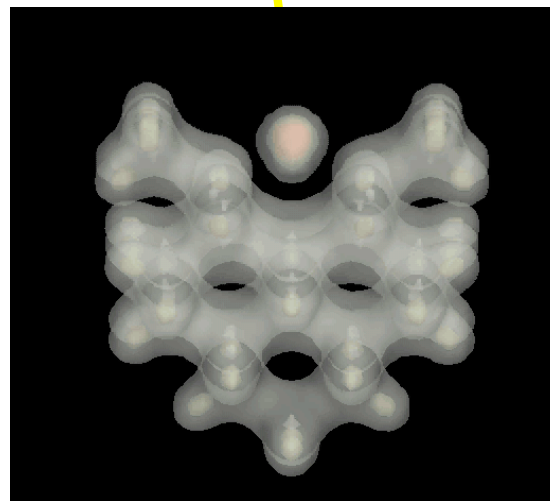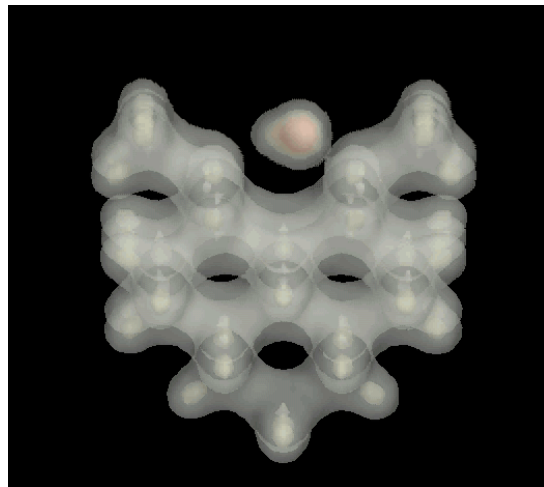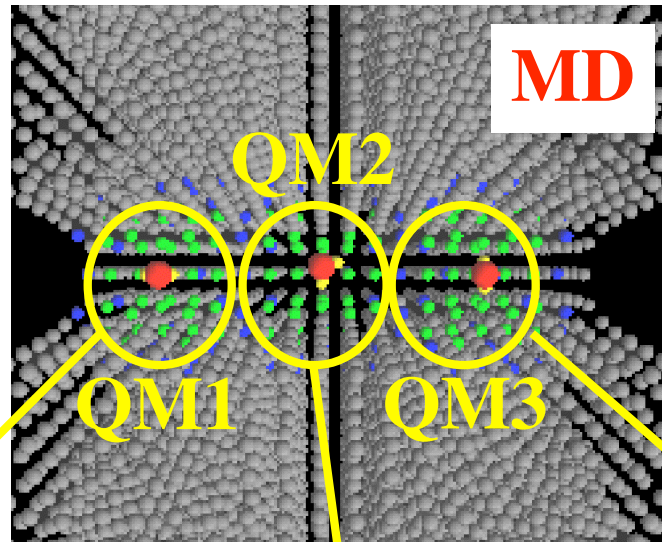
QM2

QM3

MD

GRID Computing between USA and Japan
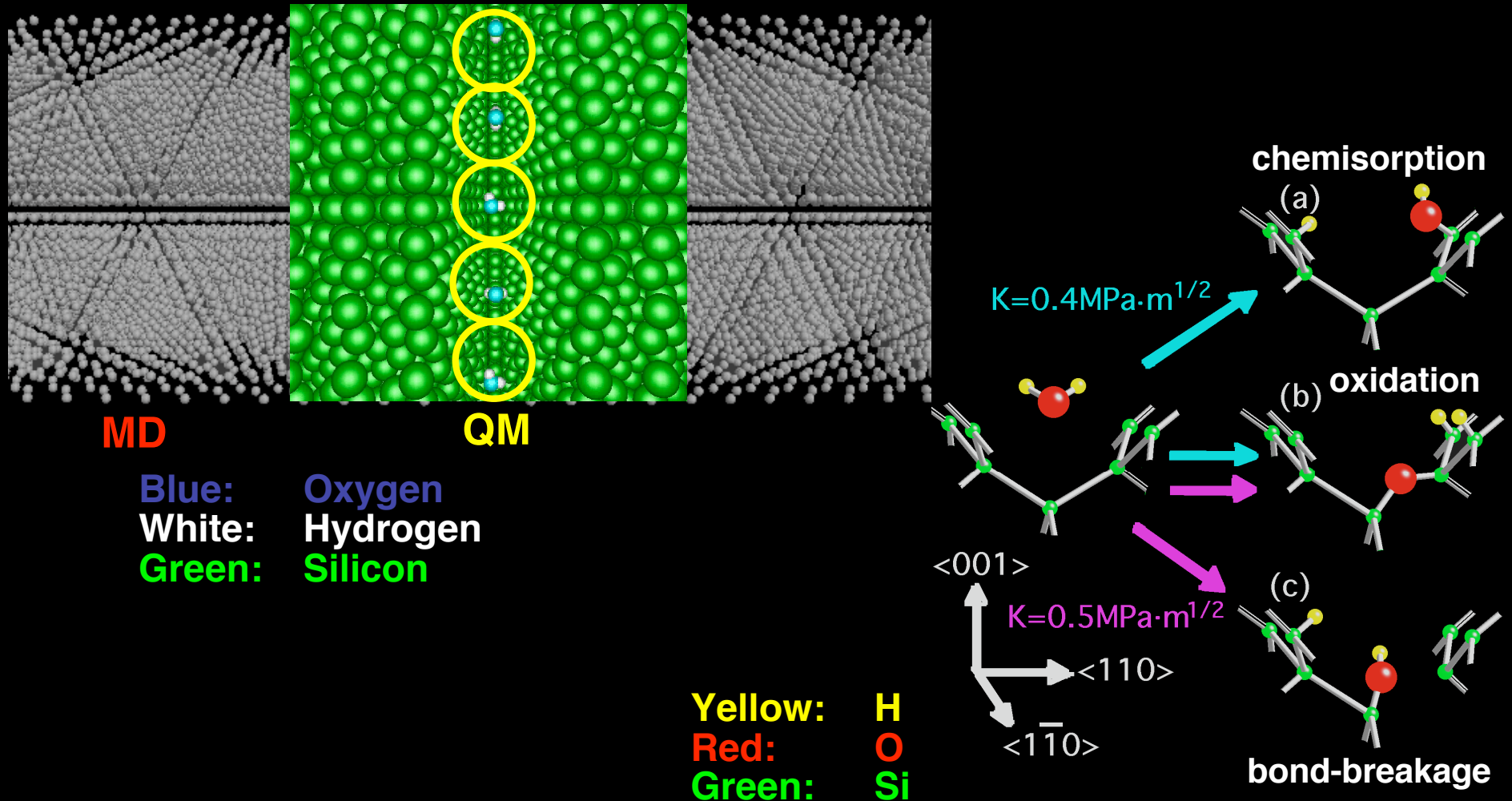
Grid Enabling: Multiple QM Partitioning

Environmentally assisted fracture:
Reaction of water molecules at the crack tip in silicon

Divide-&-conquer

US-Japan collaboration on environmentally-assisted fracture

Reaction of H_2O molecules at a Si crack tip

MD **QM**

Blue: Oxygen
White: Hydrogen
Green: Silicon

Yellow: H
Red: O
Green: Si

chemisorption
(a)

$K=0.4MPa \cdot m^{1/2}$

(b) oxidation

(c)

$K=0.5MPa \cdot m^{1/2}$

bond-breakage
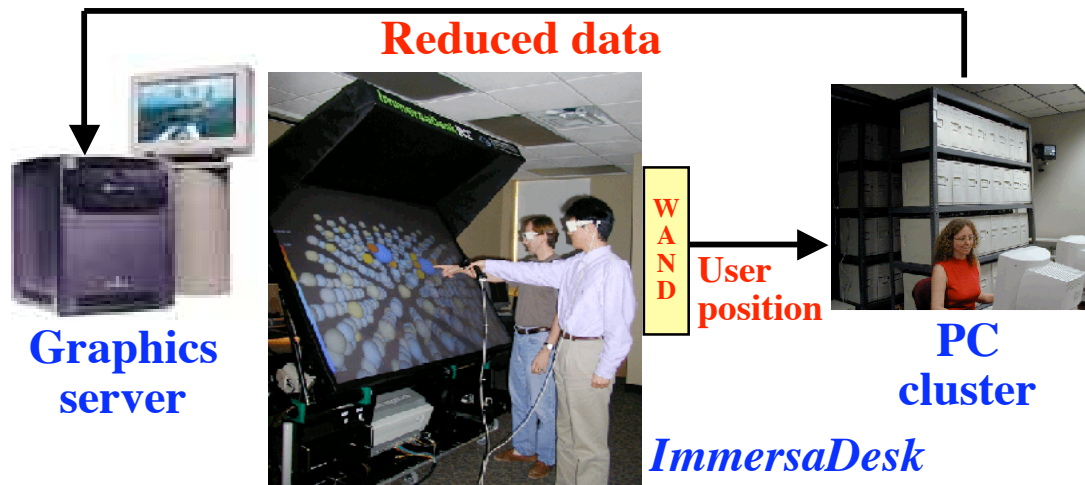
<001>
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Significant dependence of the reaction on stress intensity factor
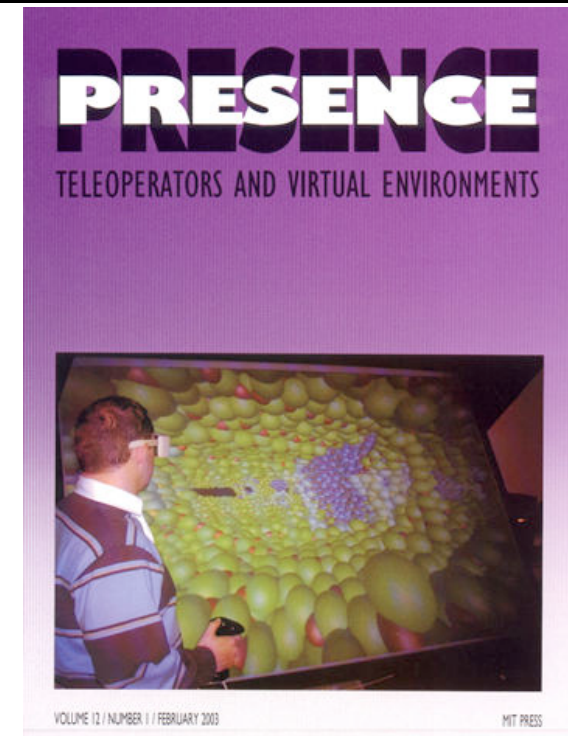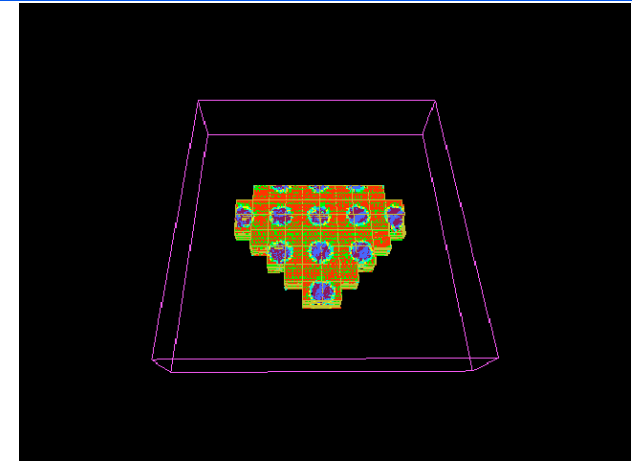
Summary_Research

- **Confined silica glass subjected to dynamic compressive loading**
    - > **Kinks at the crack tip coalesce with nanocavities to form a wing crack**
    - > **Wing-crack segments can propagate at supersonic speeds, but the crack heals due to confinement**

- **Nanoindentation in silicon carbide**
    - > **Nucleation of dislocations in crystalline SiC**
    - > **Dislocation loops cause amorphization under the indenter**

- **Collaborative GRID Computing**
    - > **USA and three universities (Niigata, Hiroshima, Yamaguchi) in Japan**
    - > **Environmental assisted fracture in silicon**

Immersive & Interactive Visualization
Billion Atom Walkthrough

- **Octree-based fast view-frustum culling**
- **Probabilistic occlusion culling**
- **Parallel/distributed processing**

Reduced data

Graphics server

W A N D

User position

PC cluster

ImmersaDesk

- **Interactive visualization of a billion-atom dataset in immersive environment**

PRESENCE

TELEOPERATORS AND VIRTUAL ENVIRONMENTS

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Education & Outreach

Education & Outreach: Computational Science Workshop for Underrepresented Groups (CSWUG)

January, 2003 at LSU

2nd Computational Science Workshop for Underrepresented Groups

Report Prepared by Student Participants and Faculty Mentors

"…I want to be able to help inspire others just as all of you in the workshop helped to inspire me…"
Tanjala Purnell, Tougaloo College

January, 2004 at USC

Computational Science Workshop for Underrepresented Groups

University of Southern California

January 5-10, 2004

Success Story of Tangela Purnell, Tougaloo College, Mississippi

"I am one of the students who recently attended your workshop, and I was just writing to sincerely thank you for selecting me to be a part of such an astounding experience. I cannot believe how much I learned in one week, and it was so much fun. I am so glad that I attended the workshop because being in undergraduate school, I do not usually get a chance to do much hands-on work, but I mainly have to do a lot of difficult programming. At one time I was so frustrated with only having to program and not getting any hands-on experience that I almost considered changing my major. However, during the workshop I was so mesmerized by all of the hands-on experience, especially when we built the parallel computer. Your workshop helped me to remember why I wanted to be a computer science major in the first place. I feel so inspired now to go on and get my PhD in computer science. I hope that you will continue the workshop for many years so that other students will be so richly enhanced, just as the workshop enhanced me. I hope that when I obtain my PhD I will be able to return to the workshop no longer as a student but as a mentor for other students. I want to be able to help inspire others just as all of you in the workshop helped to inspire me."

Tanjala Purnell a participant at our
Computational Science Workshop for
Underrepresented Groups, January 5-11, '03.

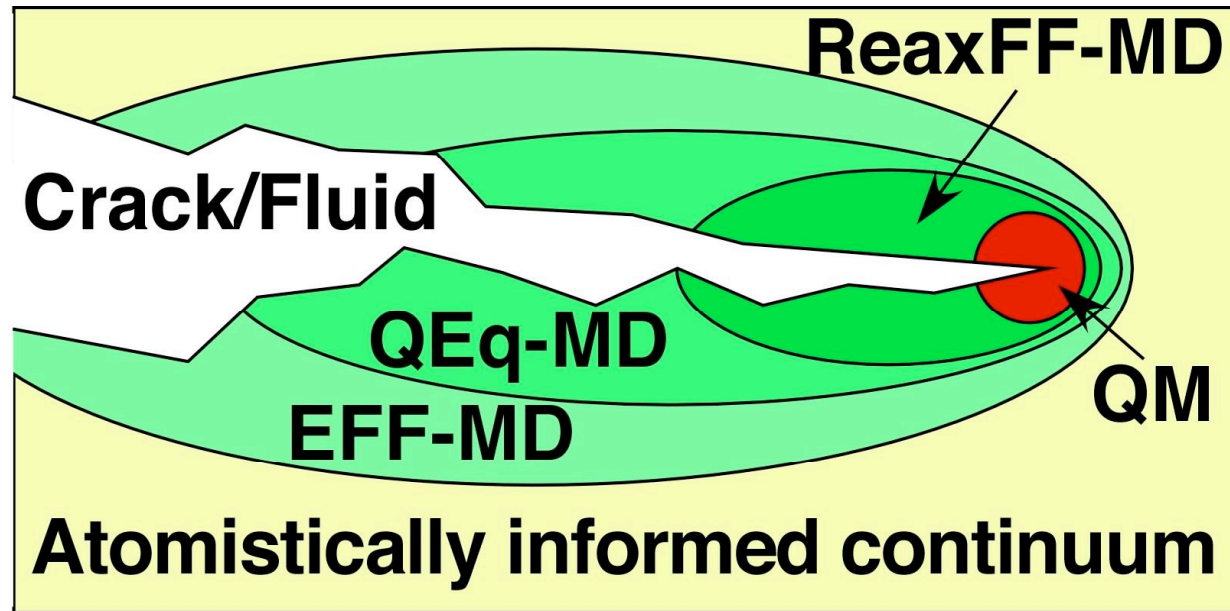Summer 2003: Internship at the University of Michigan
Summer 2004: Internship offers from Michigan, Wisconsin, Chicago, Harvard and NIH

Research
and
Education & Outreach

In Progress

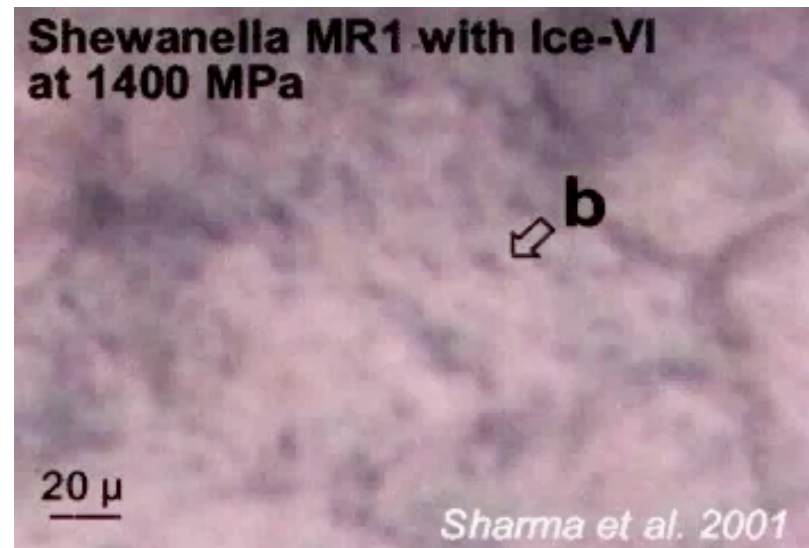# Shock-induced structural phase transformation, damage & fracture in AlN

Pressure (GPa)
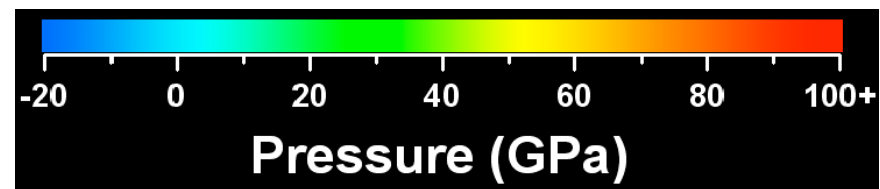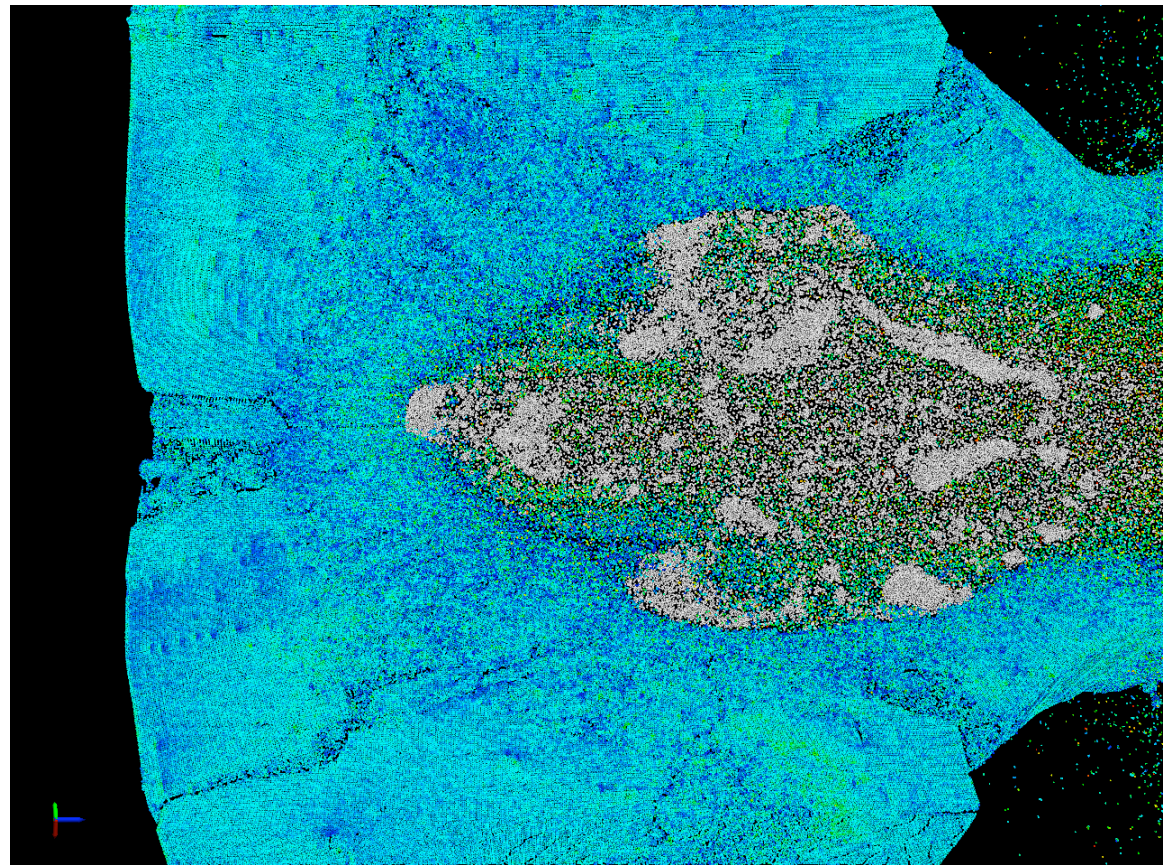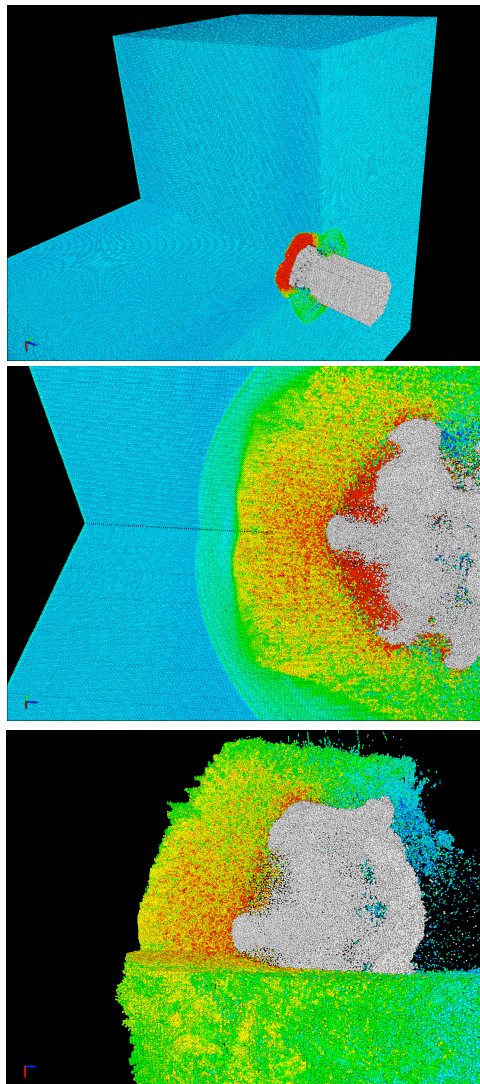
Stress Corrosion Cracking (SCC)

SCC Inhibitors

- **Ceramic coatings**
- **Self-assembled monolayers**
- **Microorganisms**

Education & Outreach: Computational Science Workshop for Underrepresented Groups
January 5-11, 2004 at USC

Education & Outreach: Computational Science Workshop for Underrepresented Groups

- **Follow-on activities with participants will include**

    > Bringing students back for summer research and to participate in a computational science conference

    > Inviting some students and faculty mentors to help organize and run the next workshop, which will be held at USC during January, 2005

    > Remote research experiences for students facilitated by the loan of the PC nodes they built at the workshop

Thank you for your attention!