ITR: Billion-atom Multiscale Simulations on a Grid

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September 1, 2002: Collaboratory for Multiscale Simulations
Departments of Materials Science & Engineering, Physics,
Computer Science, and Biomedical Engineering
University of Southern California

NSF Division of Materials Research
Computational Materials Theory Program Review
Program Managers: Dr. Bruce Taggart & Dr. Daryl Hess
Organizers: Dr. Duane Johnson & Dr. Jeongnim Kim
June 20, 2002, Urbana, IL
Outline

1. Multiscale simulation of lattice-mismatched nanopixels & nanomesas
2. Multimillion-atom molecular dynamics simulation of semiconductor nanoparticles
3. GRID computing with latency tolerant algorithms
Faculty:
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Visitors:
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Systems Manager: Monika Lee
Coordinator: Jade Ethridge
1,024 CPU System being installed at LSU under the auspices of Louisiana IT initiative.
Hybrid FE/MD Algorithm

- FE nodes & MD atoms coincide in the handshake region
- Additive hybridization
Si(111)/Si$_3$N$_4$(0001) Nanopixel

Displacement from equilibrium positions

- Full MD
- Hybrid FE/MD

[Graph showing displacement from equilibrium positions with color coding and interface markings]
Stress Domains in $\text{Si}_3\text{N}_4$/Si Nanopixels

Stress well in Si with a crystalline $\text{Si}_3\text{N}_4$ film due to lattice mismatch

Stress domains in Si due to an amorphous $\text{Si}_3\text{N}_4$ film
Epitaxially Grown Quantum Dots

Substrate-encoded size-reducing epitaxy

GaAs (001) substrate; <100> square mesas

A. Madhukar (USC)
Lattice-mismatched Growth of Epitaxial Quantum Dots on Patterned Substrates

InAs island formation on a flat GaAs(001) substrate >1.6 monolayer deposition

$\theta_{cr} = 1.6$ ML

Strain relaxation suppresses 2D→3D transformation on a patterned substrate <100nm

$\theta_{cr} = 12$ ML

GaAs/InAs: 7.2% lattice mismatch

A. Madhukar (USC)

InAs delivery: 24ML, Base: 75nm Height: 11±1 ML

Self-limiting growth of 12 ML InAs on a patterned substrate
Validation of Interatomic Potentials—GaAs

X-ray static structure factor

Phonon dispersion

Experiment (Strauch & Dorner, '90)

Theory

Amorphous GaAs

High-pressure phase transition

Experiment [Besson et al., '91]
Atomistic Stress in InAs/GaAs Square Mesa

- In-plane lattice constant in InAs overlayers exceeds the bulk value at 12 ML → self-limiting thickness
- Domain formation in larger mesas → critical lateral size for 3D island formation

Vertical displacement in the first As layer above the interface
Colloidal Quantum Dots, Rods & Tetrapods

Applications
• LED, display
• Biological labeling
• Pressure synthesis of novel materials

Collaborator: Paul Alivisatos (Chemistry, Berkeley)

High-pressure structural transformation in a GaAs nanocrystal

Nucleation at surface  Multiple domains

[from Bawendi’s group at MIT]
Multiple Domains in a GaAs Nanocrystal

Nucleation & growth of high-pressure-phase domains
Domain Fluctuations

Third domain’s growth fluctuates with time
Shape Dependence of Transformation

Transformation is sensitive to the initial shape
One billion atom simulation for one micron (1000nm) nanopixel. The simulation will be split in two parts - top 200 million atoms on a 256 CPU system and the remaining 800 million on a 1,024 CPU system for GRID computing. In GRID computing, quality of service (QoS) and latency issues serious, but not killers.

Main objective is to confirm the nature of hexagonal pattern of stress domains at the interface.
GRID Computing for an Ensemble of 64 Nanoclusters

- Nanocrystals in Lennard-Jones liquid
- Isothermal-Isobaric simulations
- Nanocrystal: 20-60 Å
- Pressure: 2.5-25 Gpa
- 90% of the particles constitute pressure medium.
- 8 to 16 processors optimum for one nanocrystal.
- In GRID computing, QoS and latency issues not serious, synchronization needed at pressure change only.
Access Grid Technology for Education and Training of Underrepresented Groups
Undergraduate Education & Training

Computational Science Workshop for Underrepresented Groups

- 19 participants from 11 institutions — Hampton, Clark-Atlanta, Morehouse, Jackson State, Mississippi State, Texas Southern, Univ. of Texas — Pan American, Xavier, Grambling, Southern & Univ. of Louisiana in Monroe

- Activities: Construction of a PC cluster from off-the-shelf components & using this parallel machine for algorithmic and simulation exercises.
Summary

1. Multiscale simulation of lattice-mismatched nanopixels & nanomesas

2. Multimillion-atom molecular dynamics simulation of semiconductor nanoparticles

3. GRID computing with latency tolerant algorithms

4. Educational and training activities using access grid
Future: Biologically-inspired Nanostructures

Bio-inspired self-assembly of epitaxical & nanoparticle quantum dots

Protein-nanotube-based nanostructures

Collaborators:
A. Madhukar (USC)
Paul Alivisatos (Berkeley)

Collaborator:
Jonathan Trent (NASA)