Material Design: Perspective and Status of MGI

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Presentation Outline

- The Material Genome Initiative
- Brief History of Mix Design and Computer Development
- Methodology Overview
  - Multiscale Characterization Tools
  - Continuum Mechanics Methods-FEM/BEM
  - Discrete Mechanics Approaches
  - Molecular Dynamics and Quantum Mechanics
  - Multiscale and Bridging Scale Methods
- Digital Specimen and Digital Test
- Digital Mix Design
- Computer-Aided/Based Mix Design Perspectives

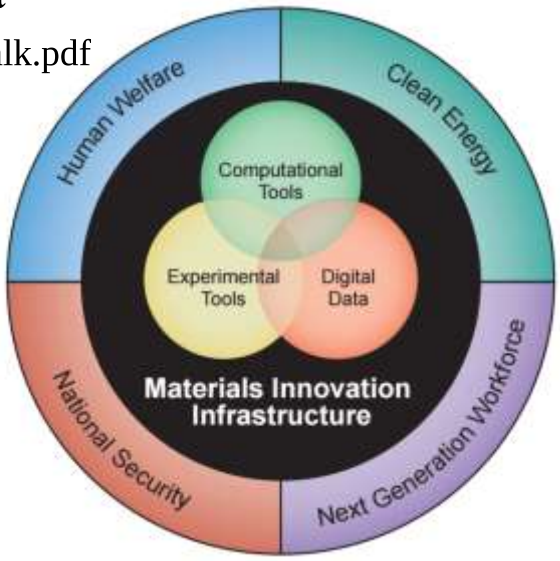
Material Genome Initiative

• "The **Materials Genome Initiative** is a multi-agency initiative designed to create a new era of policy, resources, and infrastructure that support U.S. institutions in the effort to discover, manufacture, and deploy advanced materials twice as fast, at a fraction of the cost."   2011.6.24

• "To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call the Materials Genome Initiative. The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place. We can do it faster.   --By President Obama"

https://www.whitehouse.gov/sites/default/files/docs/microsites/mgi/wadia_mgi_talk.pdf

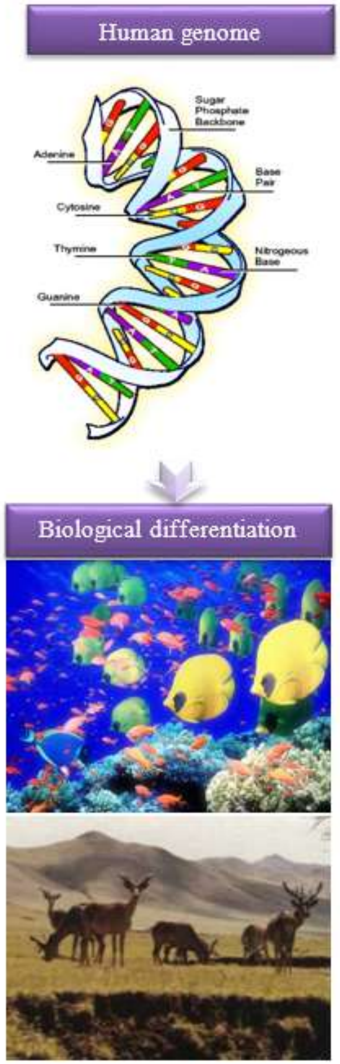
https://www.whitehouse.gov/mgi



Projects in the United States
- **NIST: CHiMaD**
- **DOE & NWU: OQMD**

Projects in China
- 材料科学系统工程发展战略研究
- 上海硅酸盐研究所:无机材料基因科学创新中心

Genome for Civil Infrastructure Materials



- **The "Genome" of Civil Materials**
  - **Mineral Compositions**
  - **Crystals Structures**
  - **Inherent Defects**
  - **Interfaces**

Significantly influence

  - **Physical Properties**
  - **Mechanical Properties**
  - **Chemical Properties**

•Linbing Wang (PI), Genome for Gravels and Sands Evolution, Chinese Natural Science Foundation REM 870,000 (2013-2016).

Methodology Overview
-What do we need? -Where are we?

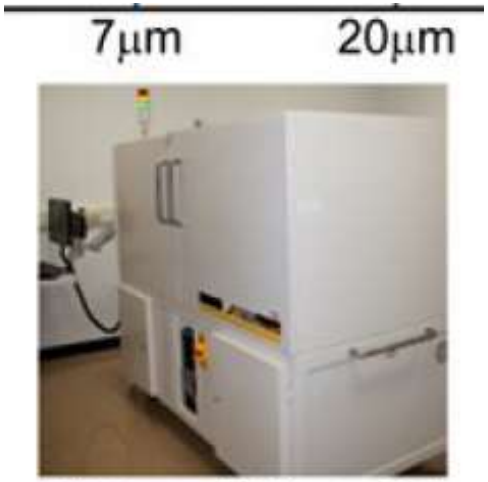
Composition, Structure, Defects and Interactions

Multiscale Characterization Tools

Microstructure Characterization Equipment

•Co-PI, Development of the Next-generation Nano-CT System for ROI-focused Scanning and Exact Interior Reconstruction, NSF, $1,360,206, 2009-2012.

• Co-PI, Acquisition of a 500nm Resolution Nano-CT Scanner, NIH, $500,000, 2009-2010.

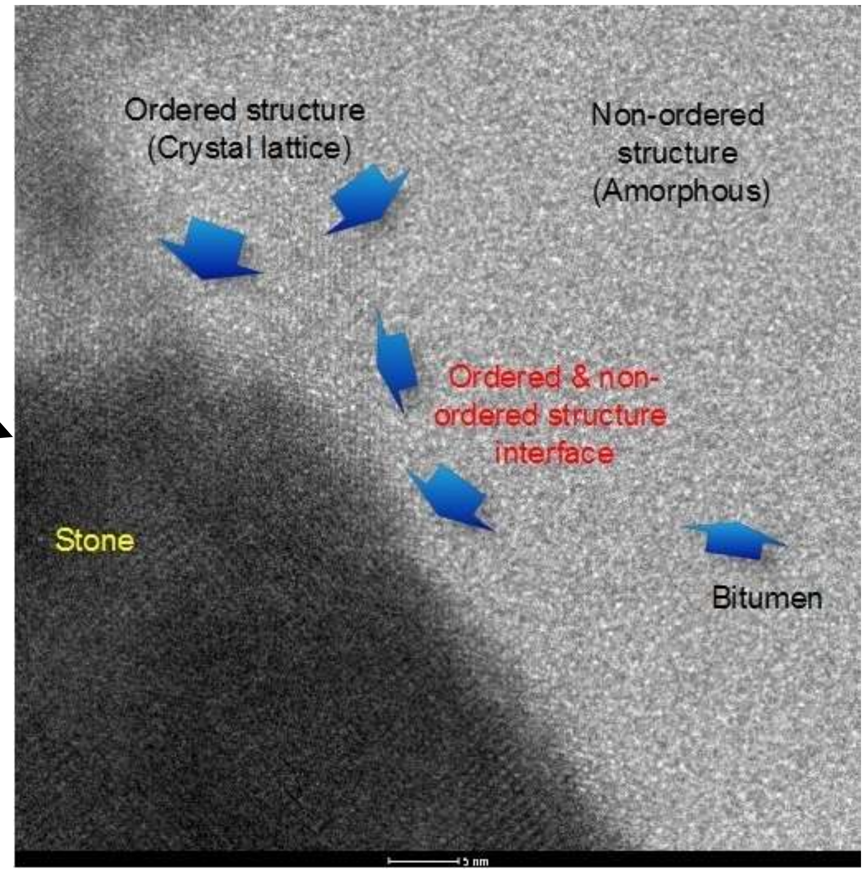


High-end Micro-CT

Nano-CT

Transmission Electron Microscope (TEM)

FEI Titan 300, in NCFL at Virginia Tech

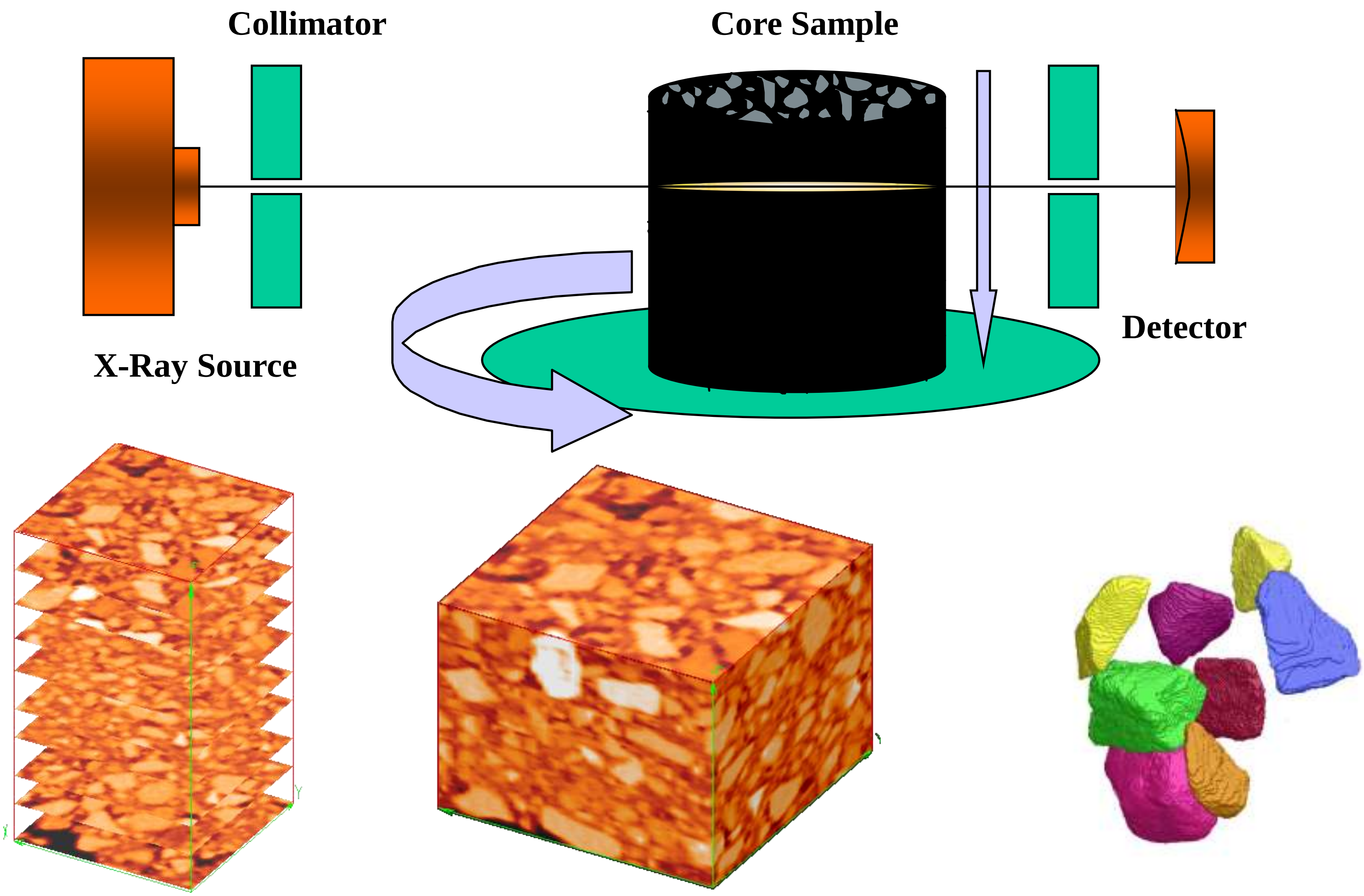


Atomistic structure at the interface by High Resolution TEM (nanoscale resolution), by TITAN at VT

Methodology Overview
-What do we need? -Where are we?

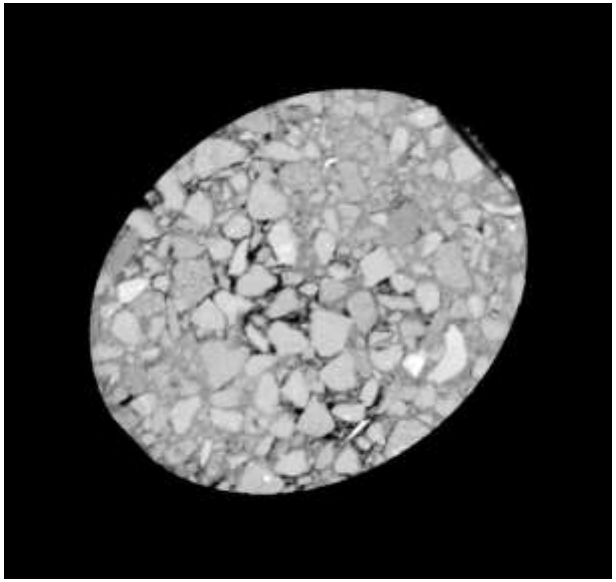
Continuum Approaches/FEM/BEM

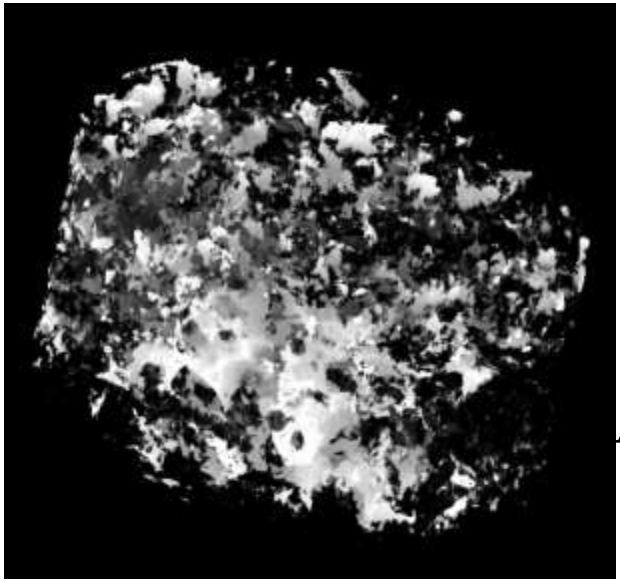
X-ray Computerized Tomography



Hounsfield and Cormack, Original Inventor, 1979 Nobel Prize Winner

Image Processing and Analysis-Quantitative Structural Parameters





Local Volume Fraction Determination

$$\mathrm{grad}\,\phi = \sqrt{\phi_1^2 + \phi_2^2 + \phi_3^2}$$

Tensor Analysis

$$f(n) = \frac{C}{4\pi}\left[1 + \phi_{ij} n_i n_j\right]$$

$$\bar{I}_1 = \left(\alpha_1 \delta_{\mathrm{ij}} + \alpha_2 R_{\mathrm{ij}}\right)\sigma_{\mathrm{ij}}$$

Specific Damaged Surface Area

$$\mathrm{S}(n) = \frac{\mathrm{S}_v}{4\pi}\left(1 + \mathrm{S}_{ij} n_i n_j\right)$$

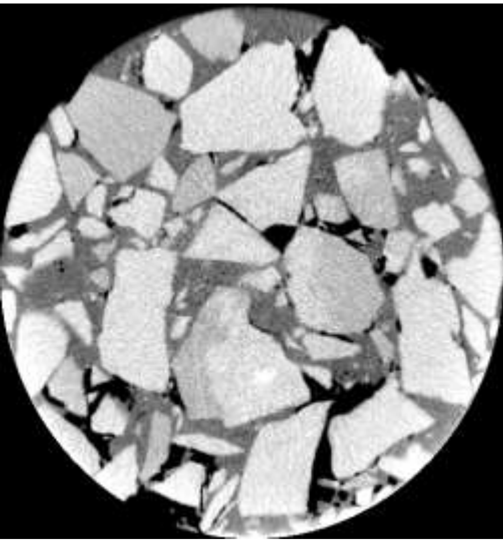
Mean Solid Path

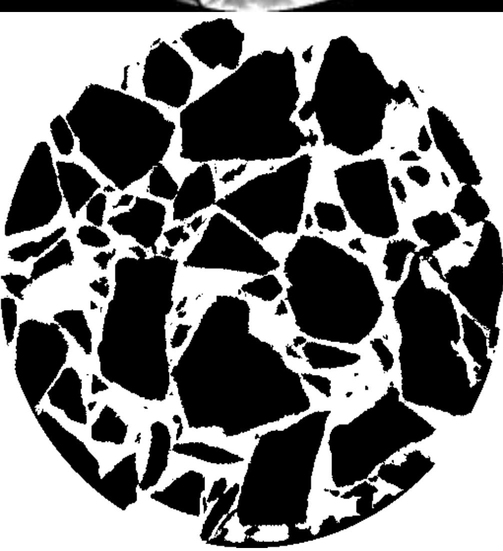
$$\lambda(\mathrm{n}) = \lambda\left(1 + \lambda_{ij} n_i n_j\right)$$

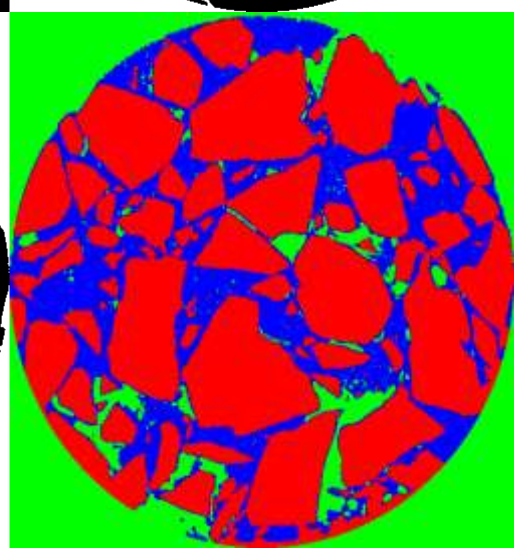
Average Size and Shape Tensor of the Defects

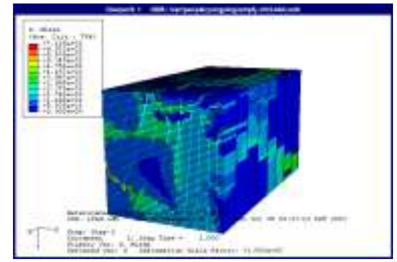
$$\delta(\mathrm{n}) = \delta\left(1 + \delta_{ij} n_i n_j\right)$$

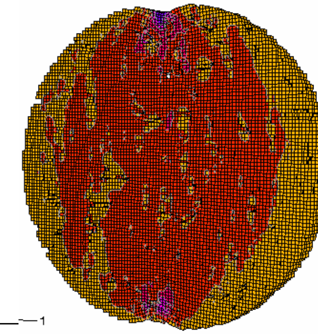
FEM Simulation, 3D 3 Constituents

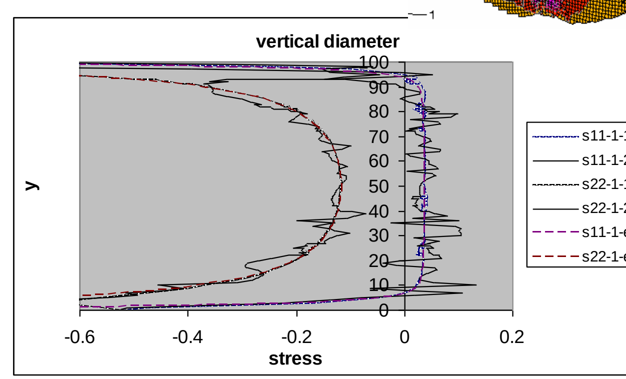


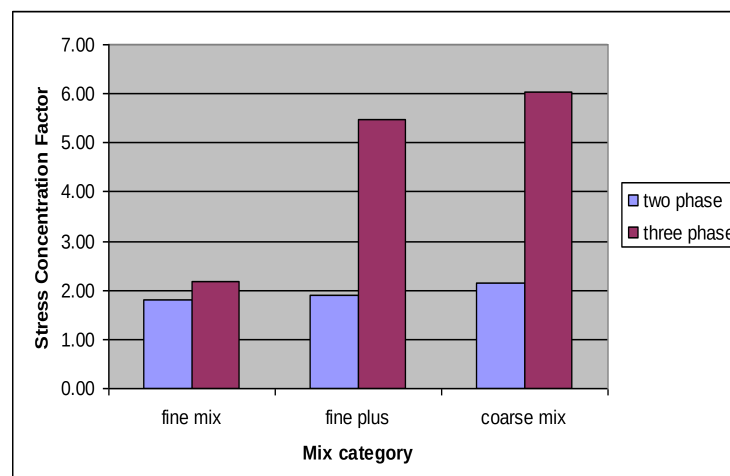












Effect of Interfacial Zone

Elastic case

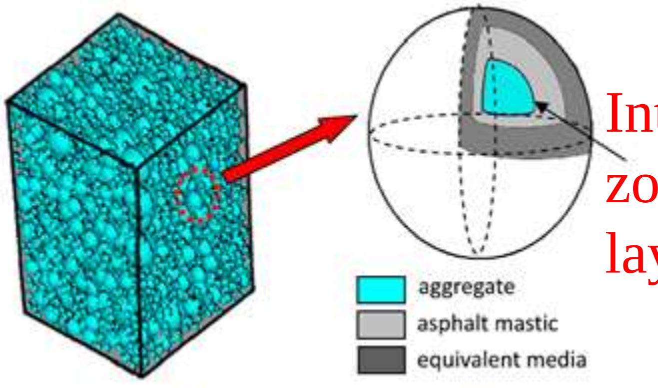
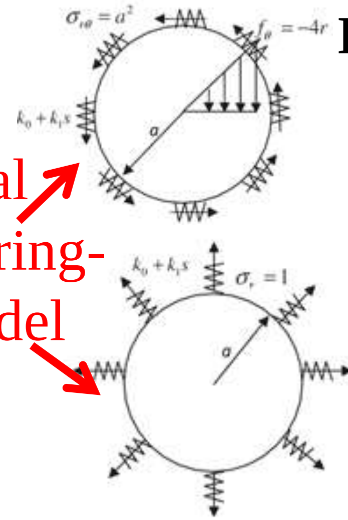
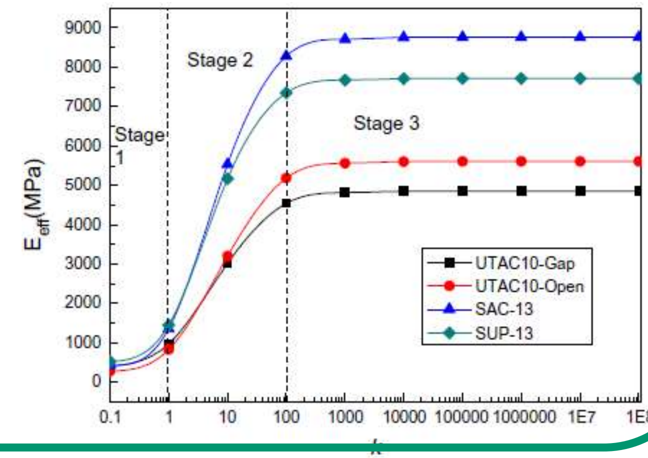


Fig. 1. 3D micromechanical model for AC with imperfect interface.

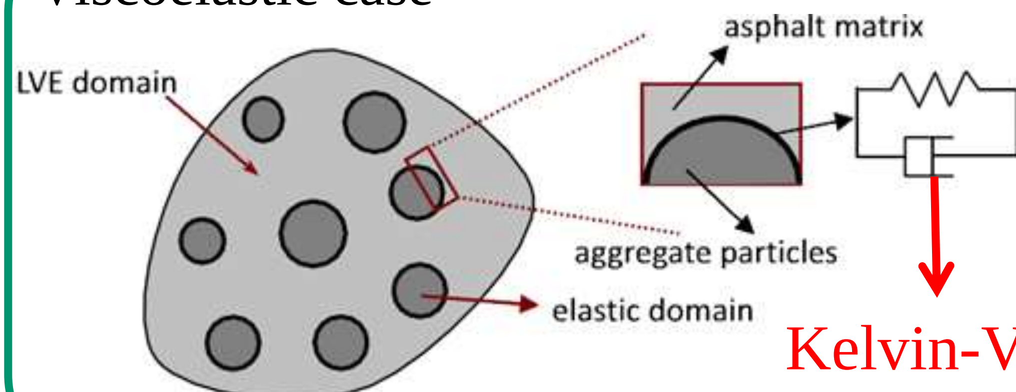
Interfacial zone: Spring-layer model



Effect of interfacial zone :3 stage

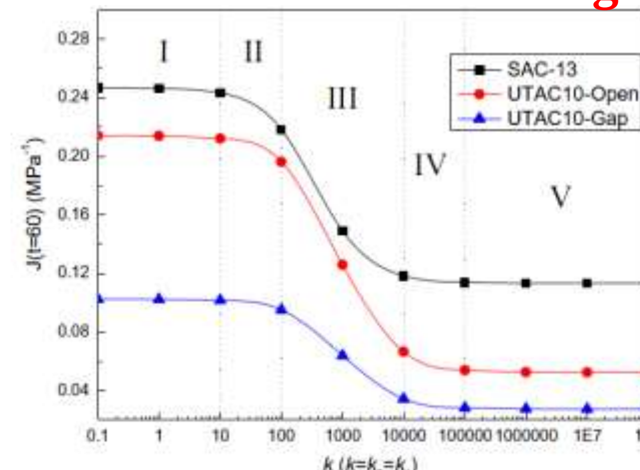


Viscoelastic case



Kelvin-Voigt Interfacial model

Effect of interfacial zone :5 stages



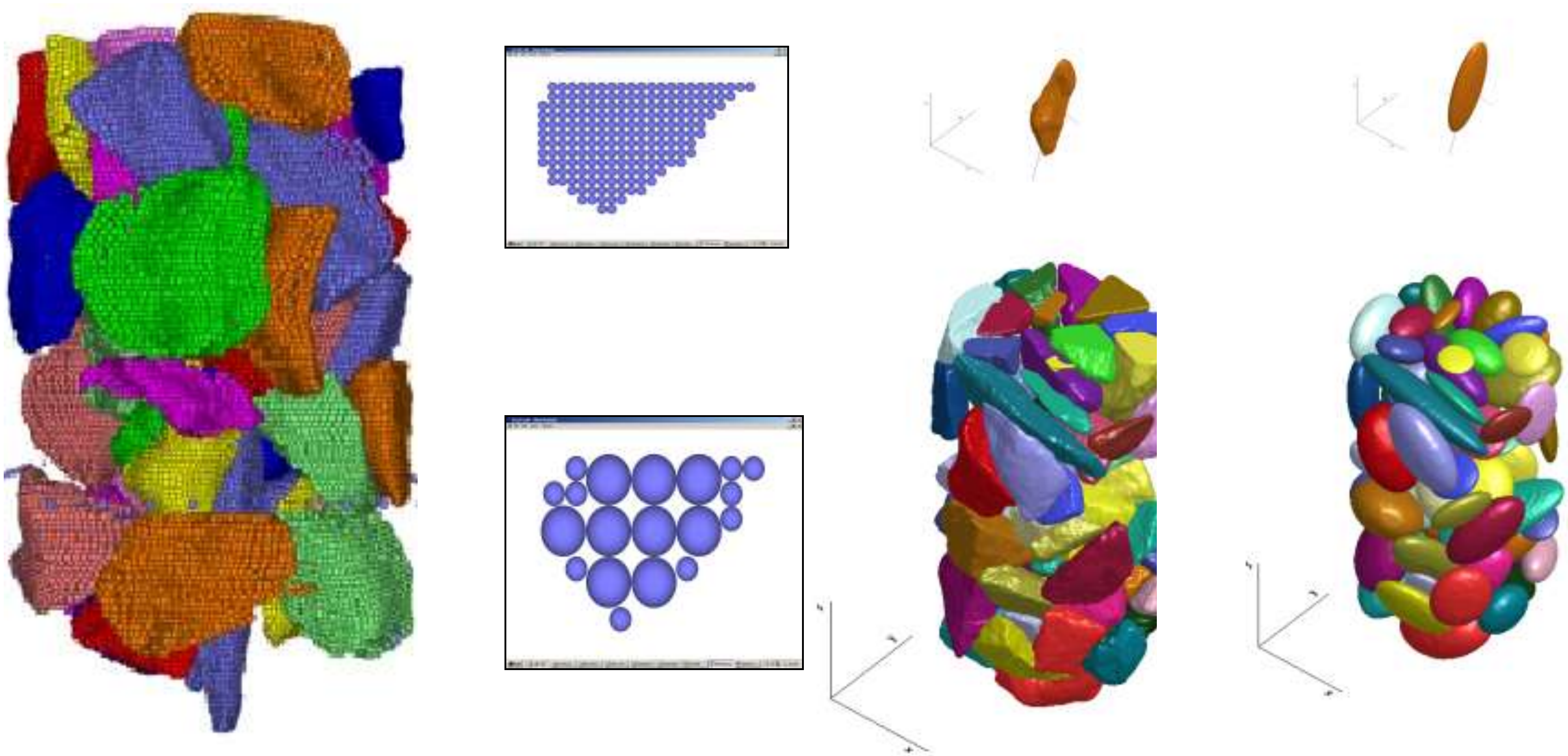
- **Xingyi Zhu. Construction and Building Materials, 49:797–806 (2013)**
- **Xingyi Zhu et al. Composites: Part B, 42:1404–1411(2011)**
- **Xingyi Zhu et al. Journal of Materials in Civil Engineering,25:328-336 (2013)**

Methodology Overview

-What do we need?-Where are we?

Discrete Element Method/ Molecular Dynamics/ Quantum Mechanics

DEM Simulation, Ellipsoid Approximation



Shape and Efficiency

DEM/MD Methods

Molecular Dynamics Simulation

Starting Point

Initial cordinates from lattice Monte Carlo simulation with initial velocities from Maxwell-Boltzman distribution

or

continue a previous MD

Calculate Forces

Calculate potential function:

$$V_{LJ}(r) = 4\varepsilon\left(\frac{\sigma^{12}}{r^{12}} - \frac{\sigma^{6}}{r^{6}}\right)$$

Calculate force on each particle:

$$F = \sum_j F_{ij}$$

Solve Equations

Integrate Newton's equations of motion for each particle:

$$\frac{dr_i}{dt^2} = \frac{F_i}{m_i}$$

Move Particles

Assign the new coordinates and velocities to each particle through Leapfrog Algorithm:

$$v_i\left(t + \frac{\Delta t}{2}\right) = v_i\left(t - \frac{\Delta t}{2}\right) + \frac{\Delta t}{m} F_i(t)$$

$$r_i(t + \Delta t) = r_i(t) + \Delta t \cdot \left(t + \frac{\Delta t}{2}\right)$$

Output

Calculate thermodynamic and static system properties:

Energies, temperatures, stress…

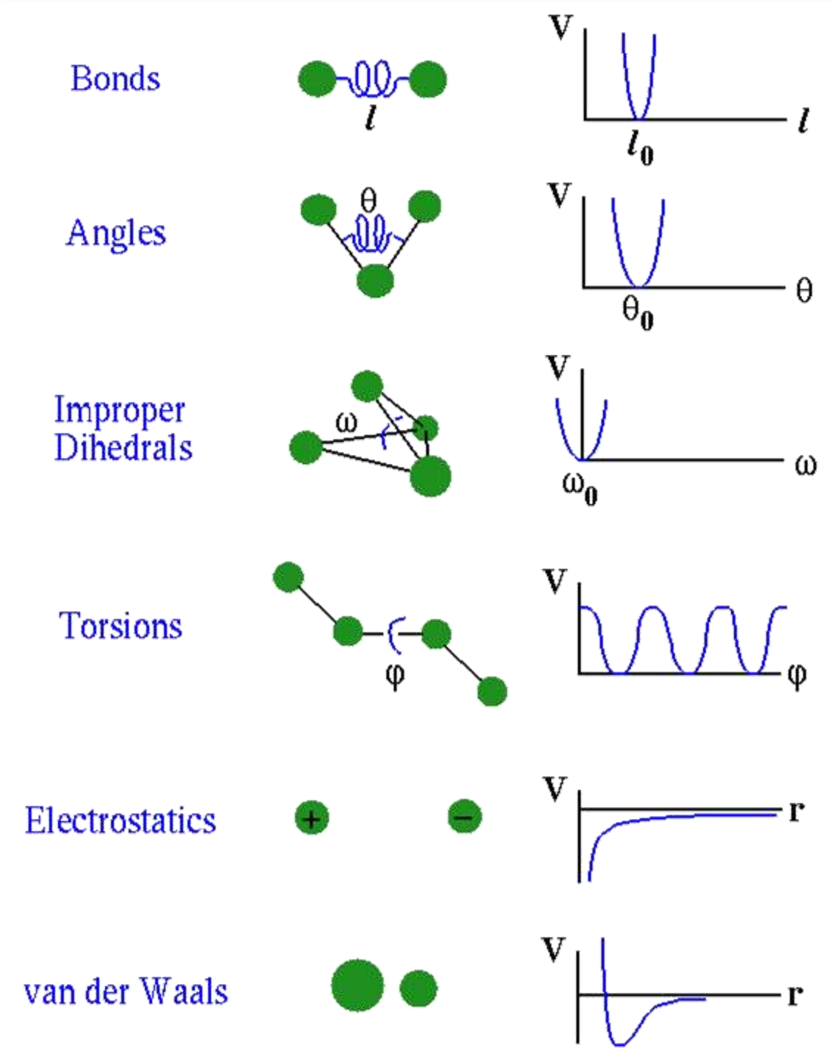
If required:

Save coordinates &velocities

save in: <trajectory file>

MD loop repeated every time step

Empirical Potential Energy Function
Equivalency-Contact Models



$$V_{bond} = \frac{1}{2} k_l (l - l_0)^2$$

$$V_{angle} = \frac{1}{2} k_\theta (\theta - \theta_0)^2$$

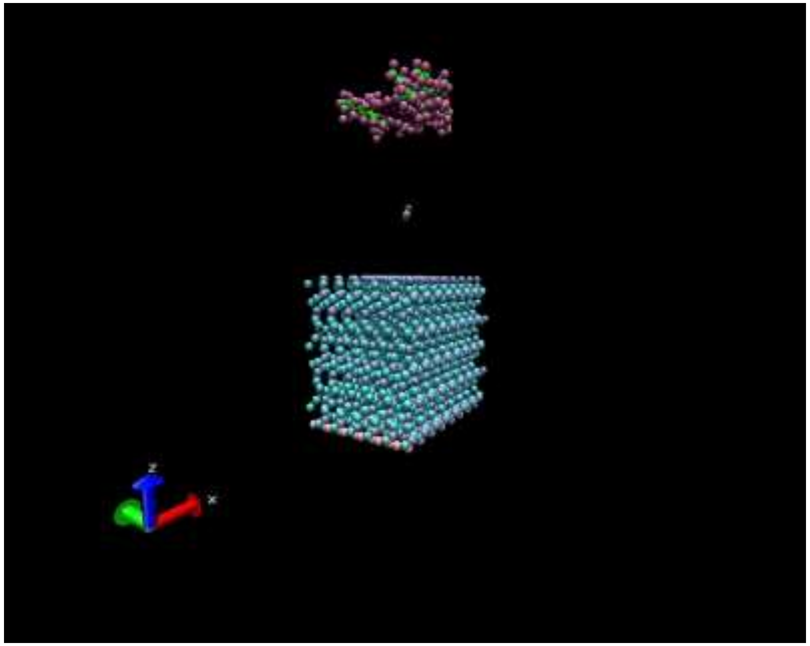
$$V_{improper} = k_\omega (1 - \cos 2\omega)$$

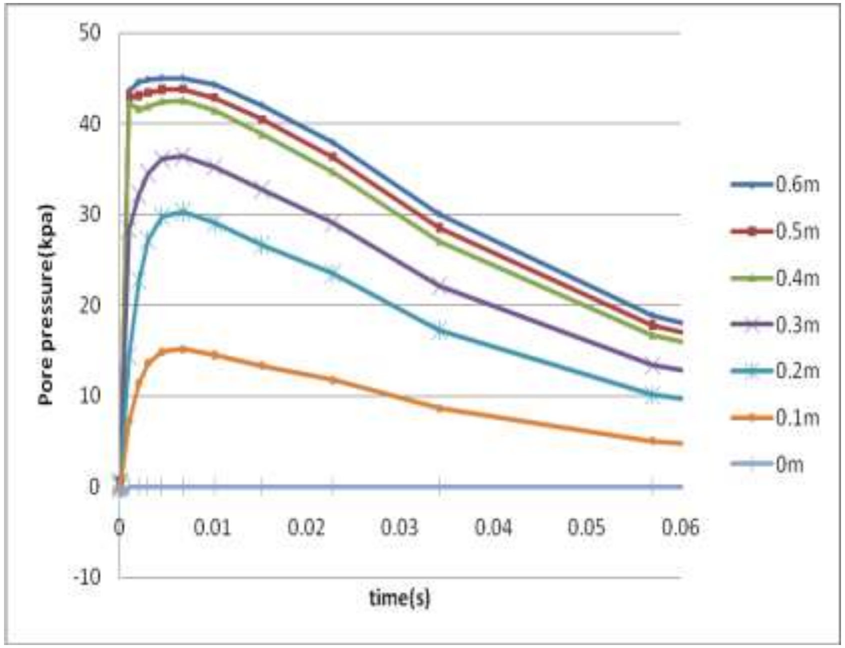
$$V_{torsion} = A_n \left[1 + \cos\left(n\varphi - \varphi_0 \right) \right]$$

$$V_{elec} = \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}$$

$$V_{vdW} = 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right]$$

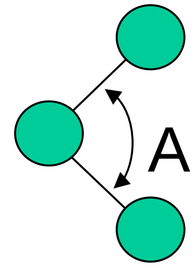
Interfacial Behavior with the Presence of Moisture in a Simple Atomistic Model





	Quartz elastic constants comparison		Calcite elastic constants comparison	
(Unit: GPa)	Calculated	Experimental	Calculated	Experimental
Bulk modulus	36.96	38 ~ 98	126.9725	129.6
Shear modulus	34.53	44	89.1558	35
Young's modulus	78.38, 80.10, 81.51	76~97	192.33, 72.78 , 41.99	72.35 ~ 88.19

ReaxFF: Advanced Features, Bill Goddard, Caltech



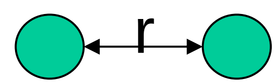
$E = k_A(A-A_0)$

Ordinary Force Fields

Fixed charges

Bonds cannot be broken, unsuitable for modeling reactions.

Examples: MM3, Dreiding, Amber, Charmm,



$E = k_r(r-r0)$

ReaxFF: first principles force field

Allow bonds to break and form, describe barriers for reactions.

All parameters from QM no empirical data !

ReaxFF: From oxidation to combustion to catalysis to shock induced chemistry but for systems with 1000s to millions of atoms

ReaxFF allows us to use to prepare the structures of complex heterogeneous systems by processes similar to experimental synthesis

Methodology Overview
-What do we need? -Where are we?

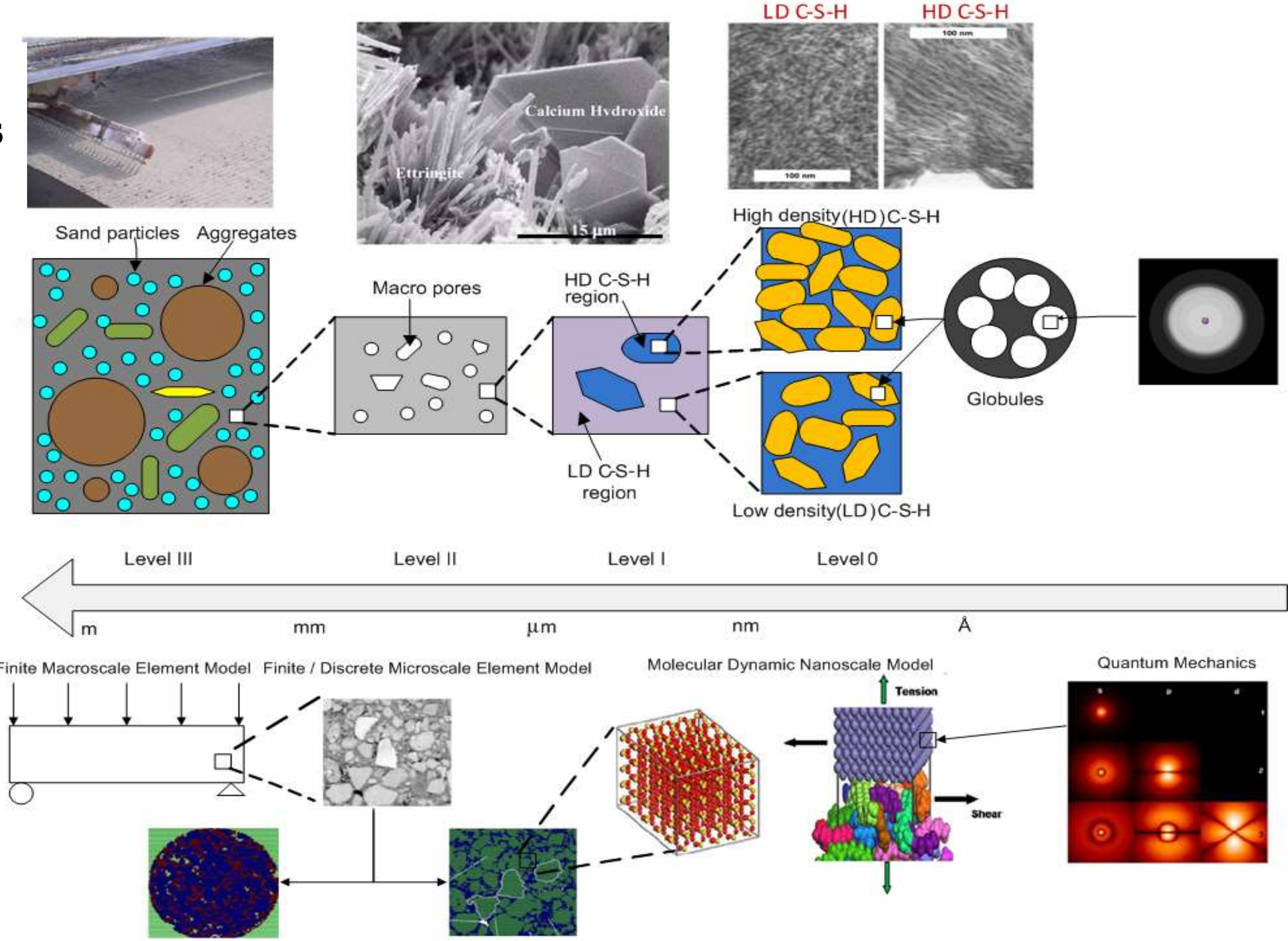
Multiscale Modeling and Bridging Scale Methods

Linbing Wang (PI), Nano Mechanics and Structure, FHWA, $1.0 Million, 2010-2015.

Multiscale and Multiphysics Modeling

Multiscale
Myltiphysics
Nature

Multiscale
Modeling
Methods



Jennings, H. M., J. W. Bullard, J. J. Thomas, J. E. Andrade, J. J. Chen, and G. W. Scherer. Characterization and modeling of ores and surfaces in cement paste: correlations to processing and properties. *Journal of Advanced Concrete Technology*, Vol. 6, 2008, pp. 5-29.

Taylor, H. F. Tobermorite/jennite- and tobermorite/calcium hydroxide-based models for the structure of C-S-H: applicability to hardened pastes of tricalcium silicate, β-dicalcium silicate, Portland cement, and blends of Portland cement with blast-furnace slag, metakaolin, or silica fume. Cement and Concrete Research, Vol. 34, 2004, 1733-1777.

http://limeworks.us/Infoall.html

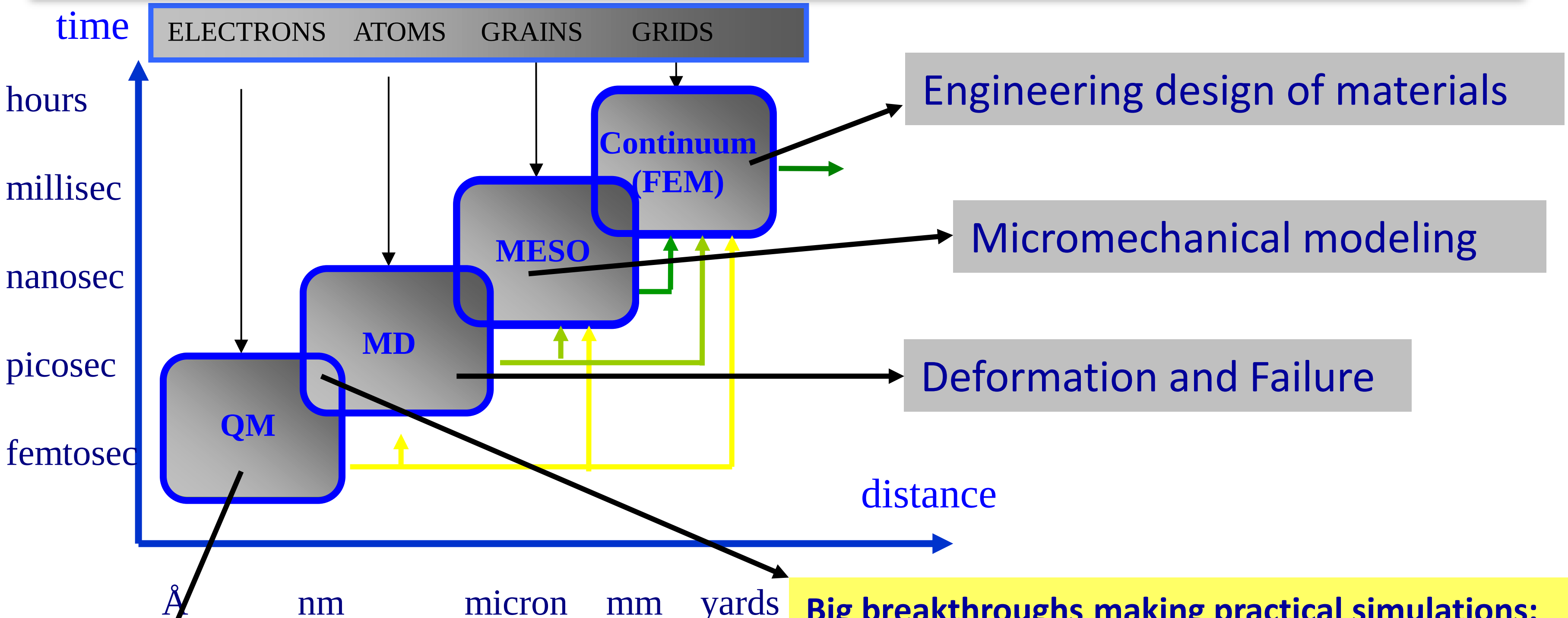
Challenge in Designing NEW Materials:

Connecting 1st Principles to Realistic Systems (Bill)

Need 1st Principles simulations of macroscale systems to predict NEW materials never before synthesized and optimize them prior to experiment

Strategy use an overlapping hierarchy of methods (paradigms) (fine scale to coarse)

Allows Design of new materials(predict hard to measure properties)



Accurate calculations for bulk phases and molecules (EOS, bond dissociation)
Chemical Reactions

Big breakthroughs making practical simulations:
ReaxFFreactive FF based on QM describe: chemistry, charge transfer, metals, oxides, organics.
eFF method large scale electron dynamics

Multiscale and Multiphysics Modeling

<table>
<tr><th colspan="9">Multiscale Modeling Method</th></tr>
<tr><th colspan="3">Hierarchy Multiscale Modeling Method</th><th colspan="6">Concurrent Multiscale Modeling Method</th></tr>
<tr><td rowspan="2">QC</td><td rowspan="2">CGMD</td><td rowspan="2">AFEM</td><td colspan="2">Handshaking</td><td rowspan="2">BSM</td><td rowspan="2">BDM</td><td rowspan="2">CADD</td><td rowspan="2">MD-DEM</td></tr>
<tr><td>FEAt</td><td>MAAD</td></tr>
</table>

Tadmor et al. Modeling materials: Continuum, Atomistic and Multiscale techniques. Cambridge University Press, 2012.
Tan et al. Advances in Mechanics 41(2), 2011, 123-139. (in Chinese)

QC = QuasiContinuum
CGMD = Coarse Grained Molecular Dynamics
AFEM = Atomic-scale Finite Element Method
FEAt = Finite Element combined with Atomistic Modeling
MAAD = Macroscopic, Atomistic, Ab initio Dynamics
BSM = Bridge Scale Method
BDM = Bridge Domain Method
CADD = Coupled Atomistic and Discrete Dislocation plasticity
MD-DEM = the combined Molecular Dynamics – Discrete Element Method

Essential Concepts :
Continuity and Weak Form
Equivalency such as Energy, Displacements, Velocity

One step closer to practical applications

Digital Specimen/Digital Test
Continuum versus Discrete

Development and Implementation of Digital Specimen and Digital Tester Technique for Infrastructure Materials

Funding Agency: Partnership for Innovation, National Science Foundation

General Concept

The digital representation of the real 3D microstructure of a physical specimen is a **Digital Specimen**. It is the digital counterpart of the physical specimen in every required detail. Computational simulation of a mechanical or physical test, which is based on digital specimens and considers every required detail of the microstructure and its evolution, is a **Digital Test**.

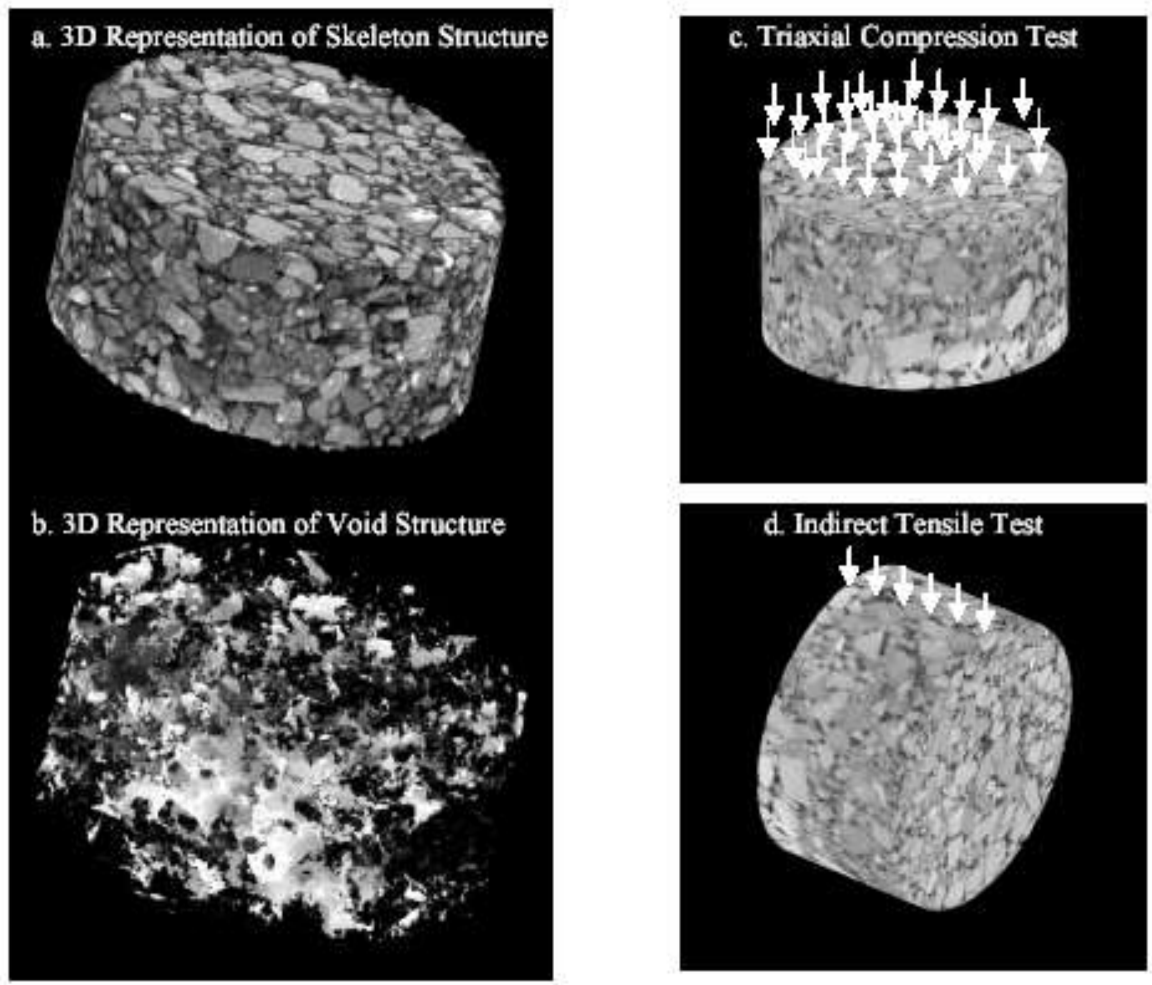
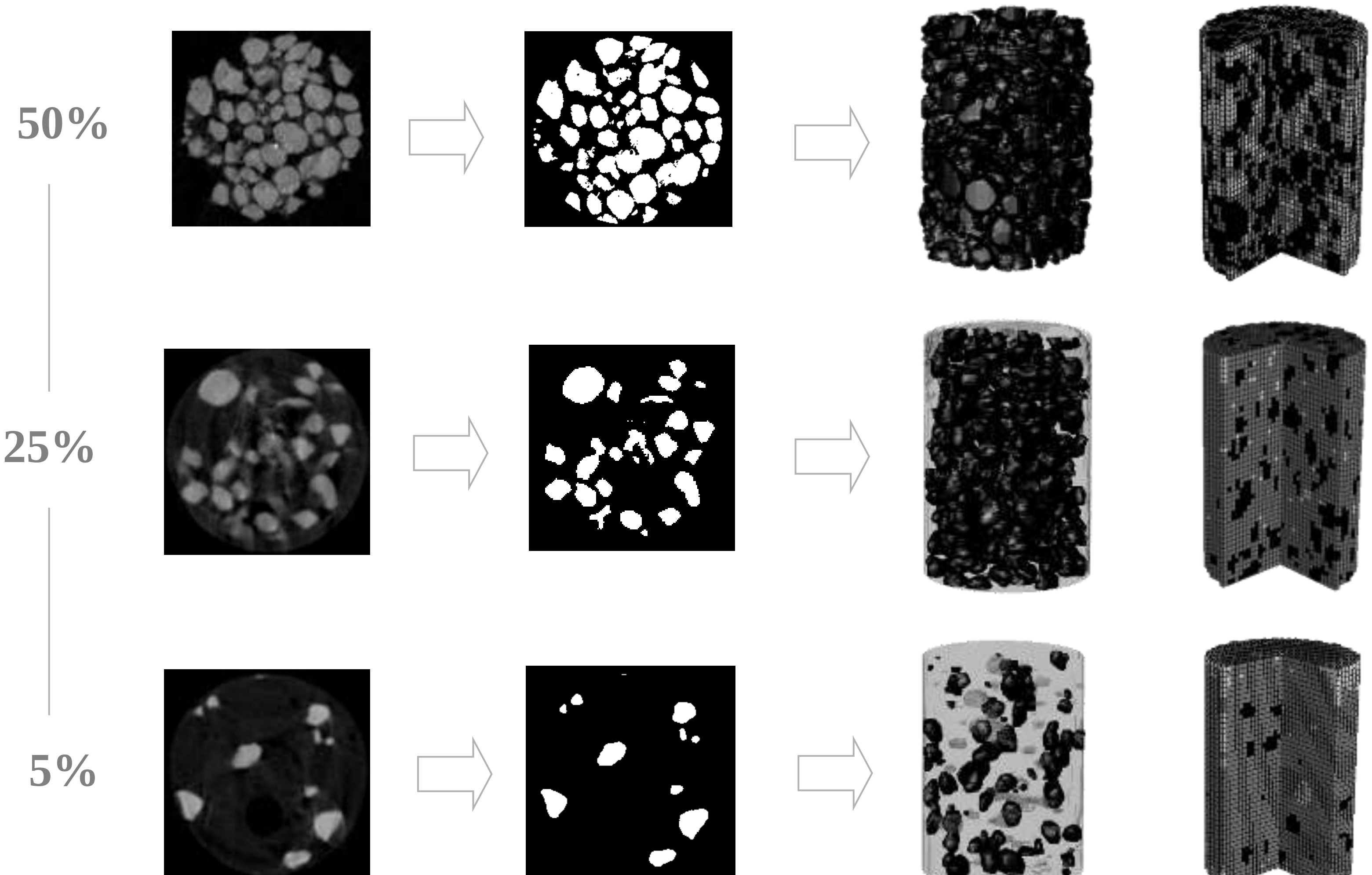


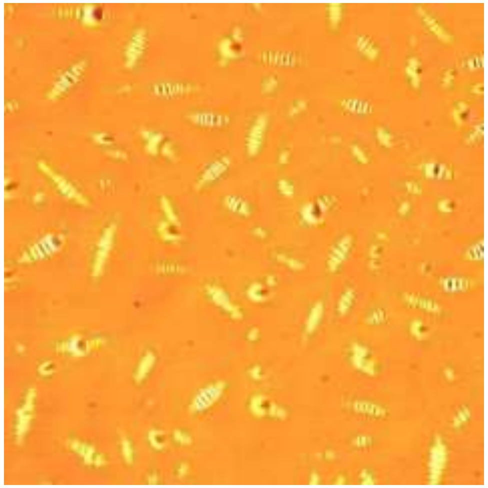
Illustration of the Concepts of Digital Specimen and Digital Test

Compression Test, Indirect Tensile Test, and APA Test

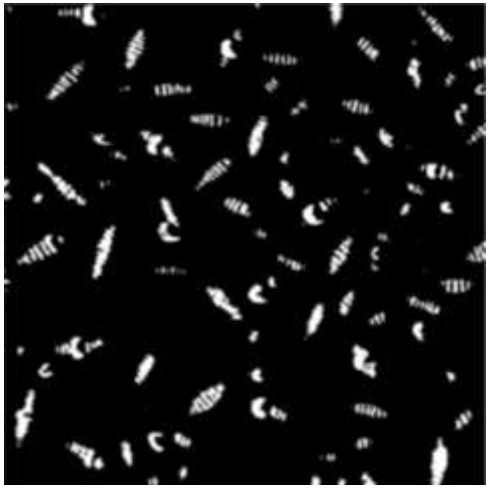


Binder Modeling, Direct Tension Simulation Sample Scanned by AFM (50 micron)

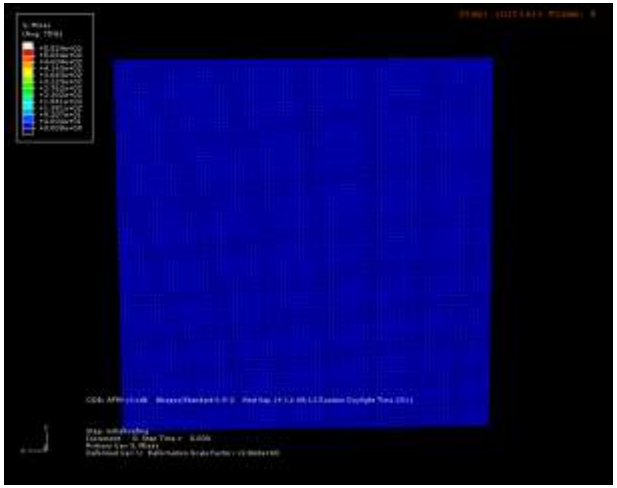
Original Image



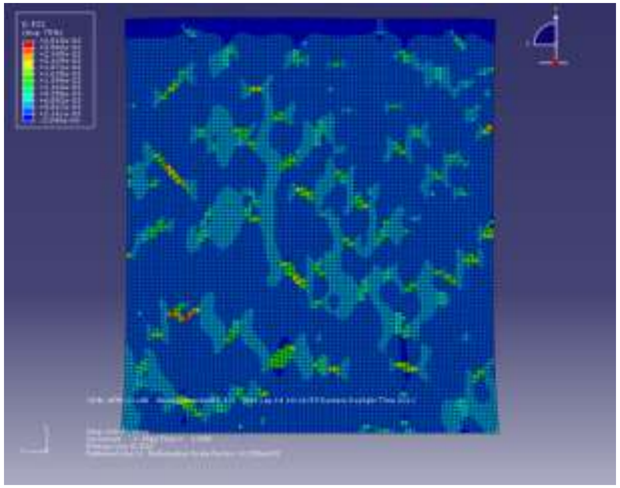
After Processing



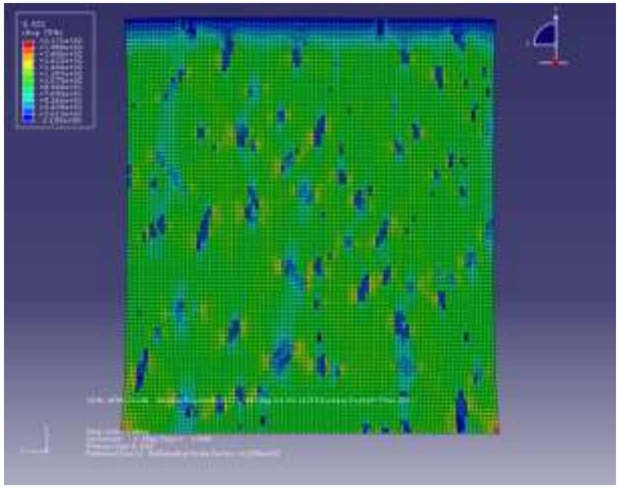
Direct Tension Simulation



Contour of Axial Strain

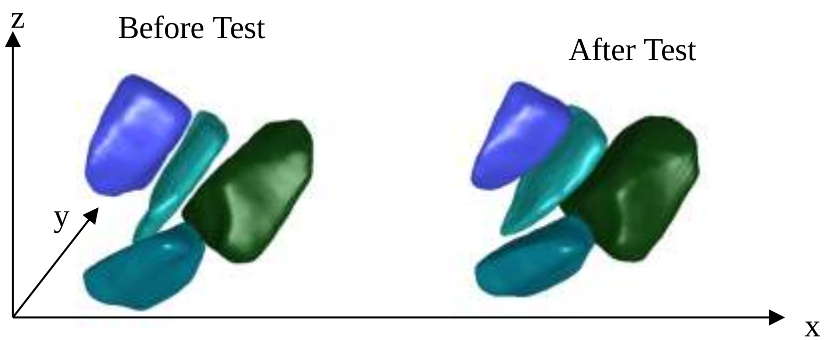


Contour of Axial Stress



Digital Specimen/Discrete View

Particle Reconstruction and Recognition



The Volume & Mass Center of Each Particle

Particle Recognition

Particle Displacements

Particle Rotations

Particle Translational Displacement:

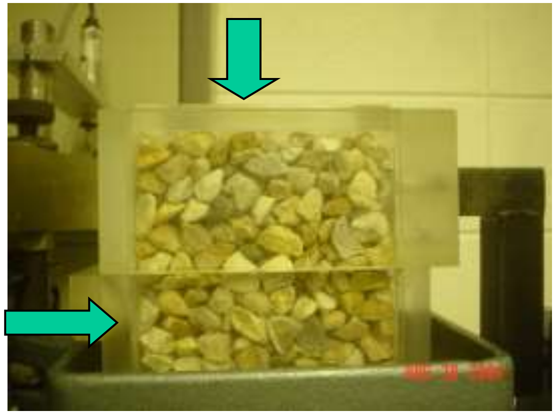
$$u = x^a - x^b; v = y^a - y^b; w = z^a - z^b$$

Particle Rotations:

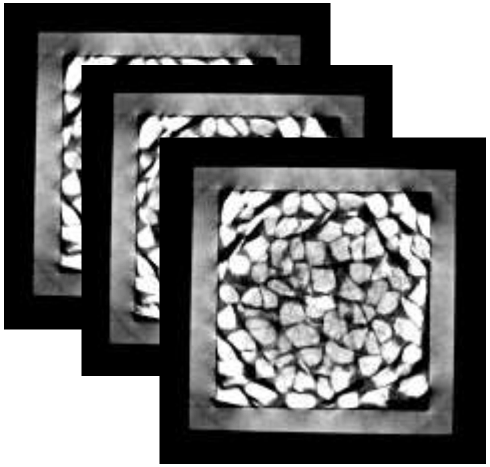
$$\Delta \vec{\Omega} = \vec{\Omega}_b - \vec{\Omega}_a$$

Digital Direct Shear Test

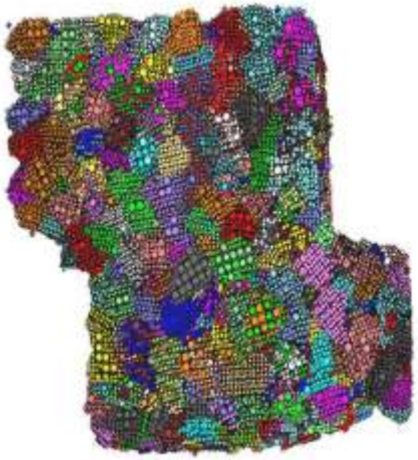
a) The ELE Direct Shear Apparatus EL28-007 series



b) The Specimen



c) The Gray images of specimen



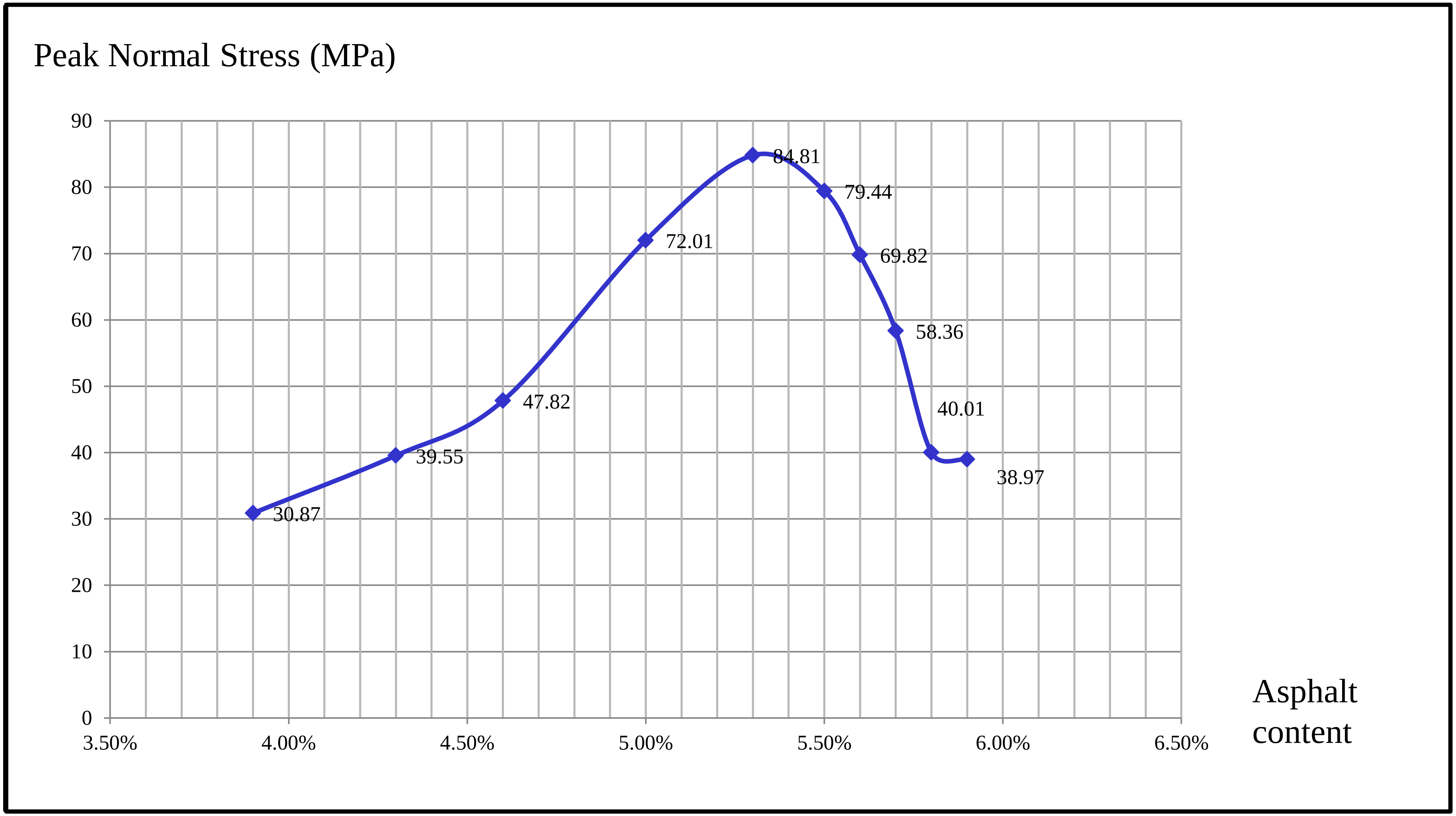
d) The digital specimen

Two steps closer to practical applications

Digital Mix Design

- PI, Digital Mix Design for Performance Optimization of AC, NSF, $289,513, 2010-2013.

Determination of Asphalt Content



FEASIBILITY AND CHALLENGES

- More advanced tools/characterization and modeling
- Database !!!
- Active researchers
- National/international collaborations
- Industrial support
- Partial replacement (now to 20-50 years later)
- Direct applications (50 years--)

Acknowledgements

NSF, FHWA, LTRC

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Thanks!

Questions?