Challenges and Limitations in Multiscale Predictive Science Simulations

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With Help from Many Colleagues

Outline

- **Multiscale Predictive Science and Simulations**
  - Radiation
  - Materials Instability, Aging, Microstructure Evolution
  - Constitutive Equations, Damage, Fracture
  - Novel Materials

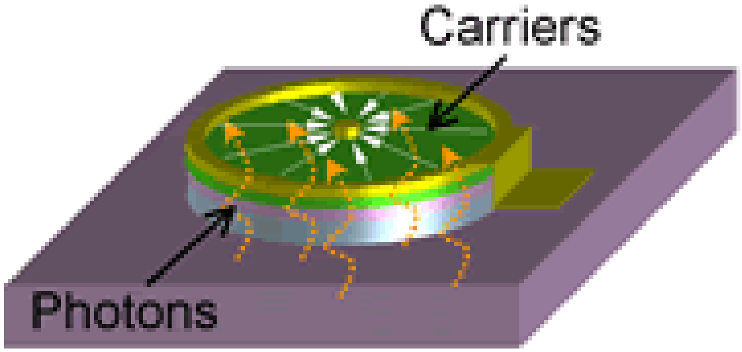
- **Integrated Computational System and Software Integration:**
  - Spans the scales QM→CM
  - Predict thermal-mechanical-electrical performance - harsh environments
  - → parallel and petaflop computation

- **Validation, Verification, and Uncertainty Quantification (V&V, UQ):**
  - Incomplete experimental information and input and model uncertainties
  - Use limited experiments/Inspections e.g. aging and radiation damage
  - Large ranges of space and time scales
  - Uncertainty Quantification to provide error bounds of the prediction

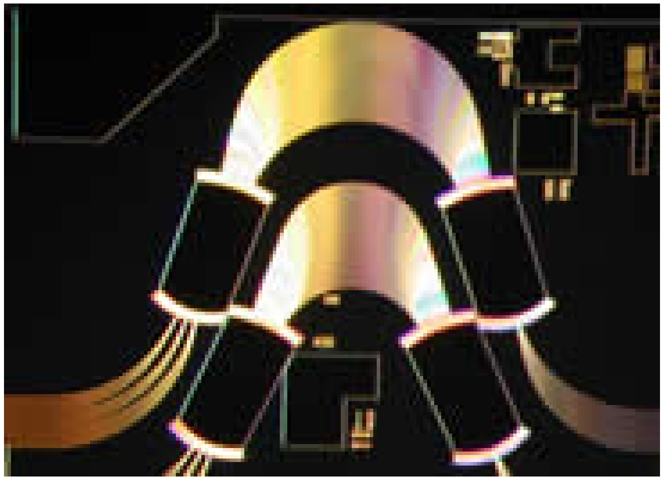
- **A focus microsystem problem to drive research and demonstrate the predictive science capabilities**

- **The design of novel materials for future microsystems**

Radiation Effects on MEMS in Satellites



Single photon detector (courtesy of H. Mohseni)



Multi-wavelength laser (courtesy of H. Mohseni)

- **Radiation accelerates diffusion of materials**
  - Material instability and aging
  - Microstructure evolution
- **Current diffusion barriers are susceptible to radiation damage**
- **Novel materials design → need multiscale simulation tools**
- **Other important design factors:**
  - Stiction, friction, and impact loading of spring contacts
  - Thermal cycling

Conclusion: Need validated and verified multiscale predictive science methodologies

Radiation Effects on Materials

- Interaction of charged particles with crystalline solid
  - E.g. energetic electrons or heavy ions
  - Electronic and elastic interactions

Electronic excitations
& Auger electrons

Frenkel pairs →
vacancy & self-interstitial atom (SIA)
(point defects)

- Modeling of radiation effects
  - Combination of molecular and quantum simulations
  - Long time scales (diffusive migration of vacancies) → Monte Carlo methods
  - Molecular models linked to multiscale continuum models
    - predict thermal-mechanical-electrical performance and reliability

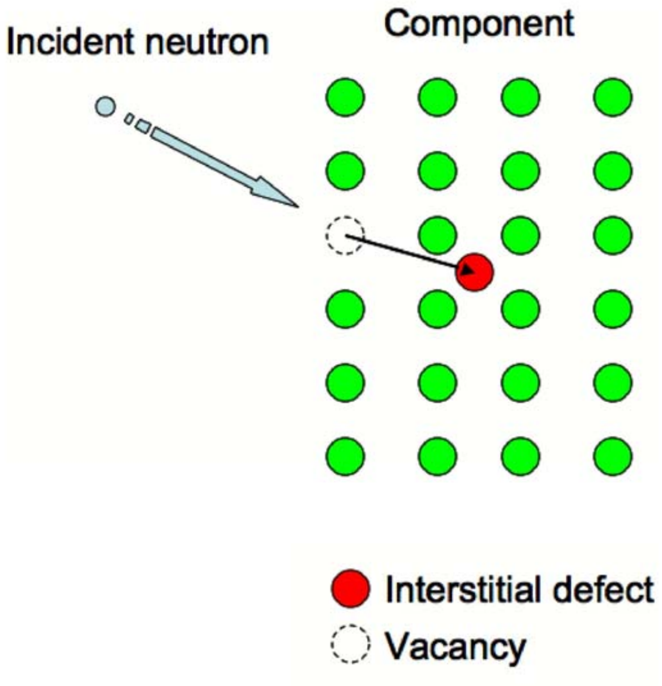
Radiation-Induced Degradation Effects

Atomic Displacement by

- particles → electrons, protons, neutrons
- high-energy photons

Long-lived effects

- Increased defect concentration
- Decreased charge carrier
  - lifetime
  - mobility
  - concentration
- Local disorder → dilation and stress
- Defects coalesce into microvoids



Transient effects

- Change in electrical conductivity

Source: Handbook of radiation effects, A. Holmer-Siedle and L. Adams, 1993.

Radiation-Induced Degradation Effects (Cont')

Ionization

- Particles: electrons, protons, and neutrons
- Phonons: high and low-energy

Long-lived effects

- Charge excitation and transport
- Bonding changes (damage)
- Decomposition

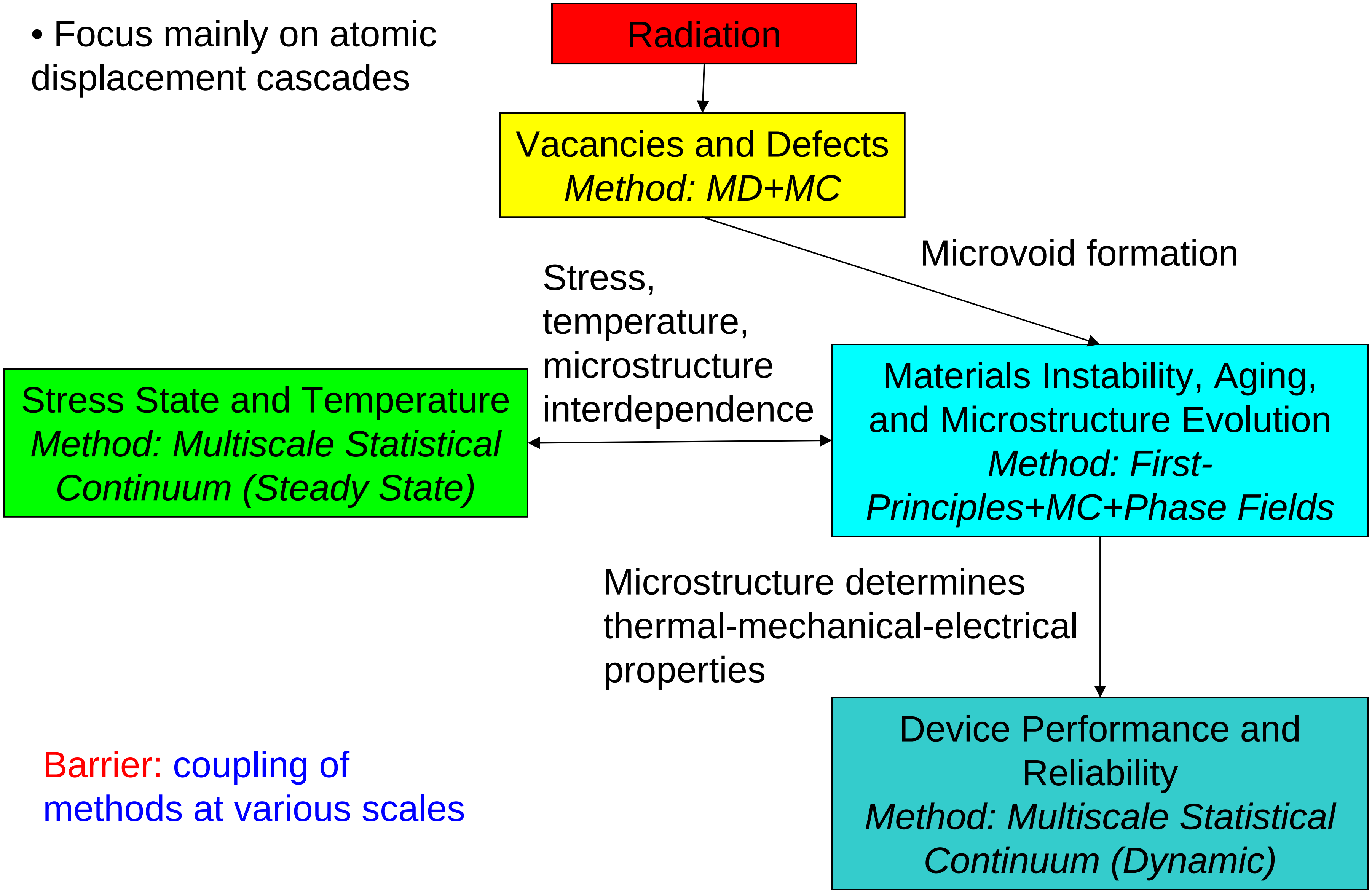
Transient effects

- Photocurrents → transient terminal voltage changes
- Latching conditions in bistable circuits
- Breakdown effects → high local currents in gas or solid state
- Short-lived color centers

Source: Handbook of radiation effects, A. Holmer-Siedle and L. Adams, 1993.

Radiation Damage Effect Schematic

- Focus mainly on atomic displacement cascades



Radiation

Vacancies and Defects
Method: MD+MC

Microvoid formation

Stress, temperature, microstructure interdependence

Stress State and Temperature
Method: Multiscale Statistical Continuum (Steady State)

Materials Instability, Aging, and Microstructure Evolution
Method: First-Principles+MC+Phase Fields

Microstructure determines thermal-mechanical-electrical properties

Device Performance and Reliability
Method: Multiscale Statistical Continuum (Dynamic)

Barrier: coupling of methods at various scales

Radiation Damage Modeling

Modeling Atomic Displacement

- MD: displacement cascade formation in small body (10 nm)^3
- MC: with ‘binary collision approximation’ (BCA) - initial defect production
- LKMC (lattice kinetic Monte Carlo): with residence time algorithm → long term radiation damage
- Free public domain codes for atomic displacement due to radiation:
  - MD: MDCASK (LLNL), MOLDYCASK (Oxford)
  - MC with BCA: SRIM (Ziegler) and MARLOWE (ORNL)

Barriers:

1. Coupling MD to MC
2. Prediction of interdiffusion between two materials using LKMC
   - Incorporation of grain boundaries, dislocations, elastic effects
3. Obtaining Input parameters (ie. activation and bonding energies) for MC or LKMC from first-principles calculations
4. Integration of above codes into LAMMPS/Tahoe

Materials Instability, Aging, and Microstructure Evolution

Material instability

- changes in thermal-mechanical-electrical properties
- vacancies, diffusion, defects, phase formation, microstructure evolution

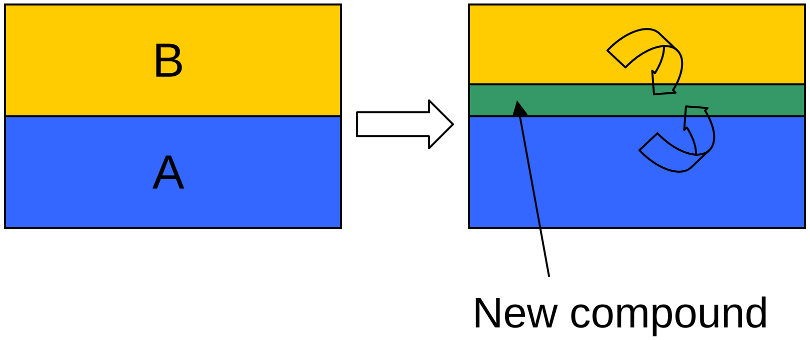
Radiation and thermal cycling

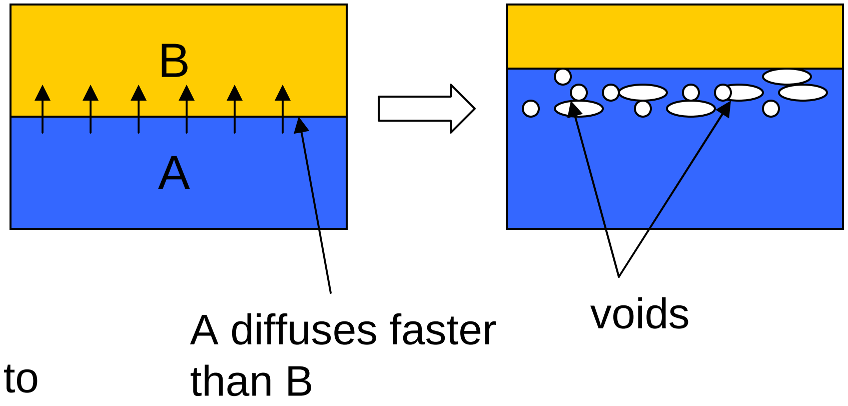
- radiation and thermal cycling are critical in micro-models
- chemical effects
  - oxidation and corrosion
  - mass diffusion and new compound formation from chemical reactions
- occur primarily at the microscale
  - kinetics governed by properties at electronic and molecular levels
- grain boundaries, dislocations, and microcracks
- interaction between quantum and micro-mechanical models
  - parametrization of microstructure model: subscale simulations

Mass Diffusion in Materials Aging

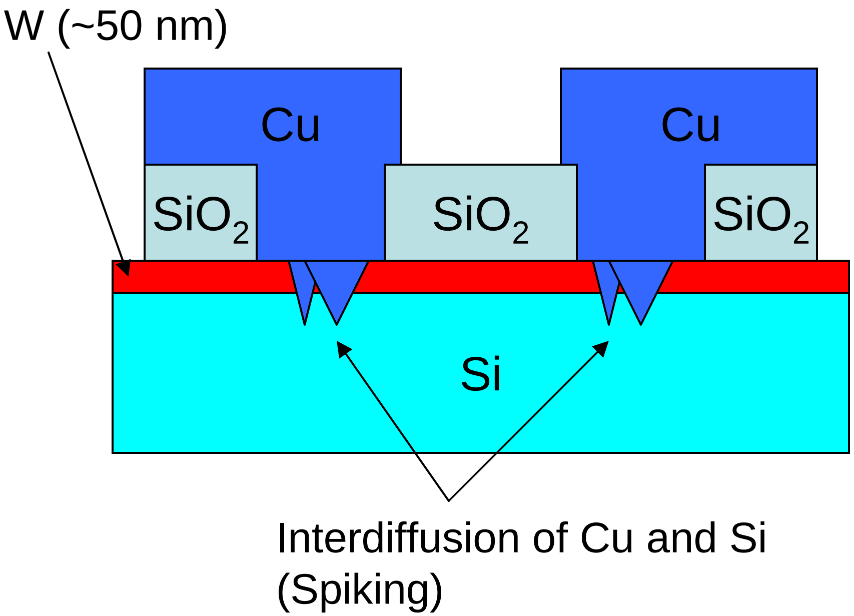
- **Compound formation** – Materials A and B interdiffuse to form new compound.

- **Kirkendall effect** – Material A diffuses faster than Material B, and voids form in A.





- **Si-Cu contacts** – copper diffuses into silicon to degrade device performance.



Complicating factors:

- These phenomena can occur simultaneously
- Diffusion depends also on temperature, electric field, microstructure, and stress state
- Typical thin film coating not enough to guard against materials aging under radiation.

Other phenomena in Microsystems

- **Thermal cycling**
- **Dynamic loading**
- **Adhesion, stiction, and arcing and damage in insulating materials that can cause electrical leakage**
- **Microstructure (ie. grain boundary, dislocations, and voids) evolution and interaction**
- **Voids diffuse into grain boundaries and grow**

- Metal-Solder reactions
- Residual thermal stresses resulting from manufacturing processes
- Creep and fatigue of solder
- Environmental effects such as oxidation and corrosion
- Tin whisker formation in solders
- Electromigration (with novel materials design, this effect can be minimized and will not be modeled)

Ultimate goal: study the selected combined effects of various critical phenomena on the long term performance and reliability of the micro-system/device

Barrier: selecting the more important phenomena for a given device

Atomistic to Microstructure Evolution Multiscale Modeling

Software codes:

FLAPW (commercial)

TB-LMTO-REC (NWU)

CEMC (NWU)

Phase Field Codes

(NWU)

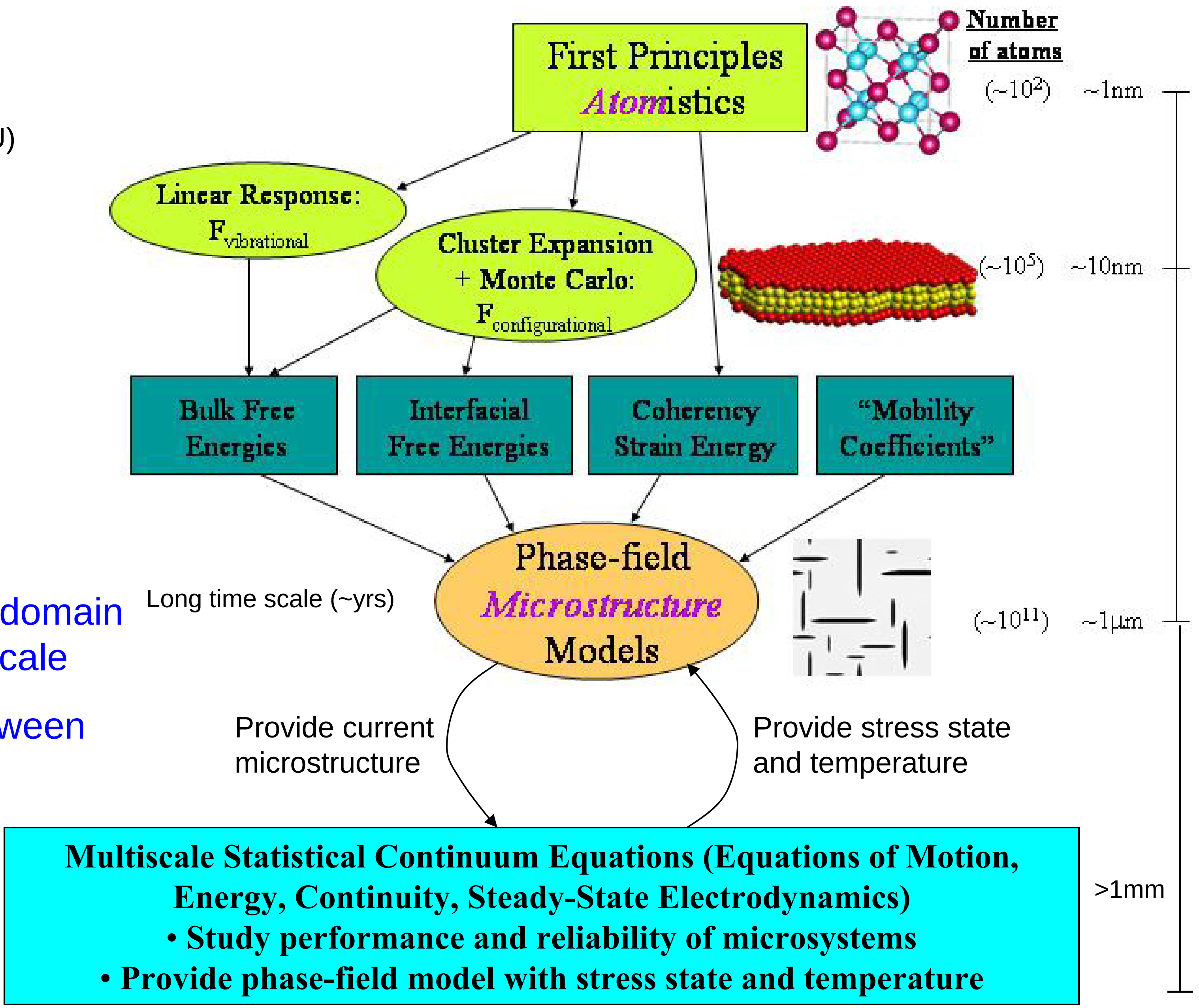
Barriers:

- determining domain size at each scale
- coupling between scales

Multiscale Statistical

Continuum

(NWU/Tahoe)



Number of atoms

First Principles *Atomistics*

(~10^2) ~1nm

Linear Response: $F_{vibrational}$

Cluster Expansion + Monte Carlo: $F_{configurational}$

(~10^5) ~10nm

Bulk Free Energies

Interfacial Free Energies

Coherency Strain Energy

"Mobility Coefficients"

Long time scale (~yrs)

Phase-field *Microstructure* Models

(~10^{11}) ~1µm

Provide current microstructure

Provide stress state and temperature

>1mm

Multiscale Statistical Continuum Equations (Equations of Motion, Energy, Continuity, Steady-State Electrodynamics)

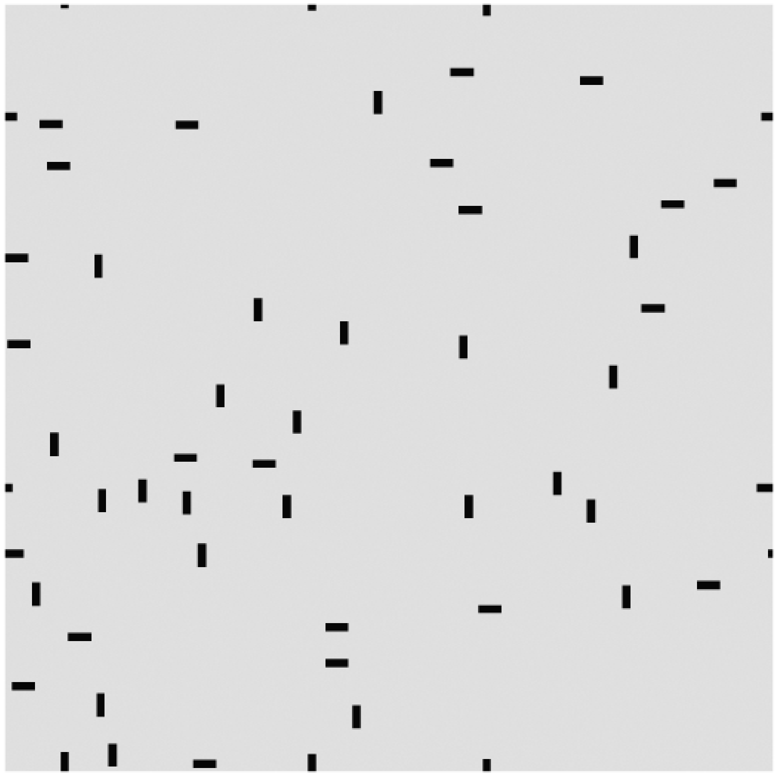
- **Study performance and reliability of microsystems**
- **Provide phase-field model with stress state and temperature**

Microstructural Evolution Multiscale Model

First-Principles / Phase-Field

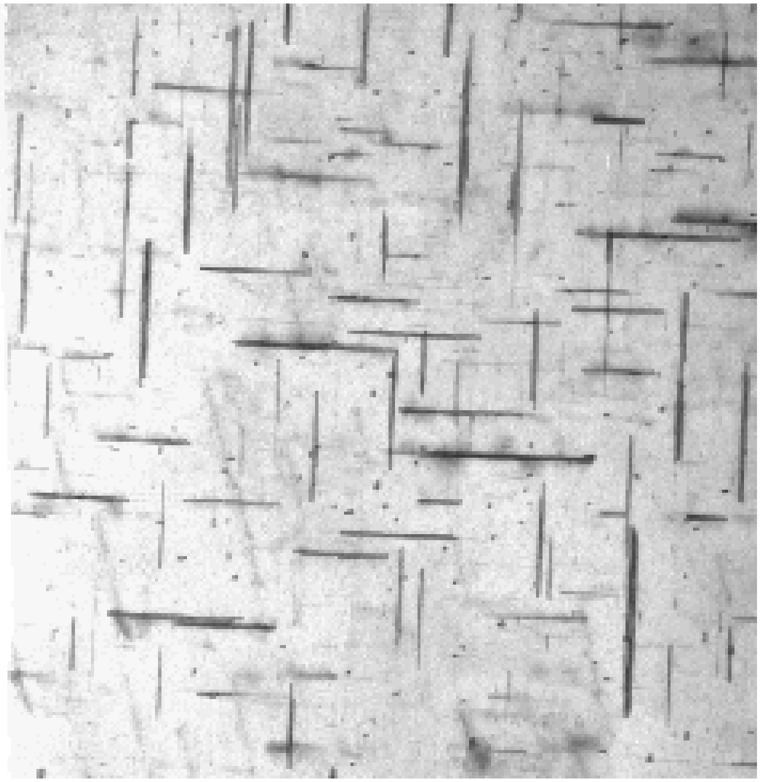
Phase Field Simulation

(All energetics taken from first-principles calculations)



TEM Micrograph of W319 Alloy

(W. Donlon et al.)



Vaithyanathan, Wolverton, and Chen,, Phys. Rev. Lett. (2002).

From Microstructure Evolution to Constitutive Equations, Damage, Fracture, and Performance

Coupled Multiscale Statistical Continuum Equations consist of various scales of:

- Continuity equations
- Momentum equations
- Energy equations
- Steady-state electrodynamics equations

Barrier: based on these equations, solve the focus problem with uncertainty quantification.

Thermal-Mechanical-Electrical-Chemical Coupling

Parameter / Variable	**Direct dependent Parameter / Variable**	**Method to Obtain Parameter**
Density (ρ)	Atomic concentration (C)	
Stress (σ)	Atomic concentration (C), Temperature (T)	
Thermal conductivity (κ)	Temperature (T), Electric current (j)	Transport theory; MD
Electrical conductivity (γ)	Temperature (T)	First principles calculation + transport theory
Temperature (T)	Electric current (j) → Joule heating	
Diffusion Coefficient (D)	Stress (σ), Temperature (T)	MC

Barrier:

- may require iterations to solve equations because of the nonlinear couplings
- thermal conductivity depends on electron-phonon interaction → hard to estimate

Multiscale Statistical Continuum Equations

Multiscale Momentum Equation

$$\nabla \bullet \boldsymbol{\sigma}^n \left(\sum_{m=0}^{m=n} \tilde{\mathbf{u}}^m \right) + \mathbf{b}^n = \rho^n \dot{\mathbf{v}}^n \quad \text{in} \quad \Omega^n$$

Multiscale Energy Equation

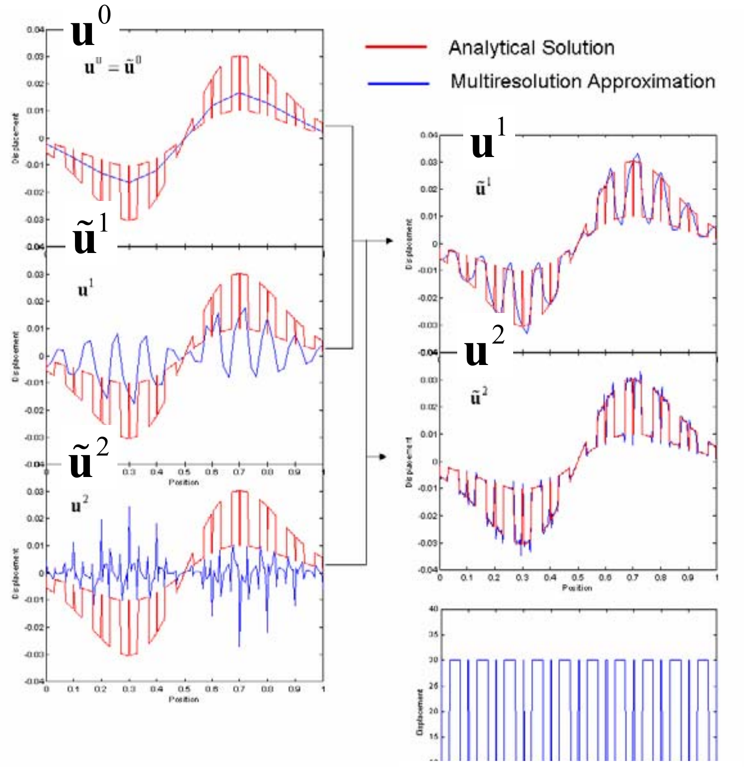
$$\kappa^n \nabla^2 \left(\sum_{m=0}^{m=n} \tilde{T}^m \right) + Q^n = \rho^n c^n \dot{T}^n \quad \text{in} \quad \Omega^n$$

Multiscale Continuity Equation

$$D^n \nabla^2 \left(\sum_{m=0}^{m=n} \tilde{C}^m \right) + W^n = \dot{C}^n \quad \text{in} \quad \Omega^n$$

Multiscale Stead-State Electrodynamics Equation

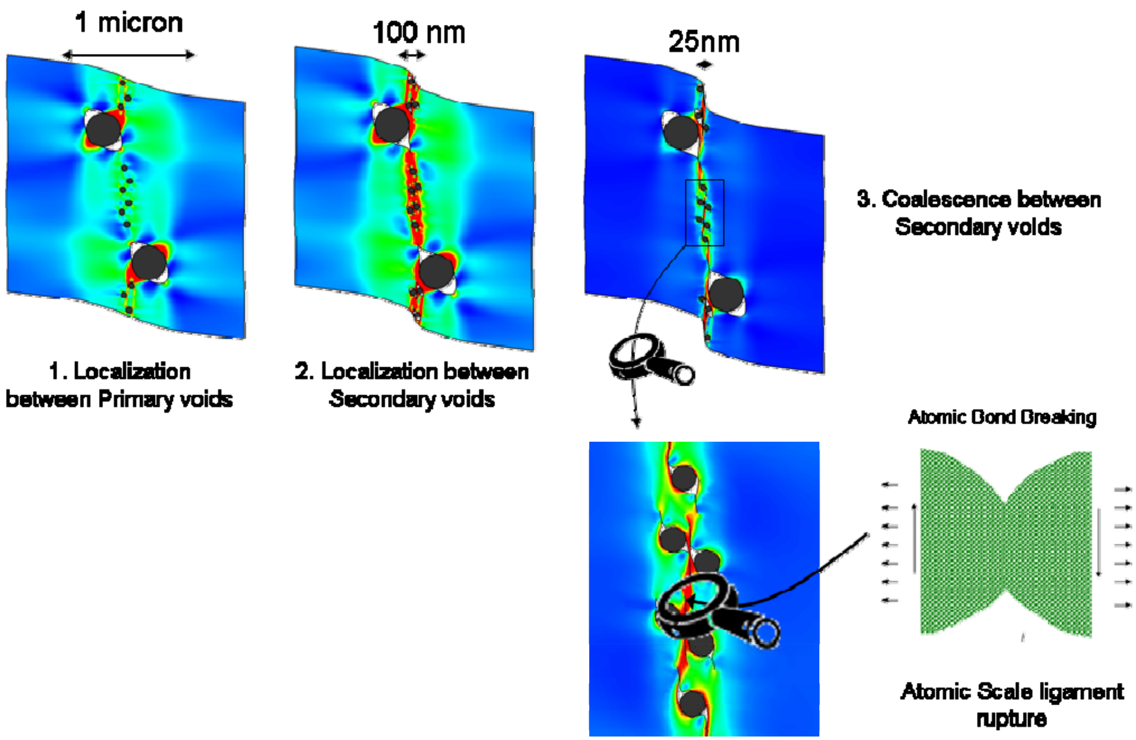
$$\nabla \bullet \left[\gamma^n \nabla \left(\sum_{m=0}^{m=n} \tilde{\phi}^m \right) \right] = 0 \quad \text{in} \quad \Omega^n$$



microstructure

Barrier: On-the-fly estimation of coarser scale constitutive relations needs to be implemented

A Four Scale Materials Design Example



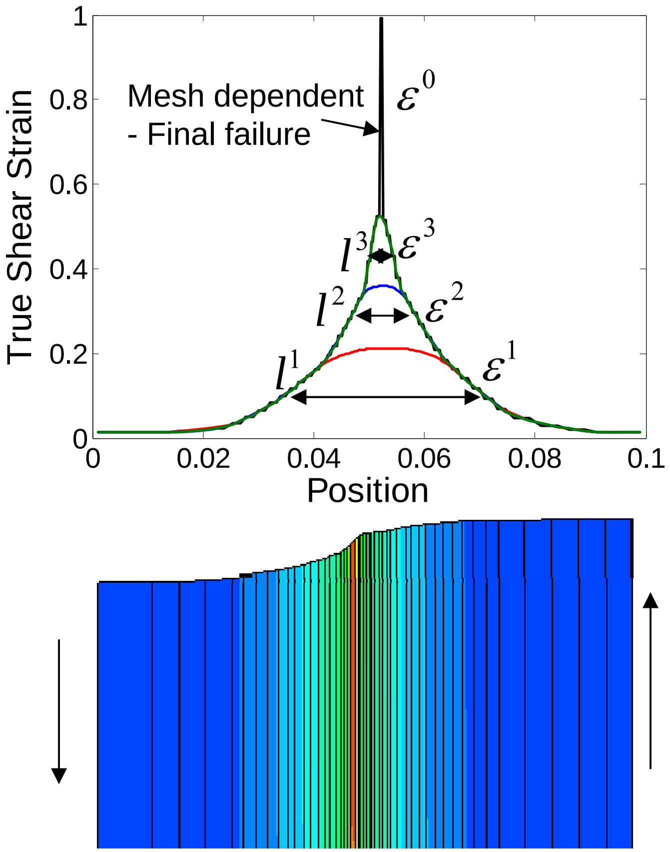
1. Localization between Primary voids

2. Localization between Secondary voids

3. Coalescence between Secondary voids

Atomic Bond Breaking

Atomic Scale ligament rupture



- Four length scales are observed in the final solution:
  1. localization between primary particles
  2. localization between secondary particles
  3. microvoid shear localization
  4. final material rupture

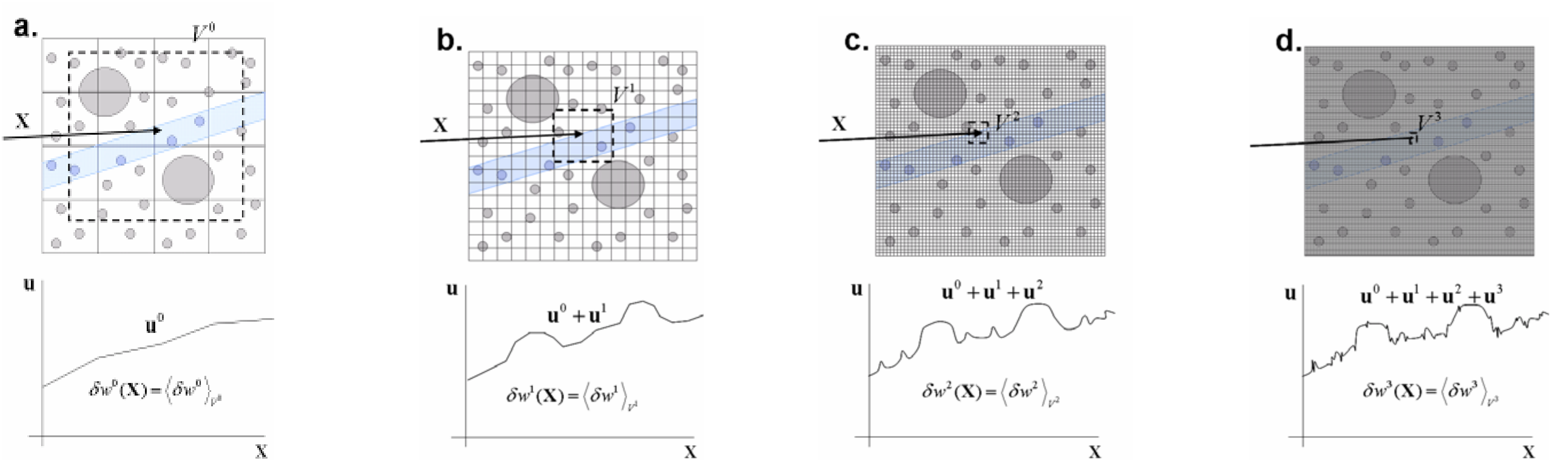
- Three scales of localization & final failure in an alloy

- Localization at scale *n* → strain field resolved to scale *n*

- The microstress at each scale has its own constitutive law

Multiresolution Imaging and Microstructure

Increasing Field & Constitutive Resolution



Small Number of degrees of freedom – suitable for average behavior

Discrete behavior of larger particles begins to be observed

Discrete behavior of smaller particles is observed

Very fine resolution – all individual micro-constituents

Small Number of pixels per km^2 – suitable for a global image

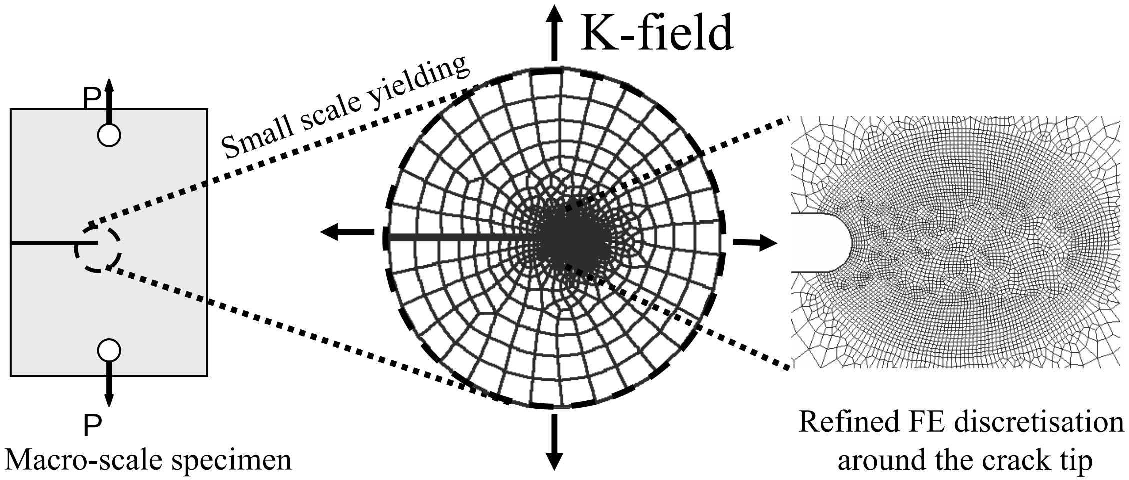
More resolution – cities can be observed

Increasing resolution – buildings can be observed

Northwestern University
- a fine institution

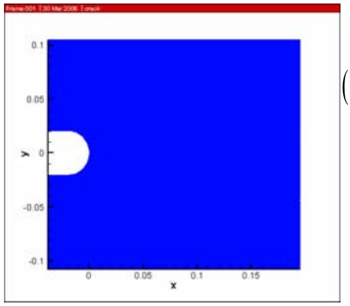
Increasing Image Resolution

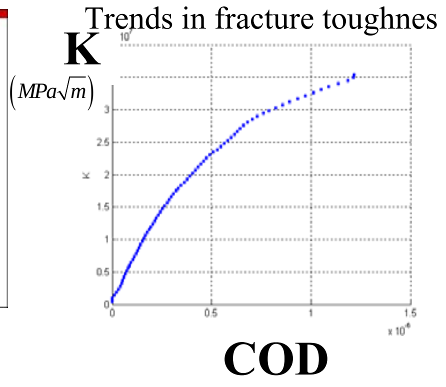
Novel Materials Design Based on Fracture Toughness



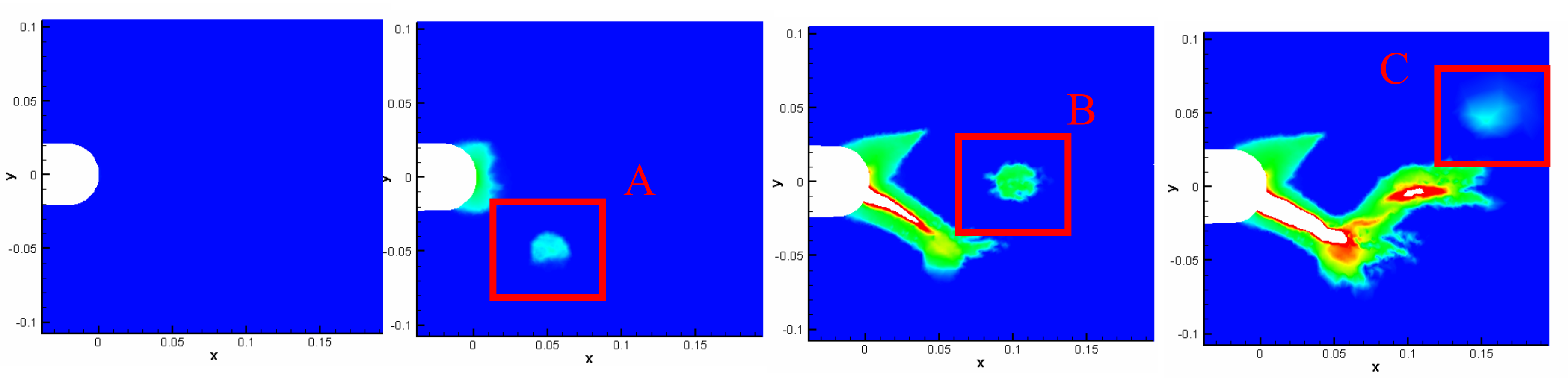
Macro-scale specimen

Refined FE discretisation around the crack tip





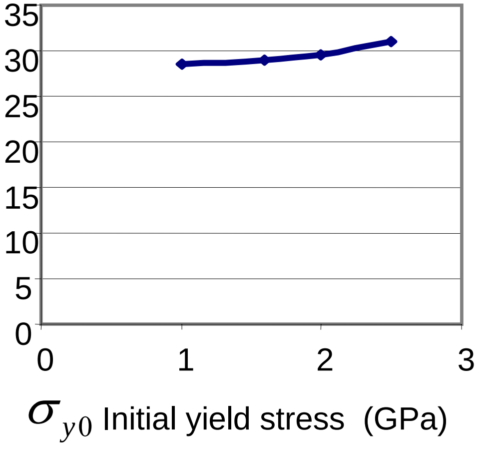
- Statistically random distribution of initial microstructure
  - particle clusters at A, B and C

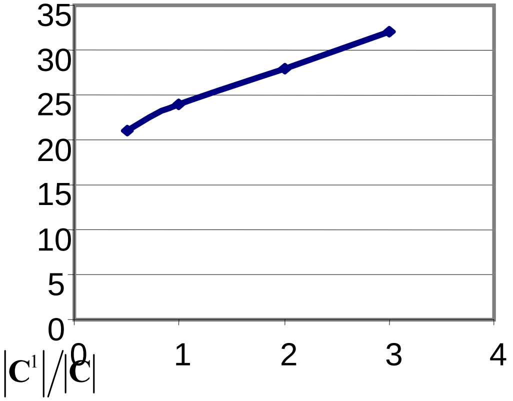


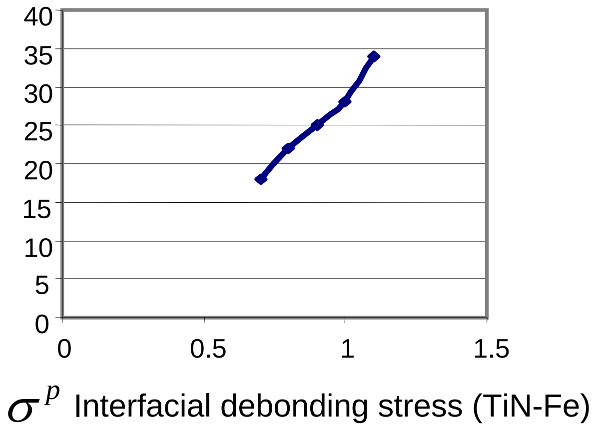
- Similar procedures can also be applied to design novel materials that are
  - Resistant to Materials Diffusion
  - Formability
  - Scratching

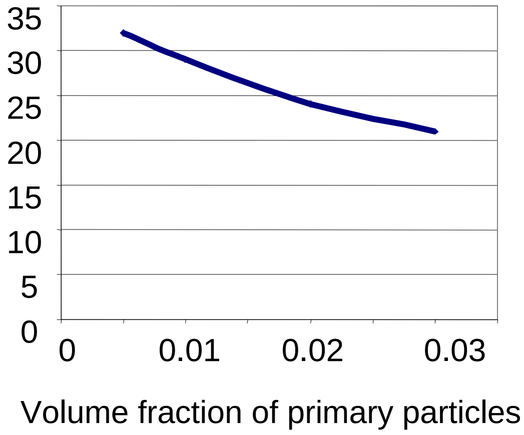
Design of Fracture Toughness

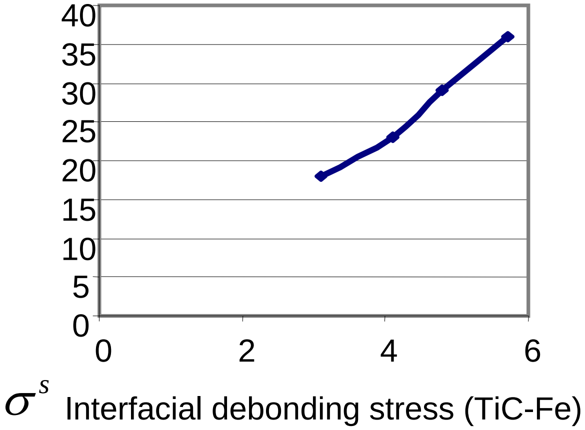
$$K_{Ic} = K_{Ic}\left(\sigma_{y0}, \frac{\left|\mathbf{C}^{1}\right|}{\left|\mathbf{C}\right|}, f^{p}, \sigma^{s}, \sigma^{p}\right)$$











(TENTATIVE NOT VALIDATED RESULTS, RESEARCH IN PROGRESS)

Computational Mathematics of Thermal-Mechanical-Electrical-Chemical Coupling

Barriers for Multiscale Momentum Equations and Their Constitutive Equations:

- Modeling Voids
  - explicitly in the full simulation
  - implicitly in multiscale continuum equation with RVE
- Microstructure evolves spatially and temporally due to diffusion
- Explicit modeling of voids accomplished by the IFEM scheme
- Propagation of microcracks emitted from voids modeled by XFEM
- Stochastic thermal-mechanical-electrical-chemical loadings due to radiation need to be formulated

Computational Mathematics of Thermal-Mechanical-Electrical-Chemical Coupling (Continue)

Barriers for Multiscale Energy, Continuity, and Steady-State Electrodynamics Equations:

- Thermal conductivity estimation given a microstructure
  - MD simulation
  - kinetic theory
  - Wiedmann-Franz law (great for metals)
- Thermal conductivity depends on electric current
- Joule heating
- Radiation-generated heat/charges
- Dielectric loss
- Surface heat radiation
- Estimation of diffusion coefficient (depends on both stress and temperature)

Novel Materials Design

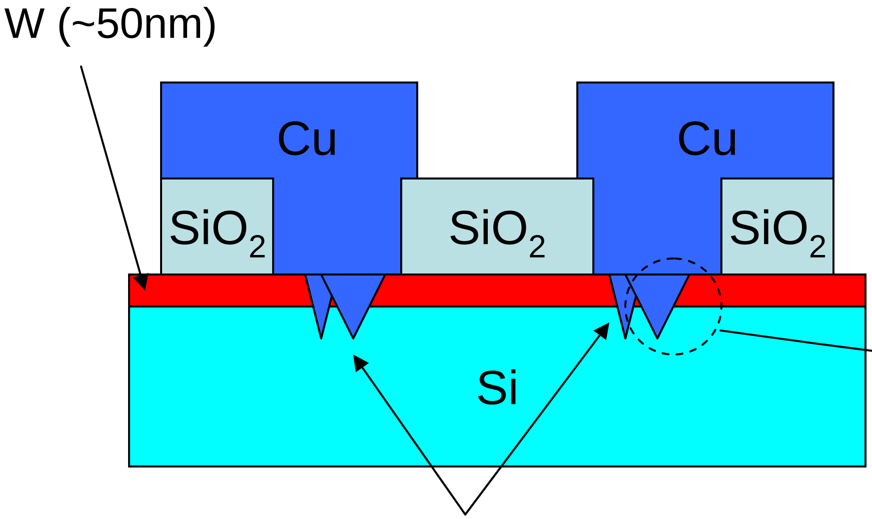
Based on the Naval Materials by design “Cybersteel 2020,” and related AFOSR and DARPA initiatives, Navy has begun a Digital 3-dimensional (D3D) project on:

“The development of the next generation of integrated research tools enabling a new level of science-based materials engineering capability keeping pace with advancing computational power.”
(Greg Olson, Northwestern)

- Slowing Down Radiation-Accelerated Diffusion
- Alkane Thiol Self-assembled Monolayers (SAM) Lubrication Coating
- Nanostructured Microactuation Shape Memory Alloys (SMA)

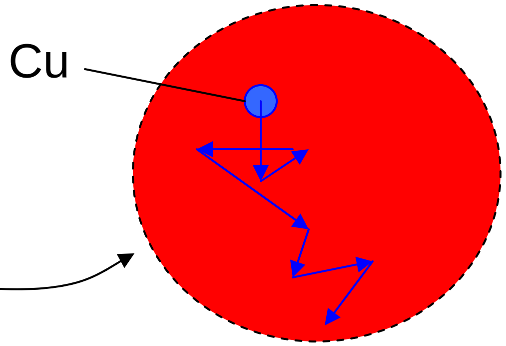
Slowing Down Radiation-Accelerated Diffusion

- Radiation environment → mass diffusion is accelerated
- Design of diffusion barrier insufficient to slow diffusion (long term)
- Add silver particles to tungsten diffusion barrier → traps copper particles

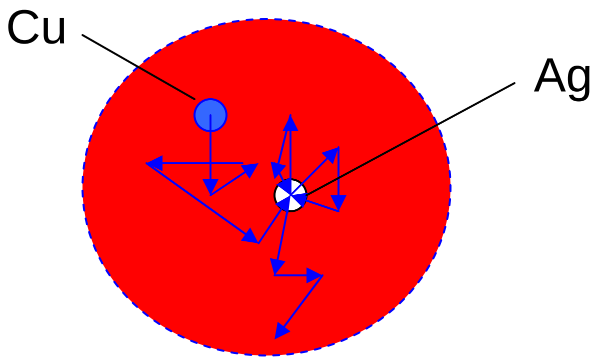


Interdiffusion of Cu and Si (Spiking)

- Microscopically, copper (Cu) particles exhibit random walk in the diffusion barrier:



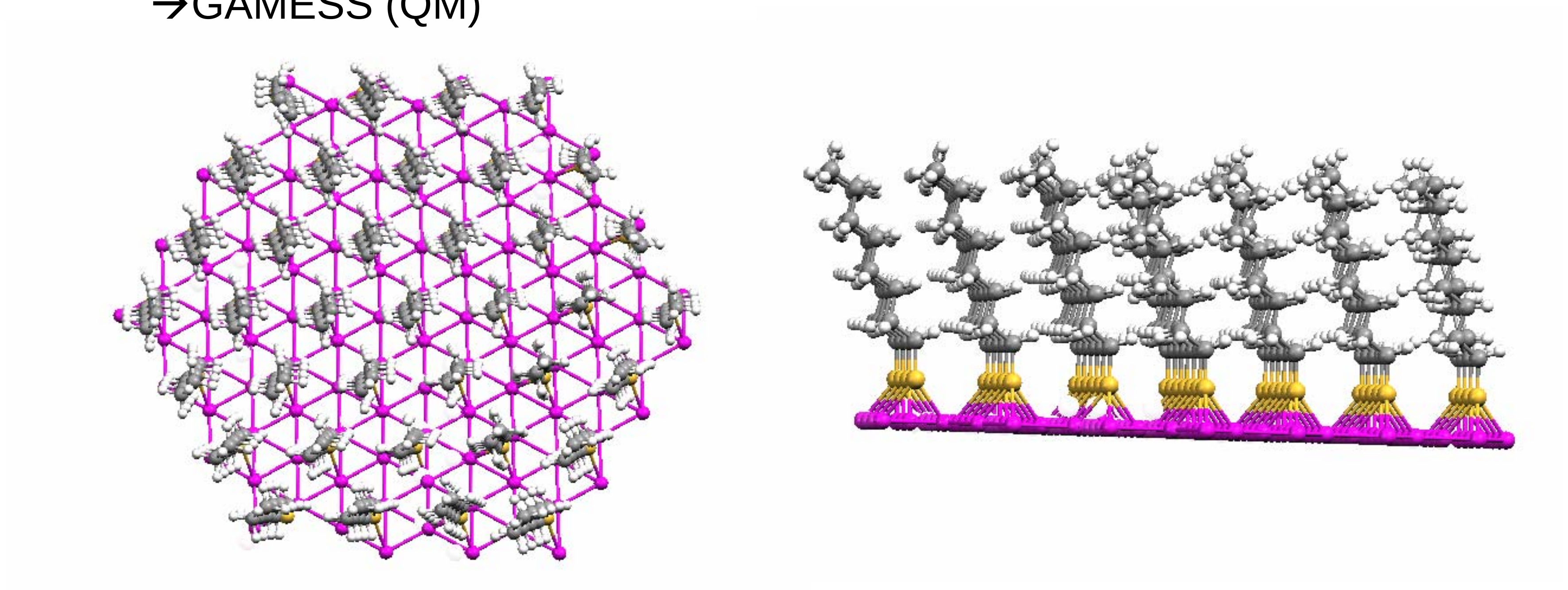
- Silver (Ag) particle in the tungsten (W) barrier layer trap copper (Cu) particles: diffusion path is longer.



Comment: The multiscale predictive science simulation system will allow us to design better material systems to guard against diffusion

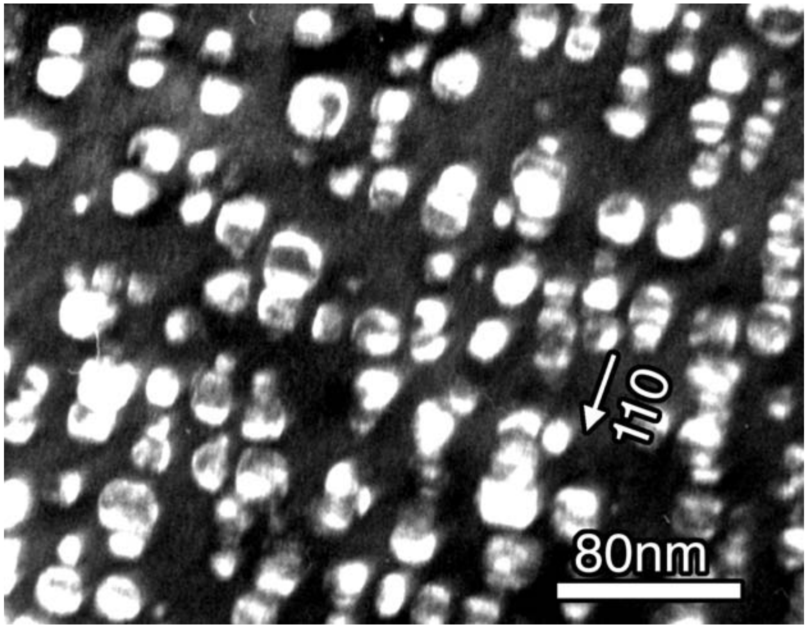
Radiation-Induced Degradation of Alkane Thiol Self-Assembled Monolayers (SAM)

- Study degradation of SAM resulting from chemical reaction with atom/ion projectiles
- SAM is model for coating or lubricant.
- Chemical degradation
  - formation of free radicals and surface ions
  - roughens the surface
- Involves QM/MM coupling
  - QM and MM computations based on free open source AMES lab code →GAMESS (QM)



Troya and Schatz, J. Chem. Phys., ***120*** *(2004).*

Nanostructured Microactuation Shape Memory Alloys



Concept: High strength SMAs for higher output stress and greatly enhanced cyclic life

Applications: High power density microactuation systems and nonlinear-compliant tribological coatings

Predictive Science: Nanodispersion precipitation strengthening and martensite kinetic theory

Integrated Software Design

- Multiscale predictive science software system - integrate many single-scale tools into an integrated systems mutliscale, multiphysics modeling
- Provide a set of components for multiscale simulation that can effectively couple the various single scale tools
  - Take advantage of existing tools in this process including the DOE Tahoe code that supports MD and continbuum
- Other codes to be integrated
  - Quantum: TB-LMTO-REC (NWU), GAMESS (NWU)
  - MD: LAMMPS (DOE), MDCASK (LLNL, radiation)
  - Phase field models (NWU)
  - Continuum: Multiscale Statistical Continuum Equations (NWU), IEFEM (NWU), XFEM (NWU)
  - Adaptive Continuum/Atomistic Multiscale: Multiscale Adapt (RPI)
  - Uncertainty quantification: OPTDOE, SORA, SSA, BPM, libuq, DAKOTA (SNL), Sundance (SNL)

Integrated Software Design

- Barriers:
  - Effective means to integrate a wide variety of different tools into a tool capable solving the full range of multiscale, multiphysics problems
    - Wide range of different capabilities needed - existing programs provide only a subset of what is needed
    - Must be able to take advantage of existing tools due to time and effort required to redo them from scratch
    - Existing tool are not easily changed or integrated
  - Supporting the level of computation needed - Even with adaptive multiscale methods petascale computed required
    - Parallelization to petascale requires extreme scalability - few of the individual tools have been scales to 1,000’s of processors, getting to the 100,000’s for petascale will be a challenge
    - The use of multiple coupled tools will compound the parallization challenge
    - The application of adaptive mutliscale methods further complicates parallelization because of the required dynamic laod balancing

Verification Plan

- Perform code and calculation verification
- Code verification based on benchmark solutions
    - analytical solutions to manufactured solutions of increasing complexity
- Multiscale statistical continuum code verified by peta-flop direct numerical simulations (DNS)
- Convergence of direct numerical simulations studied with LANL group
    - ‘three-mesh refinement’ method
    - don’t require knowledge of ‘exact’ solution

Barrier**:** Verification of atomistic scale methods and coupling of methods

Validation Plan

- Validation → limited number of experiments
- Measurement of material degradation and microstructure evolution
  - radiation and thermal aging
  - mimicked by ion or electron beams (in-situ SEM or TEM)
  - TEM and X-ray diffractions
  - 3D atom probe (3DAP) allows very fast imaging
- MEMS scale tests validate macro-constitutive equations
  - accelerated and unaccelerated conditions.
- Stochastic sensitivity across scales
- Lack of experimental data → validation performed by finer-scale method

Barrier: optimization of resources between experiments, modeling, and computations

Uncertainty Quantification Plan

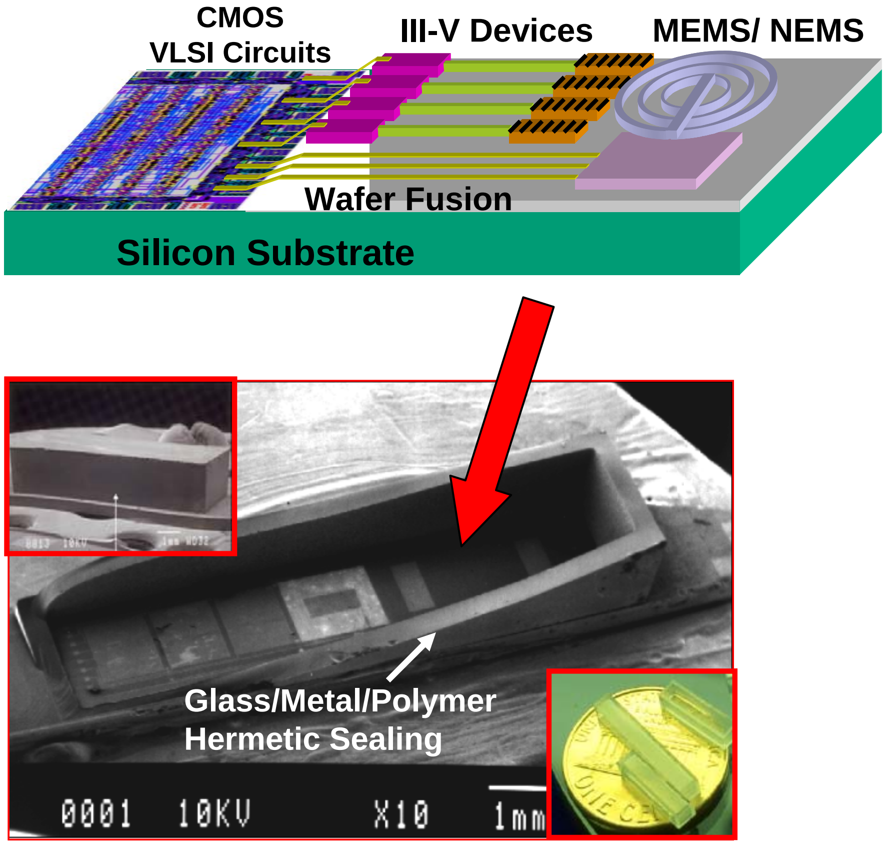
- Gage the accuracy with which information is being represented, and the significance of the associated loss of accuracy
- Quantify the worth of additional information
- Develop stochastic scale-bridging techniques
- Stochastic model calibration and prediction uncertainty quantification
- Efficient algorithms for uncertainty propagation and probabilistic finite elements (polynomial chaos, importance sampling, Markov Chain Monte Carlo) – all sources of uncertainty rolled up to give a predictable total output uncertainty
- Use examples from other similar problems.

Barriers:

- Quantification of information
- Input uncertainty

Select an Important Aspect of this Device as a Focus Problem

Wafer fusion techniques combined with MEMS/NEMS and conventional CMOS and compound semiconductor electronics will be used to realize a robust oscillator (clock) as the demonstration system.

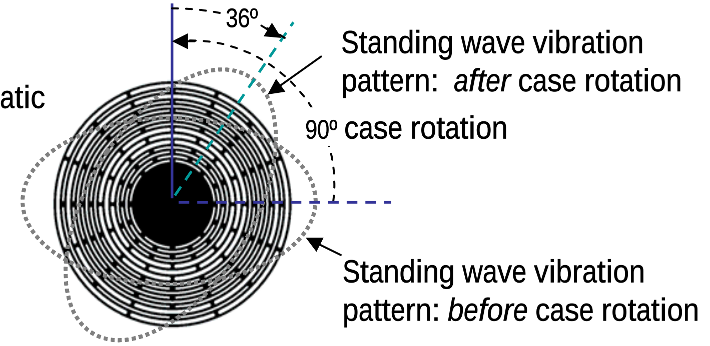


- A wide range of heterogeneous interfaces are present in this problem
- A wide range of implementations are possible (electronics, photonics, mechanical, etc)
- Long term stability of the clock is critical for many systems and applications
- Frequency of the clock provides a direct and convenient measure for the stability

Boeing Technology-Phantom Works-Disc Resonator

Principle of Operation:

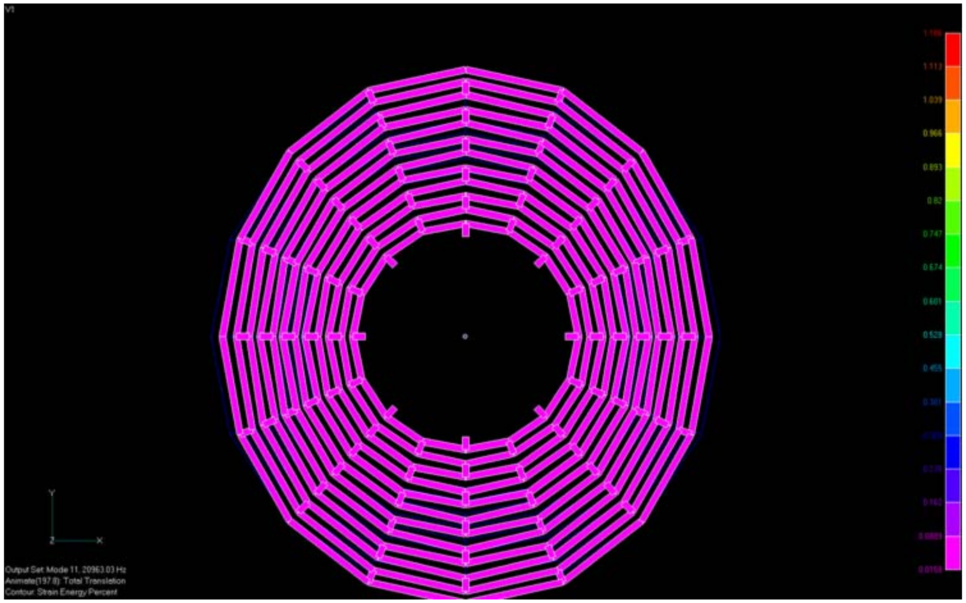
*Etched disc
w/ internal electrostatic
sense, drive & trim



*US Patent: 7,040,163
May 9, 2006

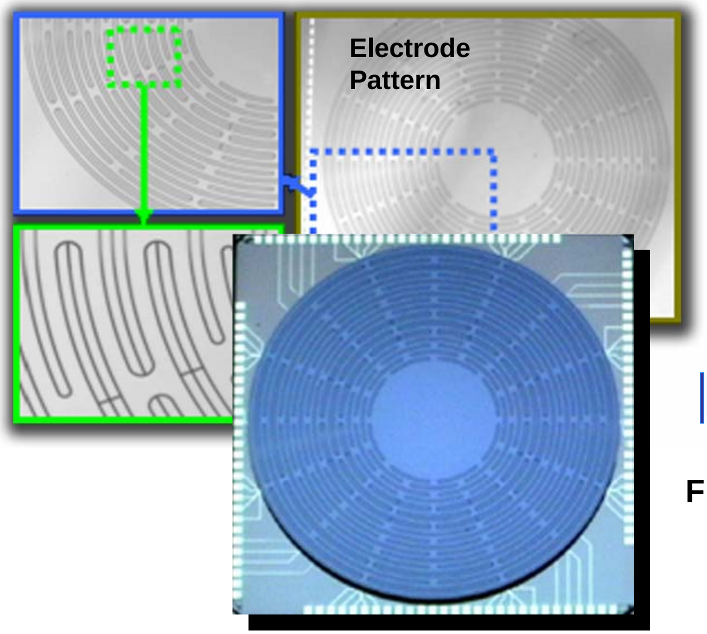
Disc Resonator Gyroscope

[First conception/ FEA]



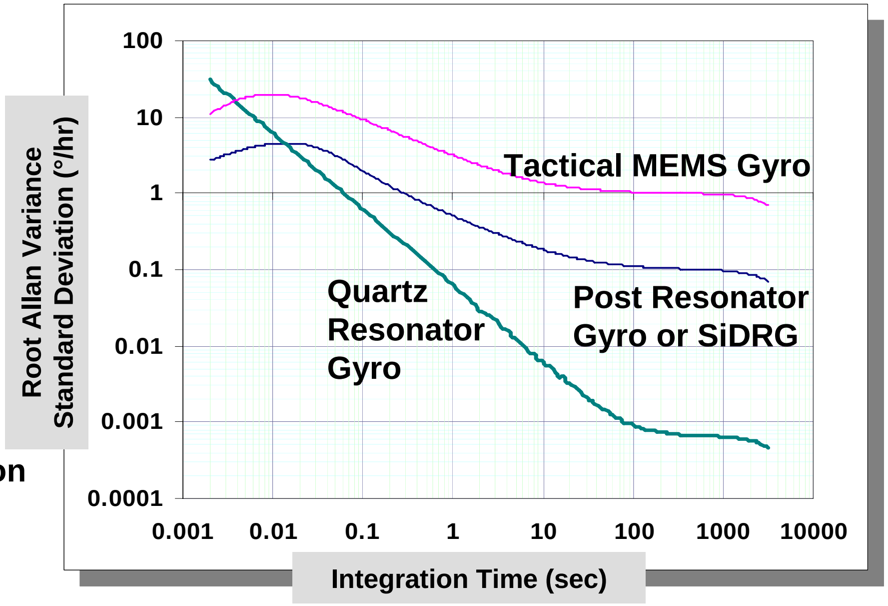
A Reliable Navigation Grade Standing-Wave MEMS Gyro

Existing Silicon Standing-Wave MEMS Resonator



From Silicon to Quartz

Projected Quartz Gyro Performance Exceeds That of Existing Resonators



Fused quartz material properties along with integrated electronics promises navigation-grade performance within the desired volume

Gyro Performance Metrics	Silicon DRG	*NGIMG Goals*
Bias stability (°/hr)	0.25	0.01
ARW (°/√ hr)	0.01	0.001
Power (watts)	2 (discreet electronics)	0.005 (ASIC)
Volume (cm³)	~10 (discreet electronics)	1 (ASIC)

Our Program Develops an Ideal Gyro

- **High-Q nav-grade performance**
- **Large signal-to-noise ratio sensing**
- **Low-cost (2D fabrication)**
- **Small (1 cm^3)**
- **Reliable**
- **Low Power(5mW)**

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Conclusions

- Aim to develop multiscale predictive science tools to model radiation-induced damages and materials aging in microsystems
- Long-term materials instability, aging, and microstructure evolution modeled by coupling first-principles, Monte Carlo, and phase field models
- Develop multiscale statistical continuum equations to check device performance and reliability based on current microstructure
- Verification, validation, and uncertainty quantification of multiscale methodologies
- Novel materials design to slow down radiation damage and materials diffusion, and design to minimize stiction and adhesion, and arcing of spring contacts
- A focus problem to drive research and demonstrate the predictive science capabilities