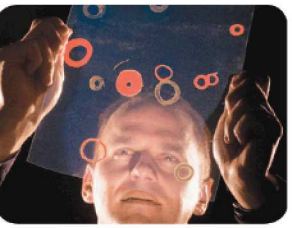
Need for Uncertainty Quantification in Multiscale Material Modeling

SAND2018-2335C



Stephen M. Foiles

Sandia National Laboratories

Albuquerque, NM

Symposium on "Building an ICME Infrastructure"

TMS Annual Meeting

March 14-15, 2018

Phoenix, AZ

Personal Experience: Small slice of the challenge

- In late 80's there was a controversy between two groups using x-ray scattering to determine grain boundary structure

Acta metall. Vol. 36, No. 12, pp. 3103–3122, 1988
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0001-6160/88 $3.00 + 0.00

QUANTITATIVE X-RAY DIFFRACTION STUDY OF THE ATOMIC STRUCTURE OF THE $\Sigma = 5(\theta = 36.9°)$ [001] TWIST BOUNDARY IN GOLD

M. R. FITZSIMMONS and S. L. SASS
Department of Materials Science and Engineering, Cornell University, Ithaca, NY 14853, U.S.A.

(*Received* 7 *December* 1987; *in revised form* 24 *March* 1988)

PHYSICAL REVIEW B VOLUME 40, NUMBER 5 15 AUGUST 1989-I

Structures of [001] twist boundaries in gold. II. Results obtained by x-ray diffraction and computer simulation

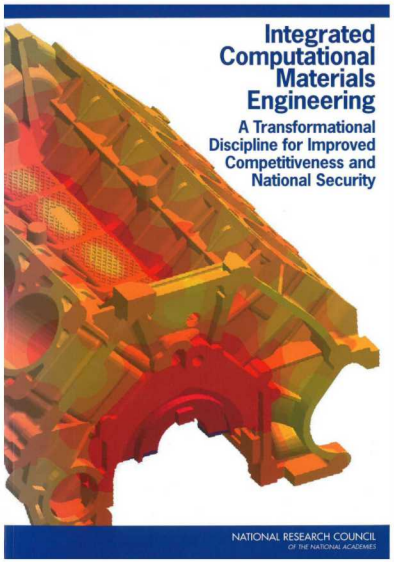
I. Majid, P. D. Bristowe, and R. W. Balluffi
Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 21 November 1988; revised manuscript received 27 February 1989)

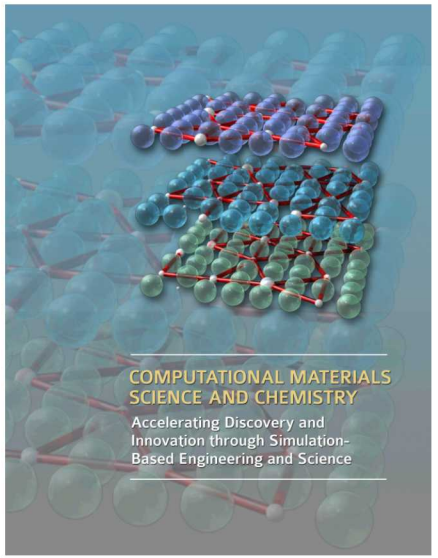
- I performed atomistic simulations that agreed with MIT group
- After an extensive discussion of experimental error analysis, Michael Fitzsimmons asked a ***simple troubling question***

What are the error bars on your calculation?

National Initiatives encourage the increased use of material modeling

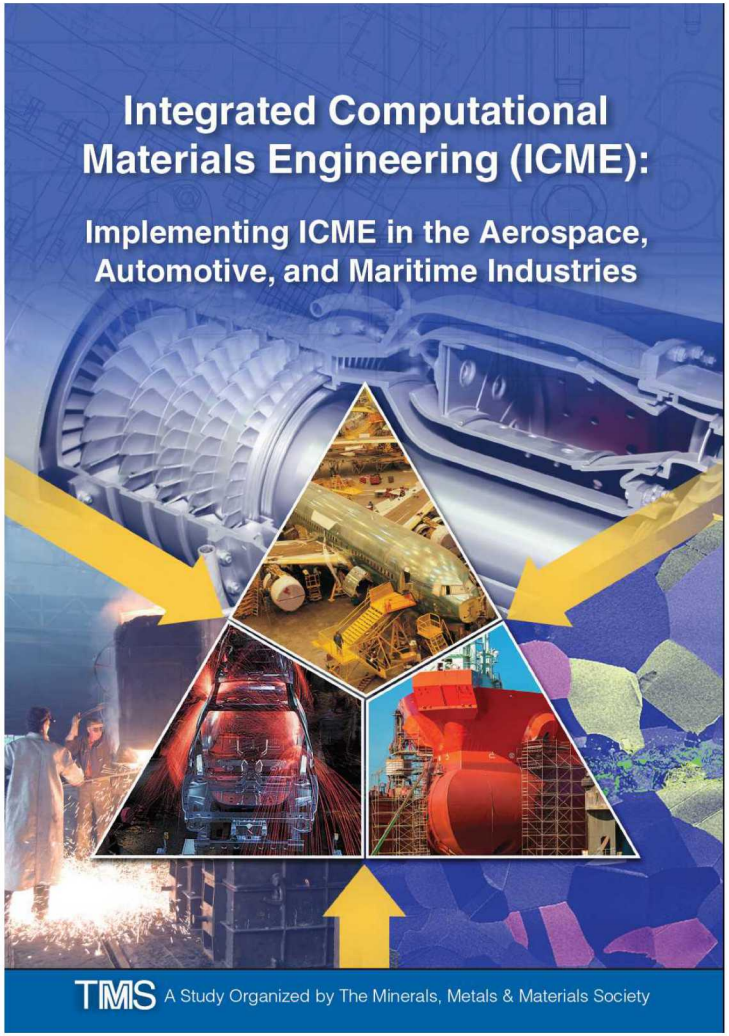
- ICME
  - Need for *more rapid and cost effective* materials design/qualification
  - Integrate materials modeling at multiple scales with experiments/data
  - Championed by The Minerals, Metals and Materials Society (TMS)
- Materials Genome
  - Need for *more rapid and cost effect* materials discovery
  - Combine materials modeling and materials databases to facilitate discovery of novel new materials
  - Sponsored by White House Office of Scientific and Technology Policy (OSTP)





Recent TMS study identified obstacles to ICME implementation

- Business case for ICME
- Effective V&V, Risk Mitigation and Tolerance of Models
- Adequate Standards, Data and Integration
- Integration among Product Design, Structures, Materials and Manufacturing
- Personnel with ICME Expertise
- Manage and Mitigate Uncertainty Quantification and Risk
- Long-term ICME Advancement



Cultural trend in materials modeling

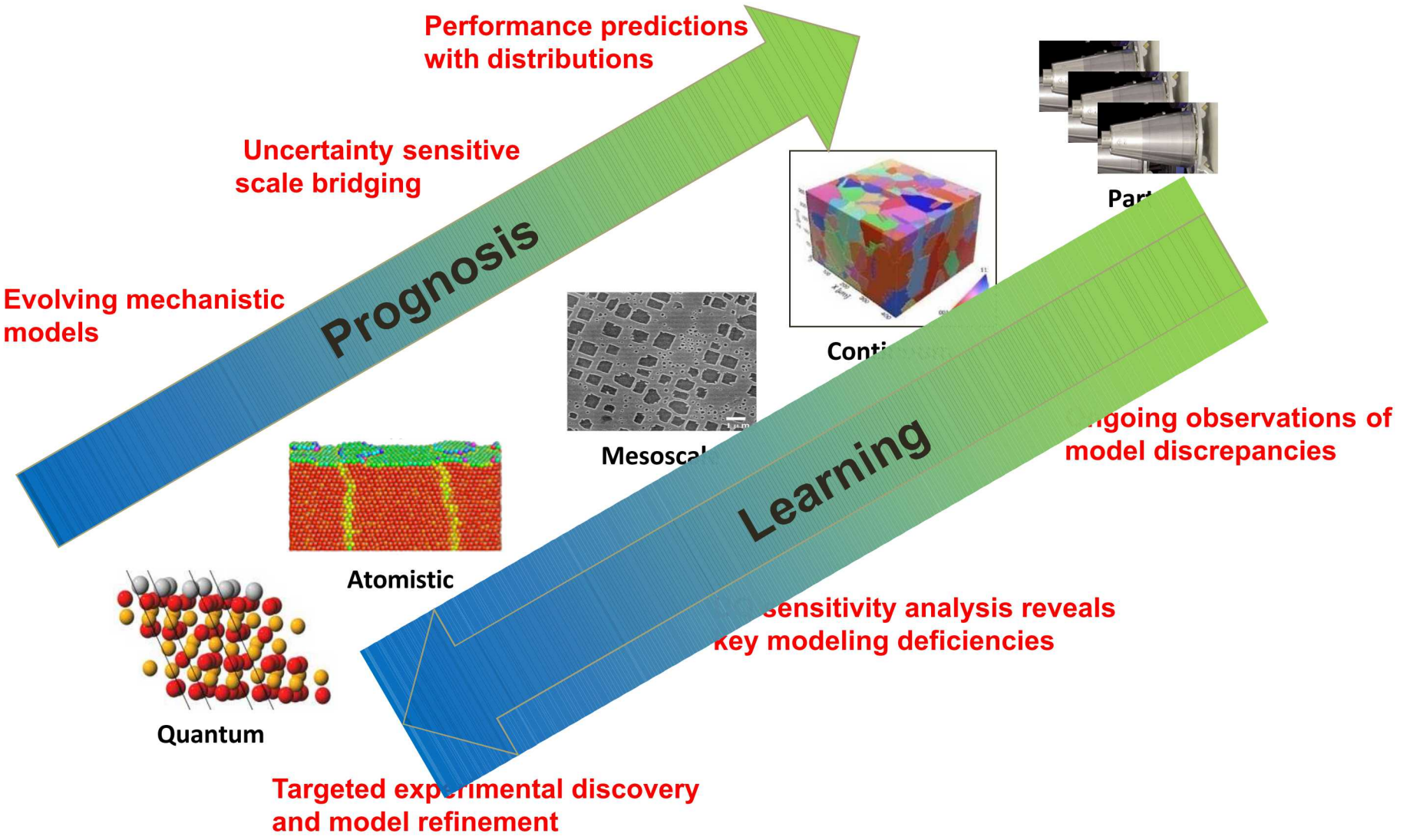
- Historically, materials modeling *at sub-continuum levels* often focused on qualitative understanding and description of trends
  - Use of simple model systems
  - Evaluate interpretations of experimental results
  - Results analyzed to reveal general behaviors/principles
- Increasingly, materials modeling is being used to provide quantitative input into materials design/evaluation
  - Emphasis on models that fit specific materials systems
  - Determination of quantities that are difficult/expensive/impossible to determine experimentally
  - Phenomena that cross multiple length/time scales
- *Development of error estimation/uncertainly quantification for sub-continuum methods is in its infancy*

WARNING! WARNING! WARNING!

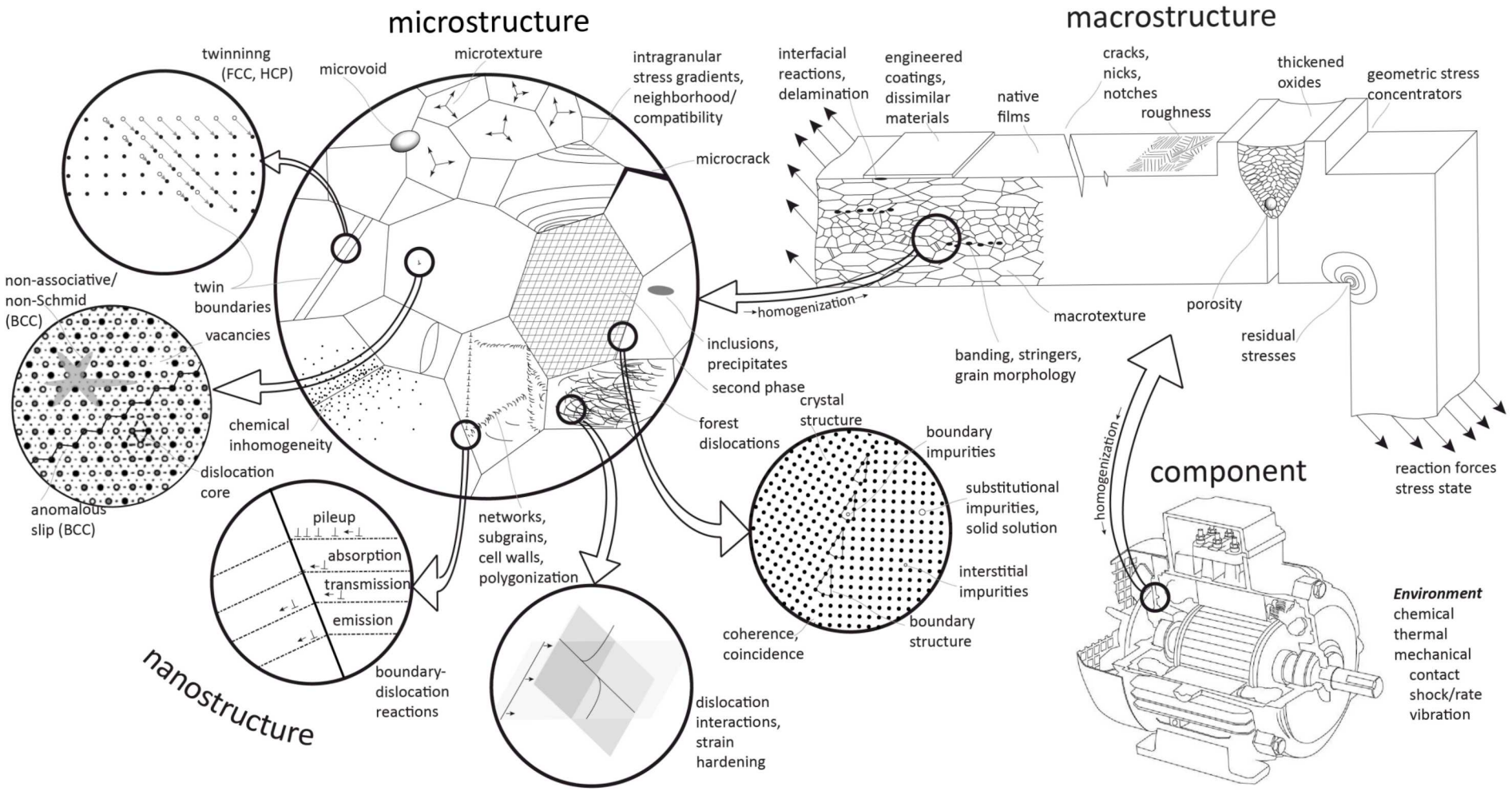
YAMMS*

*Yet Another Multiscale Modeling Slide

Multiscale Uncertainty propagation provides a platform for evolving knowledge



Multiscale Material Modeling is not a simple linear march up length scale



Multiple processes on separate and overlapping length/time scales

Aleatoric Uncertainty

- Latin: aleator = gambler
- Uncertainty due to *inherent randomness*
  - "How many heads for 100 coin flips"
- Outcomes can be described in terms of a probability distribution
  - Additional information can refine distribution, but *not* reduce uncertainty

- Example: Radiation cascade
  - Displacement damage from a neutron collision varies due to
    - Exact impact conditions
    - Thermal vibrations

Often, materials modeling ignores the inherent distribution of responses

- **estimate the mean behavior and move on**

Epistemic Uncertainty

- Greek: episteme = knowledge
- Uncertainty due to *lack of knowledge*
  - Incomplete or incorrect understanding/model/data
- Not describable with a probability distribution
  - Additional information can reduce this uncertainty

- Example: Radiation cascade
  - MD predictions limited incomplete knowledge of
    - Interatomic potentials
    - Deviations from Born-Oppenheimer approximation
    - Electron-phonon coupling

Majority of materials community knows this uncertainty exists but does not know how to treat it, so it is not explicitly incorporated

Example: Propagate variation across scales

- Goal: predict the variation of the critical resolved yield stress of a nanocrystalline Ni film due to fabrication induced variation of initial residual stress
  - Part of a program at Purdue to understand the reliability of a micro-electromechanical (MEMS) switch
  - Work supported by DOE through the ASC PSAAP (Predictive Science Academic Alliance Program)

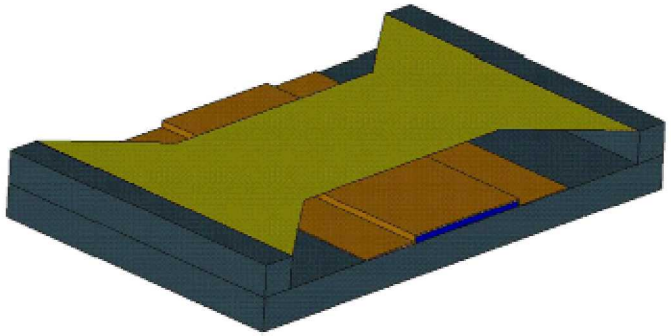
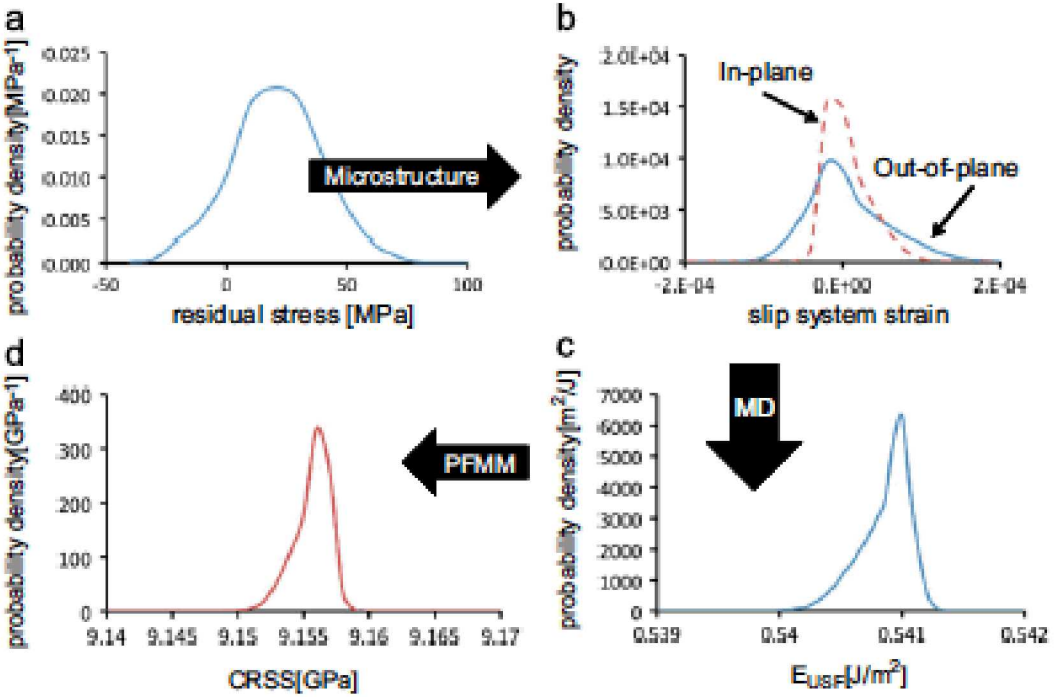


Fig. 1. Schematic representation of the RF MEMS device. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Koslowski and Strachan, Reliability Engineering and System Safety 96, 1161 (2011)

Propagation of initial residual stress variation to variation of yield stress

- Measured variation in the residual stress
- Consider 1000 model microstructures to determine range of strain on slip systems
- Use MD based response function to compute the variations in the unstable stacking fault energy
- Employ phase field dislocation dynamics model to compute variation of yield stress



Conclusion: Manufacturing based variation in residual stress leads to minor changes in yield stress

Only captures Aleatoric component!

Koslowski and Strachan, Reliability Engineering and System Safety 96, 1161 (2011)

Thoughts on path forward for UQ in materials modeling

- Ultimate goal:
  - Provide level of confidence in determination of system level materials performance
- Intermediate goal:
  - Use uncertainty quantification toolsets to identify
    - How best to pass information between scales
    - Where do we most need to improve our understanding
- Near-term goal
  - Estimate uncertainty in single-scale calculations
  - Initiate a cultural shift to include uncertainty estimation in the modeling process
- Biggest challenge
  - How to incorporate epistemic uncertainty (unknown unknowns)

Molecular Dynamics:

What could possibly go wrong?

- Deviations from Born-Oppenheimer Approximation
  - Highly dynamic events, charge states, …
- Inadequate Interatomic Potentials
  - Imperfect knowledge of Born-Oppenheimer surface
    - Errors in experimental data or *ab initio*
  - Potential form – model form error
  - Transferability or lack thereof
- Bifurcation of Behavior
  - Dominant mechanism may depend on subtle differences
- Quantum Mechanical Effects
  - Zero-point energies of light elements
  - Debye Temperature often above room temperature

- Limited time scales
  - High rates and high driving forces
  - Infrequent events
  - Sampling errors & metastable states
- Structural approximations
  - Where are the atoms, *really*?
  - Simplification of geometries
  - Boundary conditions
- Multi-component systems
  - Composition and structure coupled
  - Compositional variation - equilibrium or kinetic?
- Information extraction for higher-scale models
  - Millions of coordinates -> 'Physics'
  - Identification of dominant effects

Acquiring and testing potentials Status quo and Vision (1)

- All too common reality

Student A: "I need a potential for shock simulations of Ir"

Student B at conference: "I know a gal who has a potential file for Ir from that Foiles guy"

Student A: "Great, I'll e-mail her"

Student A spends three years doing MD simulations with an undocumented potential not designed to simulate shock

- Current 'good' process

Student: "I need a potential for shock simulations of Ir"

Advisor: "Check the potentials available from documented repositories like NIST, KIM, …"

Student: "I found a well-documented potential on KIM. It even gets the stable and unstable stacking faults right!"

Student spends three years doing MD simulations with a sensible potential, but is it right?

Acquiring and testing potentials Status quo and Vision (2)

- Current 'better' process

Student: "I need a potential for shock simulations of Ir"

Advisor: "Check the potentials available from documented repositories like NIST, KIM, …"

Student: "I found 2 well-documented potentials"

Student spends three years doing MD simulations with both potentials. Some features consistent, some very different

- *Vision* for best case

Student: "I need a potential for shock simulations of Ir"

Advisor: "Generate an ***ensemble of potentials*** that all reproduce key features"

Student spends three years doing MD simulations with the ensemble of potentials

- Able to identify ***robust features*** of shock simulations

Why bother simulating with an ensemble of potentials?

- Experience of simulating the same thing with multiple potentials for nominally the same material shows *two outcomes*
  - *Predictions are qualitatively similar but differ quantitatively*
    - Examples: same process but different activation energy, similar defect structures but different formation energies, …
    - **Question: What is the range of values consistent with the potential form and fitting database?**
  - *Predictions are qualitatively different*
    - *Examples: predict different orientation of interstitial dumbbell, motion mechanism of defect is qualitatively different, …*
    - **Question: What is the catalog of potential qualitative behaviors and what is the relative likelihood that a given behavior is correct consistent with the potential form and fitting database?**

Ensemble of potentials
Old idea whose time has come?

The concept of using Bayesian methods with an ensemble of potentials suggested over a decade ago

VOLUME 93, NUMBER 16 PHYSICAL REVIEW LETTERS week ending 15 OCTOBER 2004

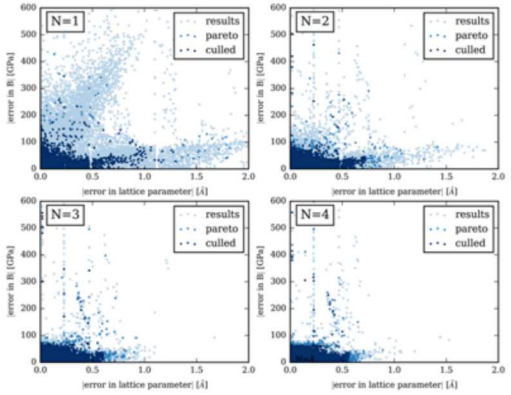
Bayesian Ensemble Approach to Error Estimation of Interatomic Potentials

Søren L. Frederiksen and Karsten W. Jacobsen
CAMP, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Kevin S. Brown and James P. Sethna
Laboratory of Atomic and Solid State Physics (LASSP), Clark Hall, Cornell University, Ithaca, New York 14853-2501, USA
(Received 18 December 2003; published 15 October 2004)

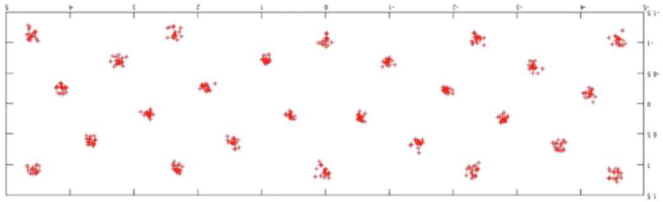
Using a Bayesian approach a general method is developed to assess error bars on predictions made by models fitted to data. The error bars are estimated from fluctuations in ensembles of models sampling the model-parameter space with a probability density set by the minimum cost. The method is applied to the development of interatomic potentials for molybdenum using various potential forms and databases based on atomic forces. The calculated error bars on elastic constants, gamma-surface energies, structural energies, and dislocation properties are shown to provide realistic estimates of the actual errors for the potentials.

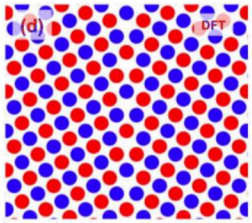
- Methods are being developed to enable automated development of ensembles
  - Example: Ragassa, et al, "Rational Design and Parametric Uncertainty Analysis of Classical Interatomic Potentials" - Tues AM, this meeting



Faceting of $\Sigma 5$ grain boundary in Fe: Do Calculations and Experiment Agree?

Structures of individual facets ***OK***





Equilibrium Facet Length ***WRONG***

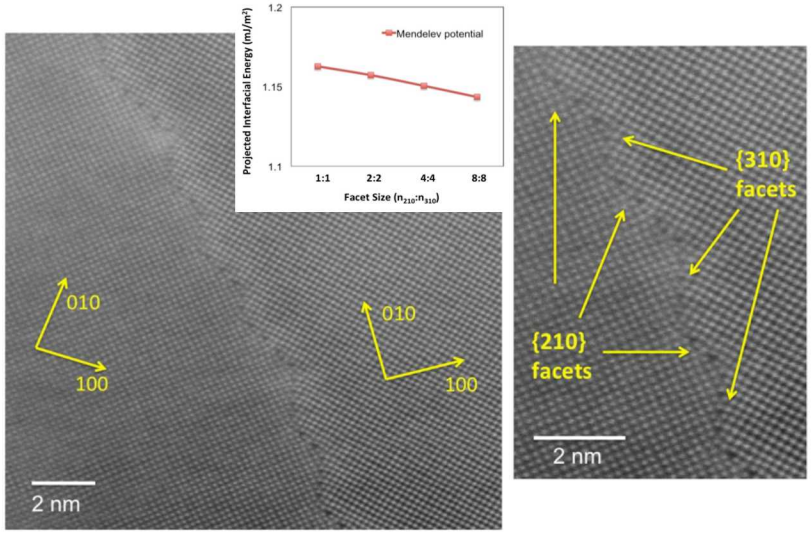
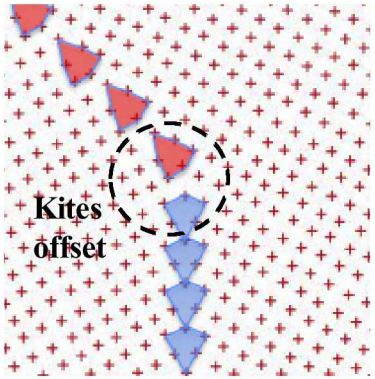


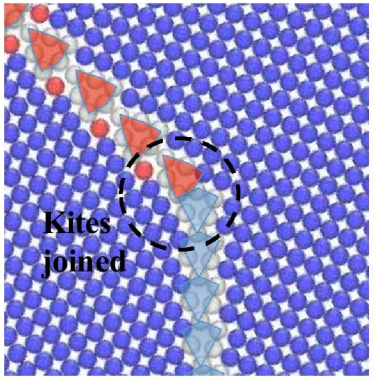
Figure 3

Junction Structure ***WRONG***

Experimental Junctions b=(1/5)(120) and (1/5)(310)



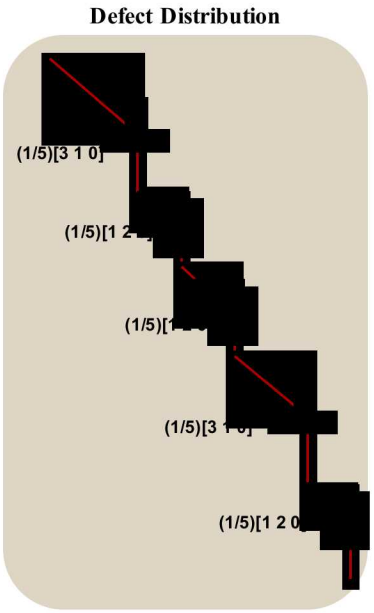
Relaxed Periodic Atomistic Structure

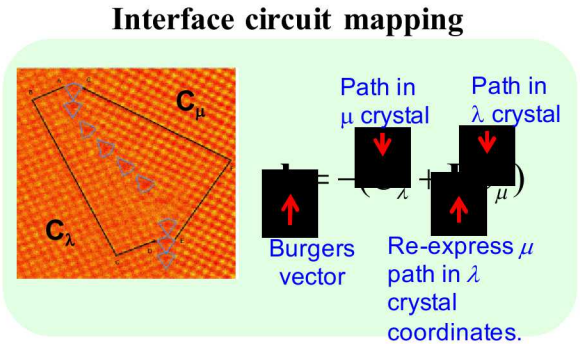


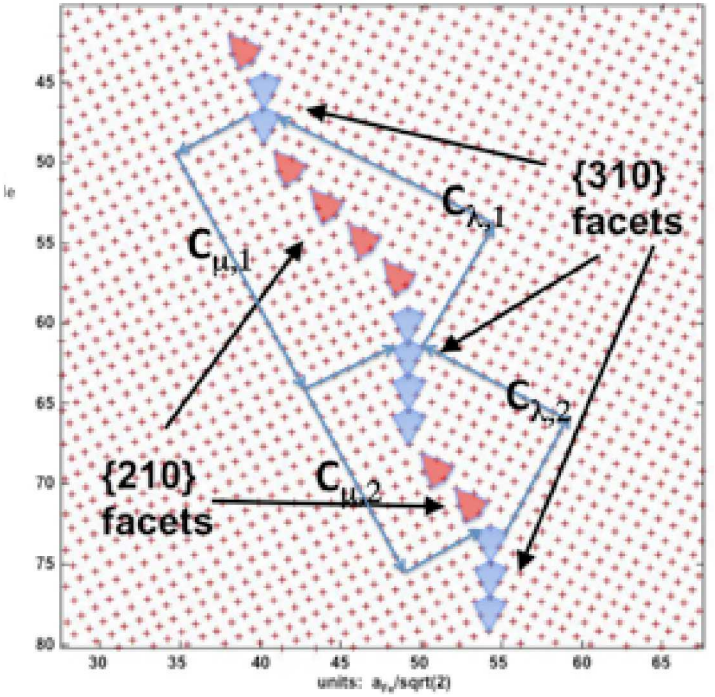
Medlin, Hattar, Zimmerman, Abdeljawad, Foiles, Acta Materialia 124, 383 (2017)

What went wrong!?!

- Simulations are Experiment are for ***DIFFERENT STRUCTURES***
  - Simulation: ***Ideal*** Σ5 misorientation
  - Experiment: ***Real-world*** Σ5 misorientation
    - $\Delta\Theta = 2.4 \pm 0.8$



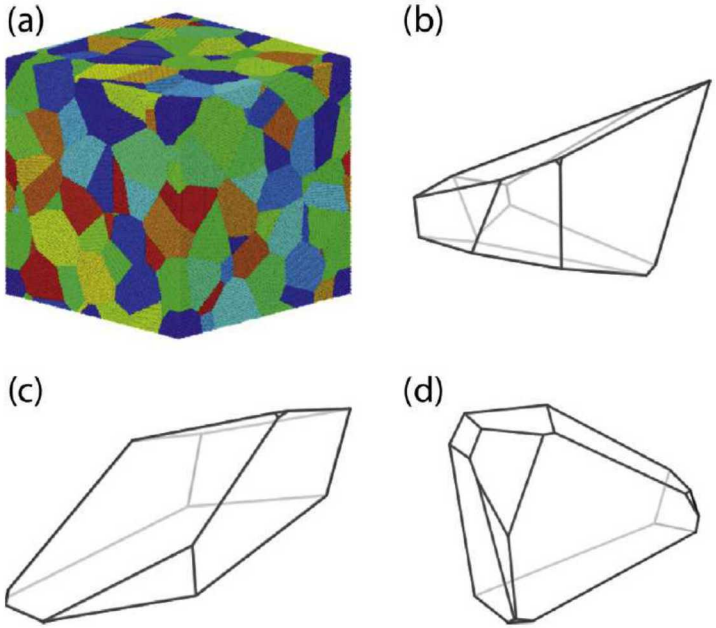


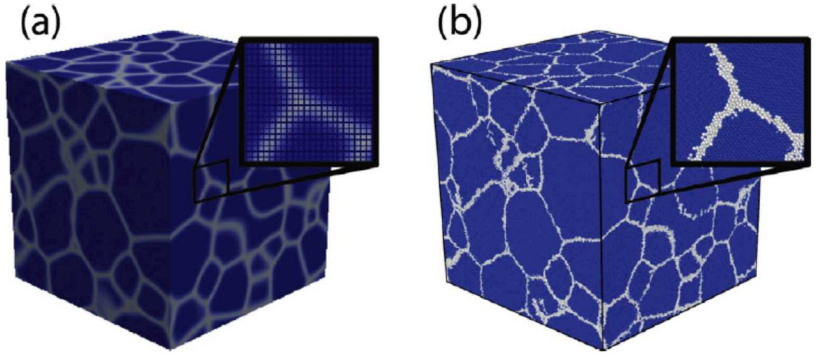


Interfacial dislocations required by Frank-Bilby equation

Medlin, Hattar, Zimmerman, Abdeljawad, Foiles, Acta Materialia 124, 383 (2017)

Do the initial conditions matter? Deformation of a nanocrystal



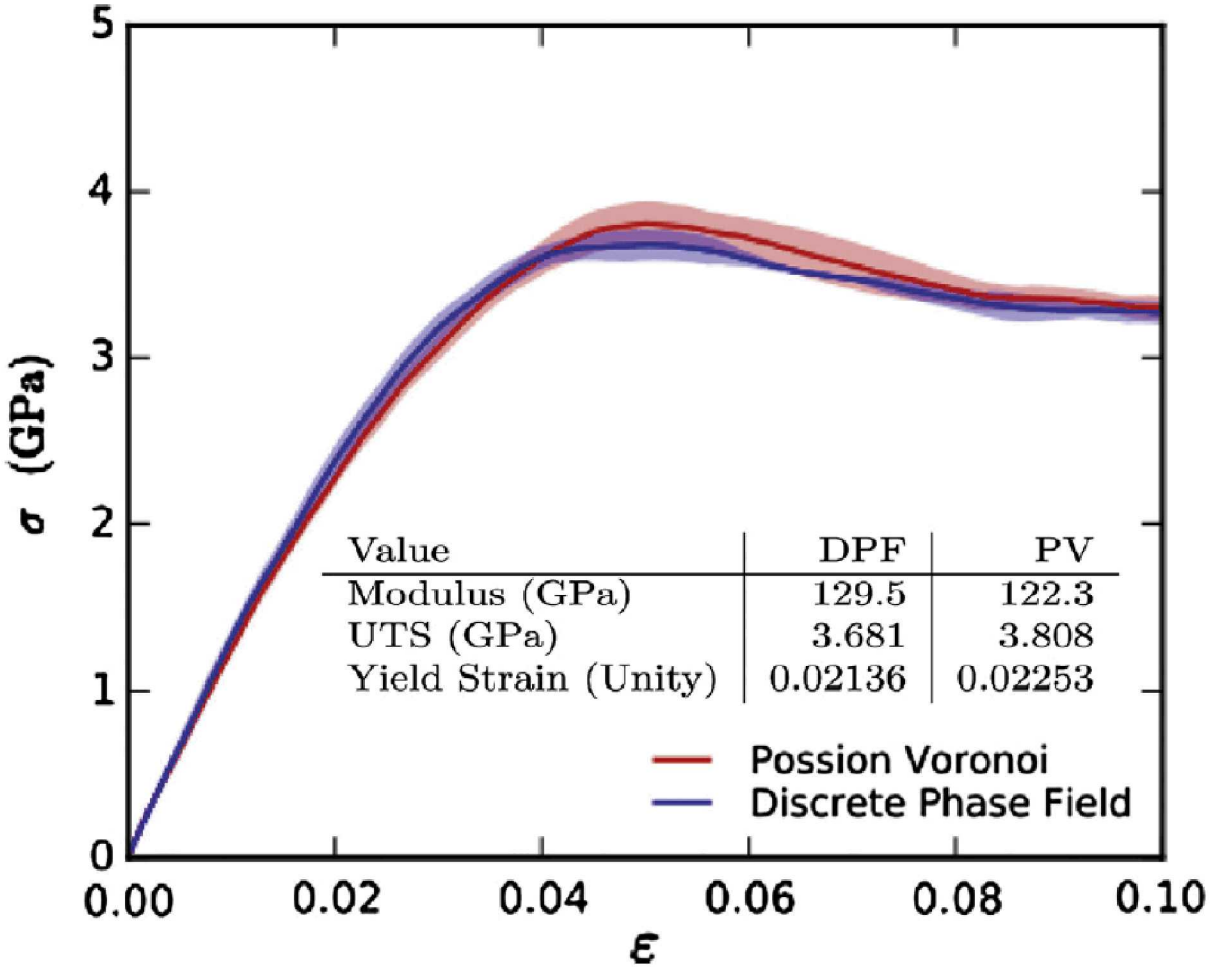


Poisson Voronoi Grain Construction
- Typical starting point for MD simulation
- Note unphysical grain properties

Discrete Phase Field Construction
- Initial grains based on isotropic phase field grain growth model

Gruber, Lim, Abdeljawad, Foiles, Tucker, Computational Materials Science 128, 29 (2017)

Initial structure has only modest effect on macroscopic response

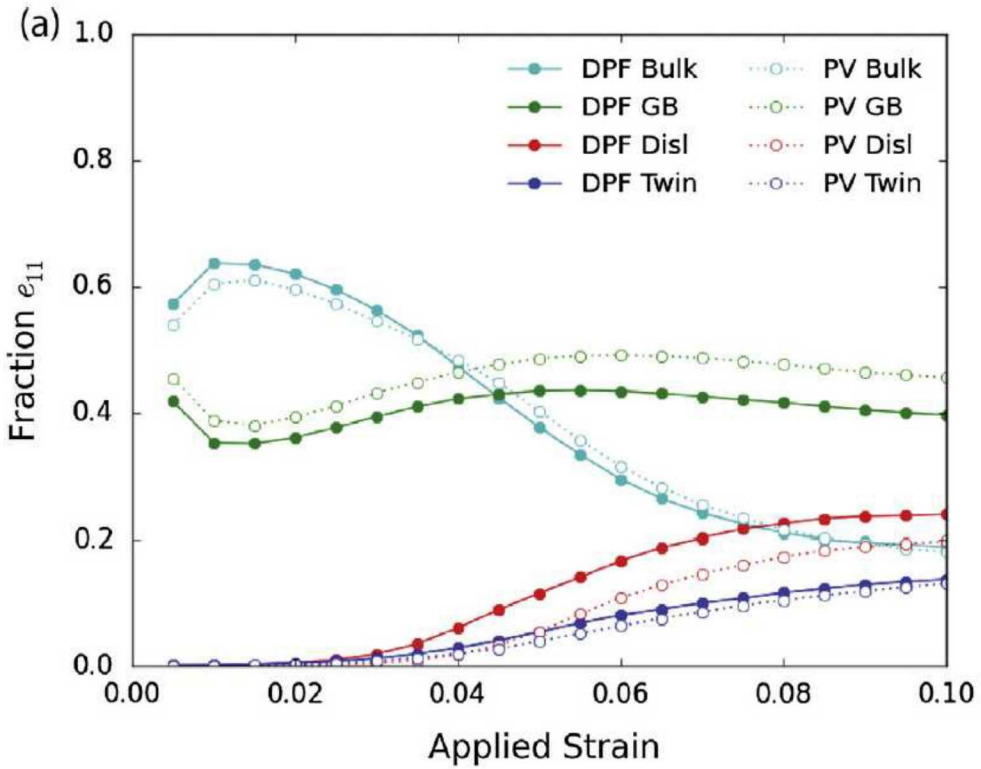


Value	DPF	PV
Modulus (GPa)	129.5	122.3
UTS (GPa)	3.681	3.808
Yield Strain (Unity)	0.02136	0.02253

Shading represents 1 standard deviation based on multiple runs

Gruber, Lim, Abdeljawad, Foiles, Tucker, Computational Materials Science 128, 29 (2017)

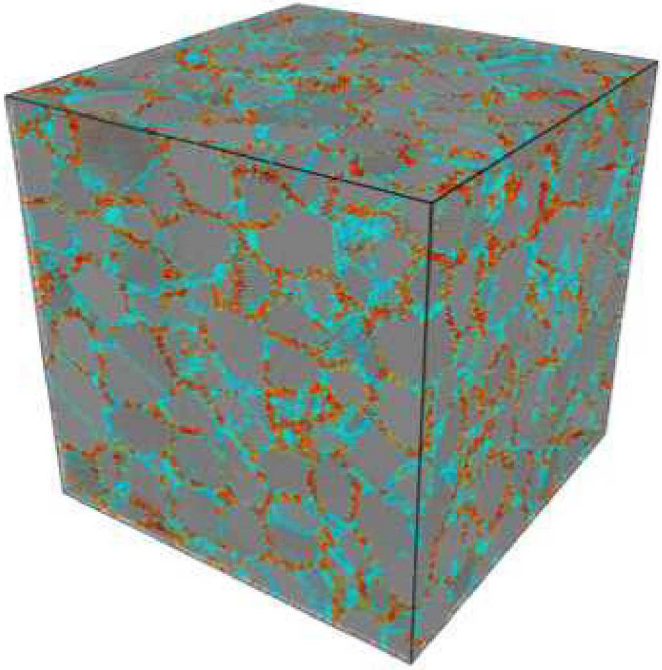
Initial structure does impact the mechanisms that operate

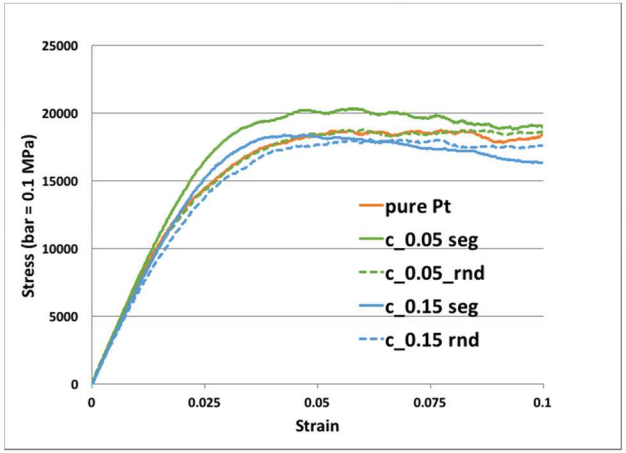


- Fraction of the deformation associated with different classes of atoms
  - Bulk, grain boundary, dislocation, twin boundary

Gruber, Lim, Abdeljawad, Foiles, Tucker, Computational Materials Science 128, 29 (2017)

Details of grain boundary segregation in a phase-separating alloy: Pt-Au





- The segregation of Au to grain boundaries is highly heterogeneous
  - Not what simple theories assume – does it matter?
  - If it does matter, how do we synthesize this for higher length scales
- This calculation assumed composition equilibrated to grain network
  - Experimental reality is often partial equilibration
  - Mechanical response depends on level of equilibration

Putting 'error bars' on MD simulations is a significant challenge

- Quantifying statistical uncertainty of results is, in principle, straight-forward, but often not done
  - Proper numerics, for example time steps
  - Multiple runs, convergence of averages
  - Convergence of system size
- How do we account for the 'uncontrolled approximation' of using classical potentials?
- Do the idealized simulation setups miss essential physics?
- For complex systems, how dependent are results on the assumptions about where the atoms are?
  - Especially problematic for multi-component systems

How do we represent all of this ambiguity/uncertainty when scaling up?

Concluding Remarks (1)

- Most studies of UQ in materials community focus on Aleatoric uncertainty
  - Need help with the more difficult problem of epistemic uncertainty
  - Improved experiments/models can convert epistemic uncertainty into aleatoric uncertainty
- Are current materials models sufficiently accurate to justify uncertainty quantification?
  - Maybe not, but need to start learning how to incorporate UQ so we are ready when the models are good enough
- Most materials scientists are not trained in the underlying mathematics and information theory
  - Need for changes in materials science curricula
  - This is identified in the plans for ICME and Materials Genome

Concluding Remarks (2)

- Is there are role for "expert opinion"?
  - Many engineering decisions made on basis of experience/judgment
- Existing community software/codes are not designed to consider UQ
  - Codes generally follow deterministic evolution
  - Need to incorporate techniques such as automatic differentiation and interval computing
- Materials Community at large is starting to think about UQ
  - Symposia at various technical society meetings such as TMS, MRS, …
  - Workshops have been held by various organization
  - UQ is still not a regular part of the sub-continuum materials modeling mindset
    - Example: Not typically required by journal reviewers