Multiscale modeling and simulation – developing solutions which link the atomistic, mesoscale, and engineering scales

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What is Materials Simulation?

- Chemical reactions – reaction energies and activation barriers for process simulation, prediction of thin film growth
- Morphology of blends, polymer mixtures
- Solubility, density, adhesion, permeation, crystallization
- Mechanical properties of composites, fluid dynamics
- E.g., morphology of blends, polymer mixtures
- E.g., solubility, density, adhesion, permeation, crystallization
- E.g., chemical reactions – reaction energies and activation barriers for process simulation, prediction of thin film growth
Problem and Modeling Approach:

- Long-wear soft contact lenses must transport $O_2$ to the evascular cornea, making high swelling in $H_2O$ desirable, but diffusion of lipids, glycoproteins etc. must then be curtailed by a suitable surface treatment.

- Molecular dynamics simulations, yields mean squared displacements, and hence diffusivities, for $O_2$ and $H_2O$ in aqueous solutions of poly(N-vinyl pyrrolidone) (PVP).

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As demonstrated by recent work by Toyota Laboratories, In Silico exploration of the alloy formulation space is a very powerful tool for materials optimization and design.

Analyzed alloys: $\text{Ti}_{1-m}X_m$

$X = \text{V, Nb, Ta, Mo, W}$

Composition can be easily varied and examined in terms of density, stability, elastic properties, etc.

Predicting Mechanical Properties for engineering design optimization

- Young's Modulus (E) is minimized at Ti\textsubscript{0.75} W\textsubscript{0.25}

![Graph showing the relationship between content of W in Ti (atomic %) and mechanical properties. The graph includes two lines: one for Young's Modulus (E) and another for Density. The E line is marked with the point where Young's Modulus is minimized at Ti\textsubscript{0.75} W\textsubscript{0.25}.]
• In cubic symmetry a low modulus requires small $C_{11} - C_{12}$

• Analysis of the results leads to a new low modulus alloy design rule:

$$C_{11} - C_{12} \approx 0 \text{ when } e/a=4.2$$

$e$ is the number of valence electrons/atom in the crystal unit cell

$a$ is the unit cell length (Å)
I-Beam Design: 4-D Optimization

- **Goal**
  - Minimize Weight
  - Minimize Deflection
  - Minimize Stress

- **Design Variables**
  - **Material**
  - Geometry Parameters
    - Beam Length
    - Beam Height
    - Flange Width
    - Flange Thickness
    - Web Thickness
3-D Optimization

Initial Design:
Deflection = 12.0
Mass = 3250000
Stress = 4.7

3D Optimized Design:
Deflection = 1.0 (reduced 92%)
Mass = 2200000 (reduced 32%)
Stress = 1.4 (reduced 70%)

4D Optimized Design:
Deflection = 1.4 (reduced 88%)
Mass = 1850000 (reduced 43%)
Stress = 1.3 (reduced 72%)

4-D Optimization provides added value over 3-D Optimization: 10% more weight savings
Multiscale modeling example: Morphology in hydrated perfluorosulfonic acid membranes

- Morphology of Nafion at the nanoscale?
- SAXS, SANS, WAXD:
  - Nanophase segregation into hydrophilic and hydrophobic domains,
  - Debate over the shape and structure of the ionic clusters: spherical, ellipsoid, or lamellar?
- Observations of the surface morphology via TEM and AFM
  - Three-phase model consisting of spherical water clusters surrounded by sulfonic acid interfaces.
  - Also observed the coalescence and growth of ionic clusters with an increasing water content using AFM.
- Use mesoscale modeling to compare and contrast with experimental observations

Results: Mesoscale simulation shows an arrangement of nearly spherical domains which exhibits a linear increase in the characteristic length as they swell and coalesce. No evidence of a lamellar ordered morphology.

Atomistic molecular dynamics simulations performed to predict the interaction energy of each pair of particle types.
Workflow of Materials Design through multiple length scales

**Molecular modeling**
- Components Parameters
  - Properties of components
  - Interactions

**Mesoscale modeling**
- Composite Parameters
  - Morphology
  - Volume fractions of components
  - Geometry of inclusions
  - Distribution/orientation of inclusions

**Overall Properties**
- Mechanical
- Elasticity, stiffness
- Swelling
- Thermal
- Expansion coefficients
- Conductivity
- Electrical
- Conductivity
- Dielectric constants
- Transport properties
- Diffusivity
- Permeability

One can also include the material as a design variable in the engineering design optimization.

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