Predictive Modeling on the Mechanical Performance of Structural Materials at Complex Environments

——— a tale of two solids by energy landscape-based atomistic modeling

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Compelling Need in Materials Performance Under Complex Environments far-from-Equilibrium

- high strain rates
- non-uniform thermo-mechanical environments
- extreme $T$, irradiation, chemistry
- non-equilibrium solidifications, large residue stresses and distortions
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Diagram:

- External stimuli
- Topological Defects
- Distribution:
  - Perfect lattice
  - Defect states

- Wide spectrum of defects identification?
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Predictive Design of Structural Materials with Desired Properties

Integrated Methodology based on Potential Energy Landscape (PEL)

Identify and Optimize pathways in PEL and processing space
Multi-scale modeling scheme: current methods & challenges

Dislocation-mediated microstructural evolution is an immensely complicated phenomenon involving multiple scales over many orders of magnitude.

Traditional MD simulations cannot be validated by in situ TEM experiments.

**Time Scale**

- **10^{-12} s**
- **10^{-6} s**
- **10^{0} s**
- **10^{6} s**

**Length Scale**

- **nm**
- **µm**
- **mm**

**Atomic-scale**

- e.g. first principle models, molecular dynamics (MD)

**Meso-scale**

- e.g. dislocation dynamics (DD), visco-plastic self-consistent (VPSC)

**Macro-scale**

- e.g. finite element method (FEM)

**Traditional MD simulations**

- Condition: 2x10^7 s^{-1}, 100 K
- Outcome: obstacle remains intact

**in situ TEM**

- Condition: 10^{-2} s^{-1}, 300 K
- Outcome: obstacle is removed by dislocation
Multi-scale modeling scheme: current methods & challenges

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**S1: Dislocation-Mediated Mechanics in Crystalline Materials**
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- Employ PEL-based techniques to provide reliable mechanisms and parameters to higher-level models such as DD, VPSC, and FEM, to enhance the capability of predictive design.

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**Proposed new modeling roadmap to capture the fundamental processes at realistic timescale**

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**Challenges in traditional scheme**

- **Atomic-scale**
  - e.g. first principle models, molecular dynamics (MD)

- **PEL-based atomistic modeling at long timescale**

**Employ PEL-based techniques to provide reliable mechanisms and parameters to higher-level models such as DD, VPSC, and FEM, to enhance the capability of predictive design.**
S2: Mechanics of Disordered Alloys (e.g. Metallic Glasses)

• Processing history dependence

• Testing condition dependence

Effective PEL-Property Relationship


\[
\frac{dE_{IS}}{dt} = \nu \cdot \exp\left(-\frac{E_A}{k_B T}\right) \cdot [E_A - E_R] + \mathcal{R}_{ext}(\mathcal{R}, \phi)
\]

coupling with external stimuli
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What's Next?