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Dynamics of Cottrell Atmospheres and Dislocations

PRESENTED BY

Ethan Epperly and Ryan Sills

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Outline

- Introduction: Dislocations, Solutes, and Dynamic Strain Aging
- Mathematical Model and Computational Considerations
- Results and Comparison with Existing Models

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- **Introduction: Dislocations, Solutes, and Dynamic Strain Aging**
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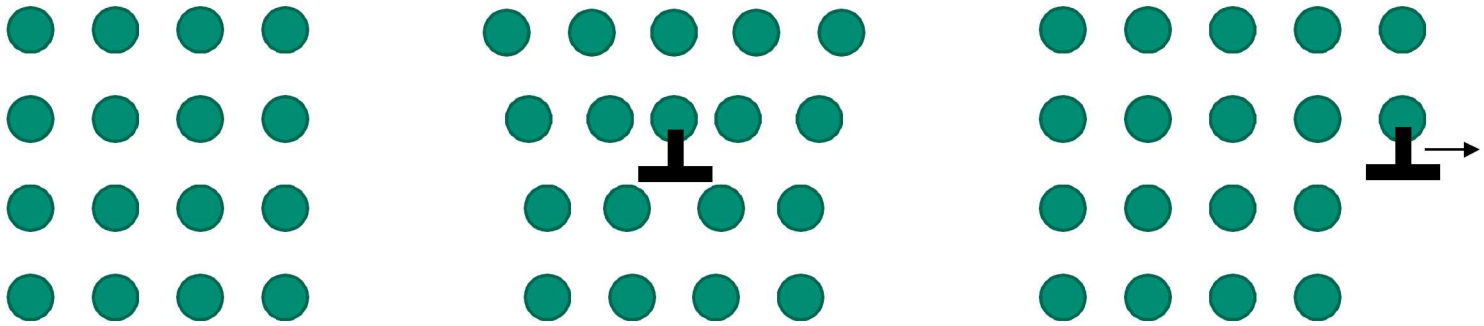
Dislocations, the Mechanism for Plastic Deformation

- At the atomic level, metals are **crystals**—their atoms exist in regular, repeating patterns. This pattern is the "crystal lattice".
- **Dislocations** are local distortions in the crystal lattice, in which an additional half-plane of atoms have been introduced.
- When a metal is subjected to loading, its dislocations move, creating permanent deformations in the metal which persist after loading is removed. This deformation is called **plastic strain**.



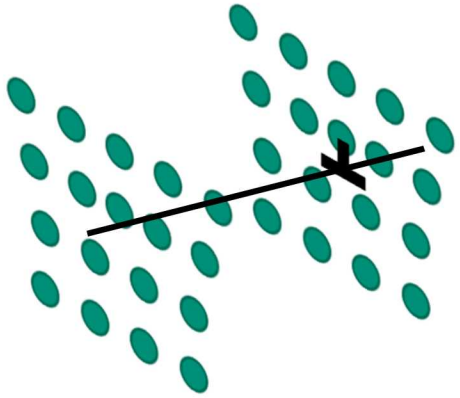
Perfect Crystal

Crystal with Dislocation

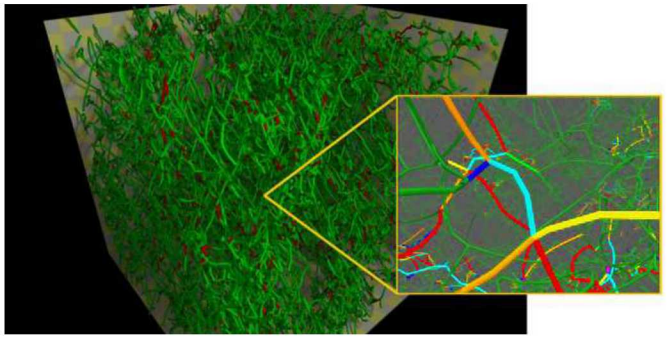
Motion of Dislocation Creates Plastic Strain

Dislocations, the Mechanism for Plastic Deformation

- Dislocations are line objects, and can curve and bend to form intricate structures.
- The strength of metals is determined by the collective action of ensembles of dislocations and their interactions with other defects.
- Understanding the behavior of dislocations through theory, experiment, and simulation has been an important area of research in materials science.



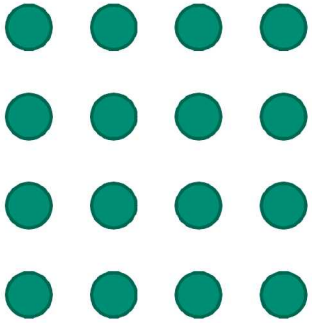
In 3D, Dislocations are Line Objects



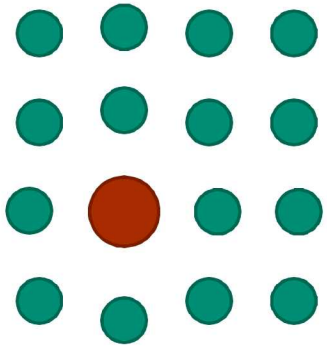
3D Discrete Dislocation Dynamics Simulations (LLNL)

Solutes, Single Atoms Different from the Surrounding Lattice

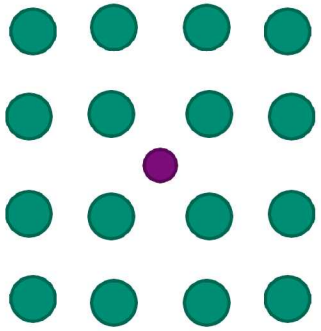
- **Solutes** are single atoms which differ from the surrounding lattice. Two types:
  - Substitutional Solutes: an atom in the lattice has been replaced (e.g. alloys like AlMg)
  - Interstitial Solutes: an atom which lies in between lattice sites (e.g. carbon in steel)
- Solutes expand (or contract) the surrounding lattice, causing a local distortion in the lattice.
- Solutes strengthen a metal by restricting the motion of dislocations.



Perfect Crystal



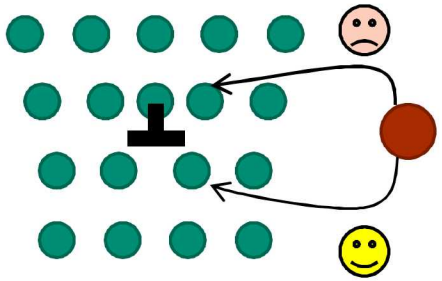
Crystal with Dislocation



Motion of Dislocation Creates Plastic Strain

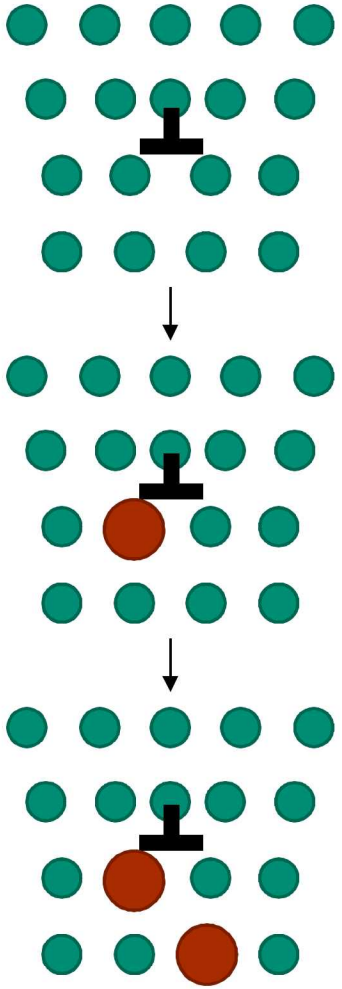
Dynamic Strain Aging

- Below the dislocation, atoms are more spread out, leading bulky solute atoms to congregate underneath the dislocations forming **Cottrell atmospheres**.



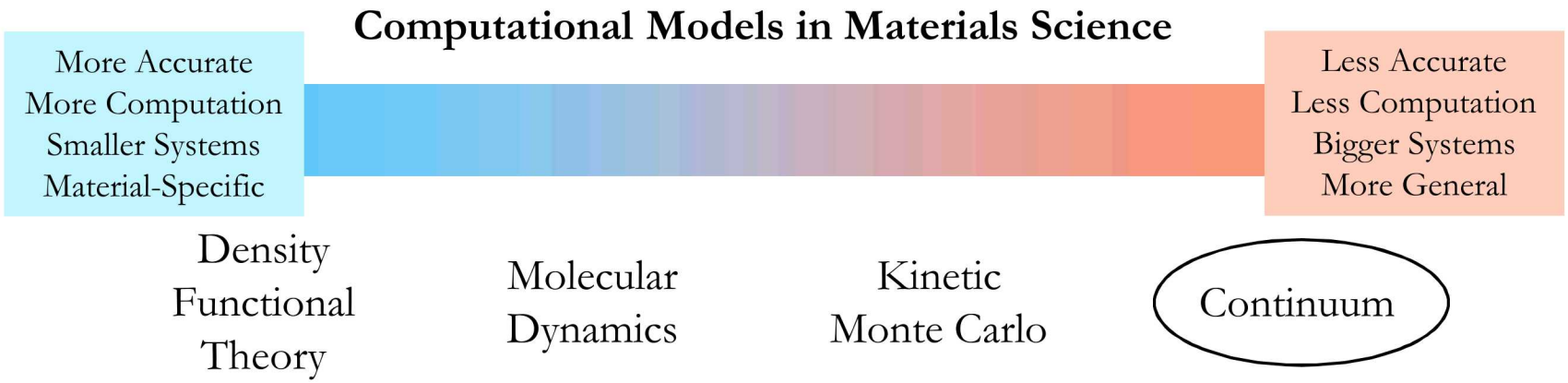
- These atmospheres restrict dislocation motion, holding them in place.
- This causes an increase in strength as dislocations arrested by their solute atmospheres are unable to move, and thus unable to produce plastic strain.
- This process is called **dynamic strain aging (DSA)**
  - "Dynamic" because solute atoms must *move* to form these atmospheres. This motion takes time, making DSA dependent on the amount of time solutes have to move.

Dynamic Strain Aging



The Problem

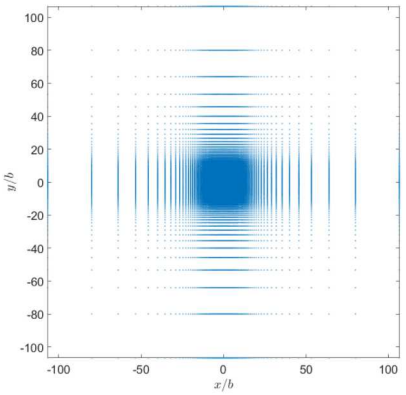
- Many theoretical/computational models of DSA exist in the literature.
  - Still a gap between predictions from theory and results of experiment.
- Two questions central to understanding DSA.
  1. How quickly do solute atmospheres form?
  2. How strongly do they restrict dislocation motion?
- We seek to understand solute-dislocations and DSA via a continuum model.
  - Continuum model gives a general understanding of many materials at the cost of perfect accuracy for any specific material.



Outline

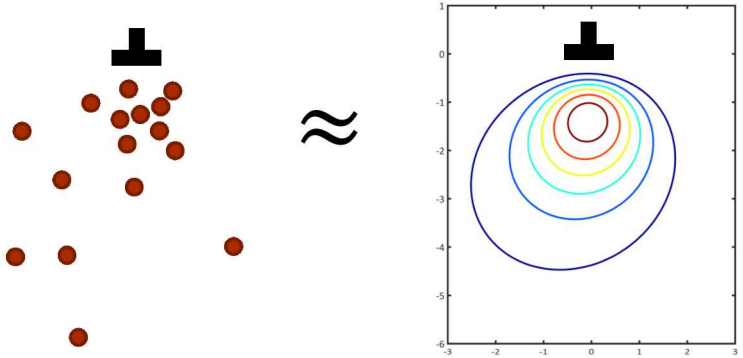
- Introduction: Dislocations, Solutes, and Dynamic Strain Aging
- **Mathematical Model and Computational Considerations**
- Results and Comparison with Existing Models

$$\frac{\partial \chi(t,\boldsymbol{x})}{\partial t} = \nabla \cdot \left(\frac{D}{k_B T} \chi(t,\boldsymbol{x}) \nabla \mu(\boldsymbol{x}) \right)$$



The Mathematical Model

- Solute distribution is modelled as a continuum concentration field $\chi(t, \boldsymbol{x})$. (a)
  - χ is the fraction of solute sites filled.
- Motion of solutes is governed by the diffusion equation (b)
- Chemical potential (c) contains enthalpic contribution $p\Delta V$ due to solute-dislocation interaction and entropic contribution $k_\mathrm{B}T \ln \chi/(1-\chi)$
- Solute concentration considered in a 2D plane perpendicular to dislocation line.



Continuum Approximation (a)

Diffusivity

Chemical Potential

$$\frac{\partial \chi(t,\boldsymbol{x})}{\partial t} = \nabla \cdot \left(\frac{D}{k_B T} \chi(t,\boldsymbol{x}) \nabla \mu(\boldsymbol{x}) \right)$$

Temperature

Diffusion Equation (b)

Solute Misfit Volume

$$\mu(\boldsymbol{x}) = p(\boldsymbol{x})\Delta V + k_\mathrm{B}T \ln\left(\frac{\chi}{1-\chi}\right)$$

Dislocation Pressure Field

Chemical Potential (c)

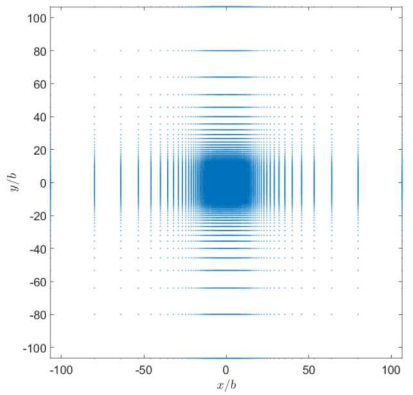
Computational and Numerical Considerations

- The diffusion equation (b) is a second-order, nonlinear, parabolic partial differential equation.
- Discretized using a second-order accurate finite difference scheme on a nonuniform mesh (d)
  - Mesh has higher density near dislocation core, where higher solute gradients are more difficult and more important to resolve.
- Time stepping is performed using the implicit trapezoidal scheme.
  - Time step sizes is controlled adaptively to bound the error per step.
- A sparse direct solver, UMFPACK, is used to solve sparse linear systems.
- Implemented in a C++ code.

Diffusion Equation (b)

$$\frac{\partial \chi(t,\boldsymbol{x})}{\partial t} = \nabla \cdot \left(\frac{D}{k_B T} \chi(t,\boldsymbol{x}) \nabla \mu(\boldsymbol{x}) \right)$$

Mesh (d)



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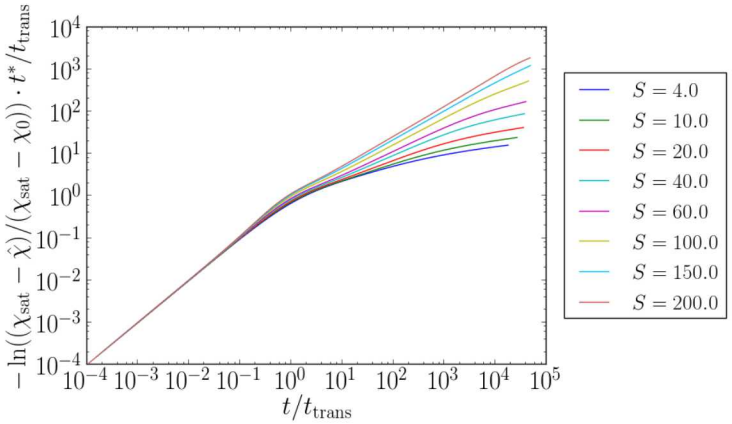
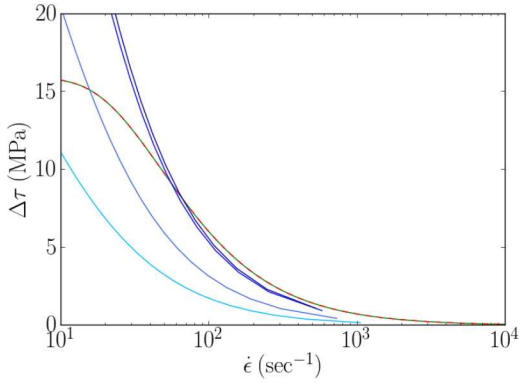
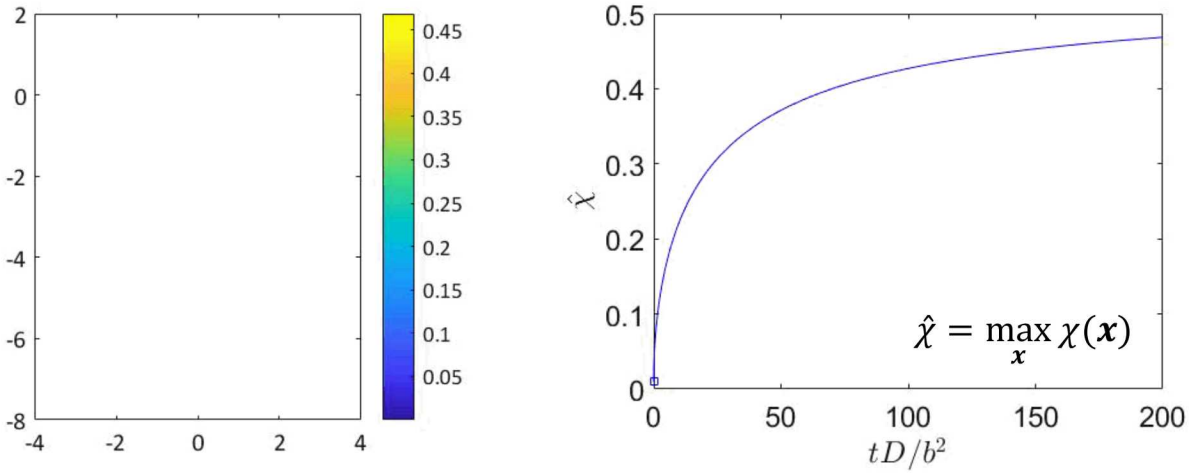




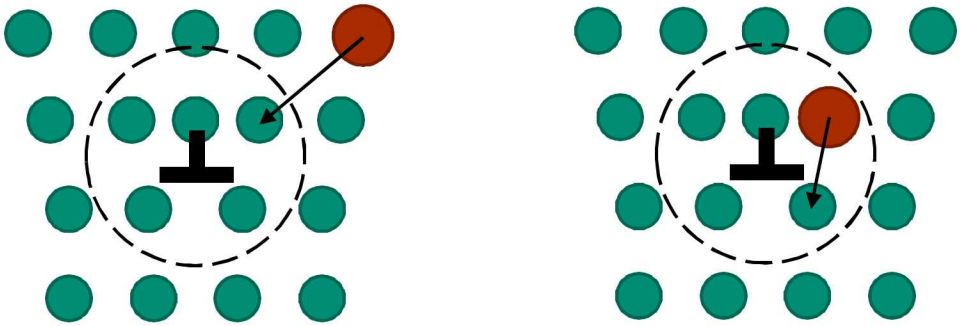
Condensation



Computational simulation of atmosphere formation allows us to predict the *rate of formation* and *strength* of atmospheres

Competing Models

- Two existing models for atmosphere formation:
  1. **Classical Continuum** (Cottrell and Bilby 1949; Louat 1981): atmosphere condensation results from solute atoms from outside the dislocation core entering the core—so called "bulk diffusion".
  2. **Cross-Core** (Curtin, Olmstead, and Hector 2006): atmosphere condensation results from solute atoms crossing from one side of the dislocation to the other.
- Both diffusion types are important: can we capture both?

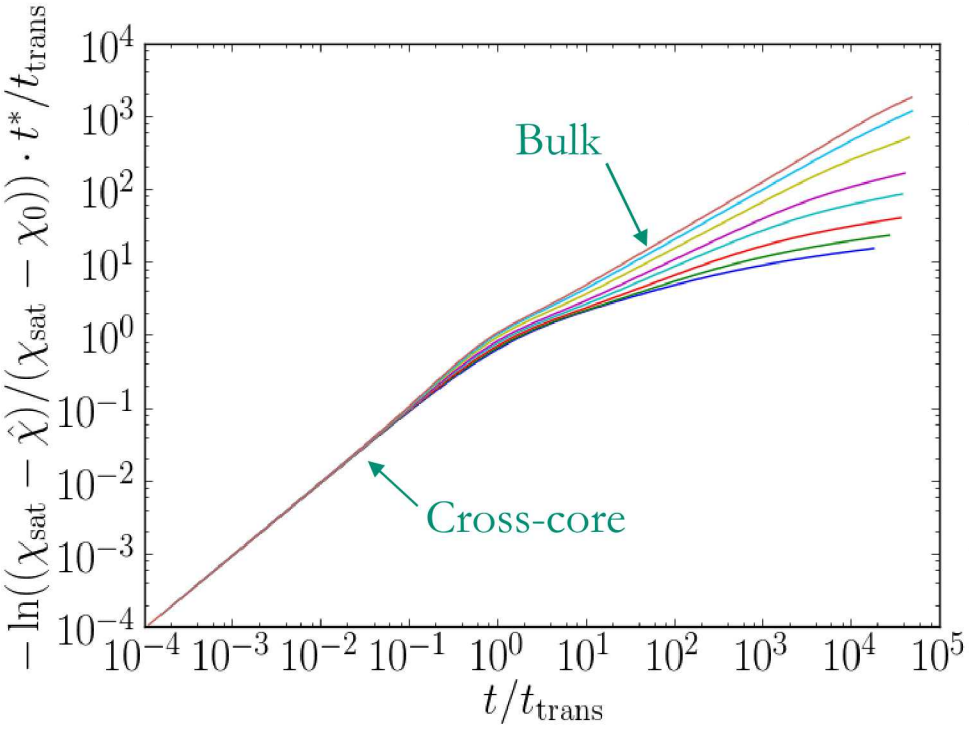


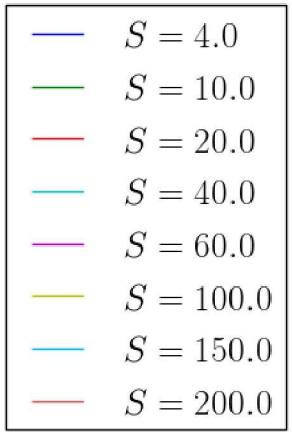
Classical Continuum

Cross-core

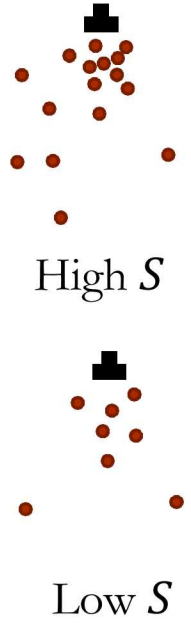
Bulk and Cross-Core Diffusion

- Our continuum model captures both the cross-core and bulk diffusion types.
- Cross-core diffusion was believed to be beyond the scope of the continuum model





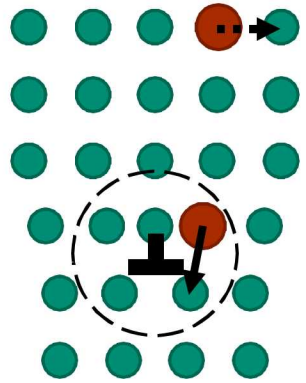
S = atmosphere strength



- Our accurate continuum computations show the classical continuum theory is based on bad assumptions and must be corrected.

Elevated Core Diffusivity

- It was observed by Picu and Zhang (2004) that the diffusivity D of solutes in the core is much higher than in the bulk. (e)
- This can be incorporated in our model by using a diffusivity function (f), rather than a diffusivity constant.



Elevated Core Diffusivity (e)

Slow

Fast

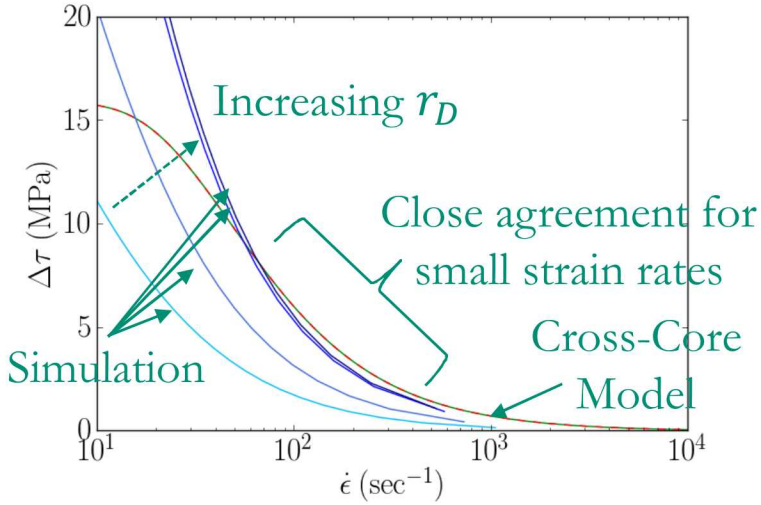
"Diffusivity Radius"

Diffusion Function (f)

$$D(\boldsymbol{x}) = D_{\mathrm{b}} + (D_{\mathrm{c}} - D_{\mathrm{b}})e^{-\|\boldsymbol{x}\|^2/2r_D^2}$$

Bulk Diffusivity

Core Diffusivity



Strengthening versus Strain Rate (g)

- By choosing a sufficiently large diffusivity radius, we are able to get reasonably close agreement between simulation (blues) and cross-core model (green). See (g)

Comparison of Models

- Two diffusion types for atmosphere formation:
  1. **Bulk**
  2. **Cross-Core**
- ~~Both diffusion types are important: can we capture both?~~ Are both diffusion types important?

	Diffusion Types		Experimental Agreement	
Model	**Bulk**	**Core**	**Timescale**	**Strength**
Classical	✓	✗	✗	✗
Cross-Core	✗	✓	✓	✓
Us	✓	✓	✓	✗

- Bulk diffusion occurs in simulations of all types (molecular dynamics, kinetic Monte Carlo, continuum), yet the best agreement with experiments is achieved by ignoring it.
- The Puzzle: How can we develop of a theoretical model of DSA which agrees with both simulation and experiment which includes bulk and core diffusion?

Conclusions

- Summary
  - Developed a continuum model of dislocation-solute interactions
  - Model is able to accurately capture both cross-core and bulk diffusion types
  - By accounting for the elevated core diffusivity, the model correctly predicts the time scale of DSA effects, but still over-predicts the strengthening
- Draft manuscript under preparation
- Acknowledgements
  - Ryan Sills, my mentor at Sandia and collaborator on this work
  - Jonathan Hu, who mentored me on a different project this summer at Sandia
  - Sandia's Student Intern Programs and my manager, Sean Stieper, who have both been immensely helpful to me performing this work year-round
- References

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