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Dynamics of Cottrell Atmospheres and Dislocations

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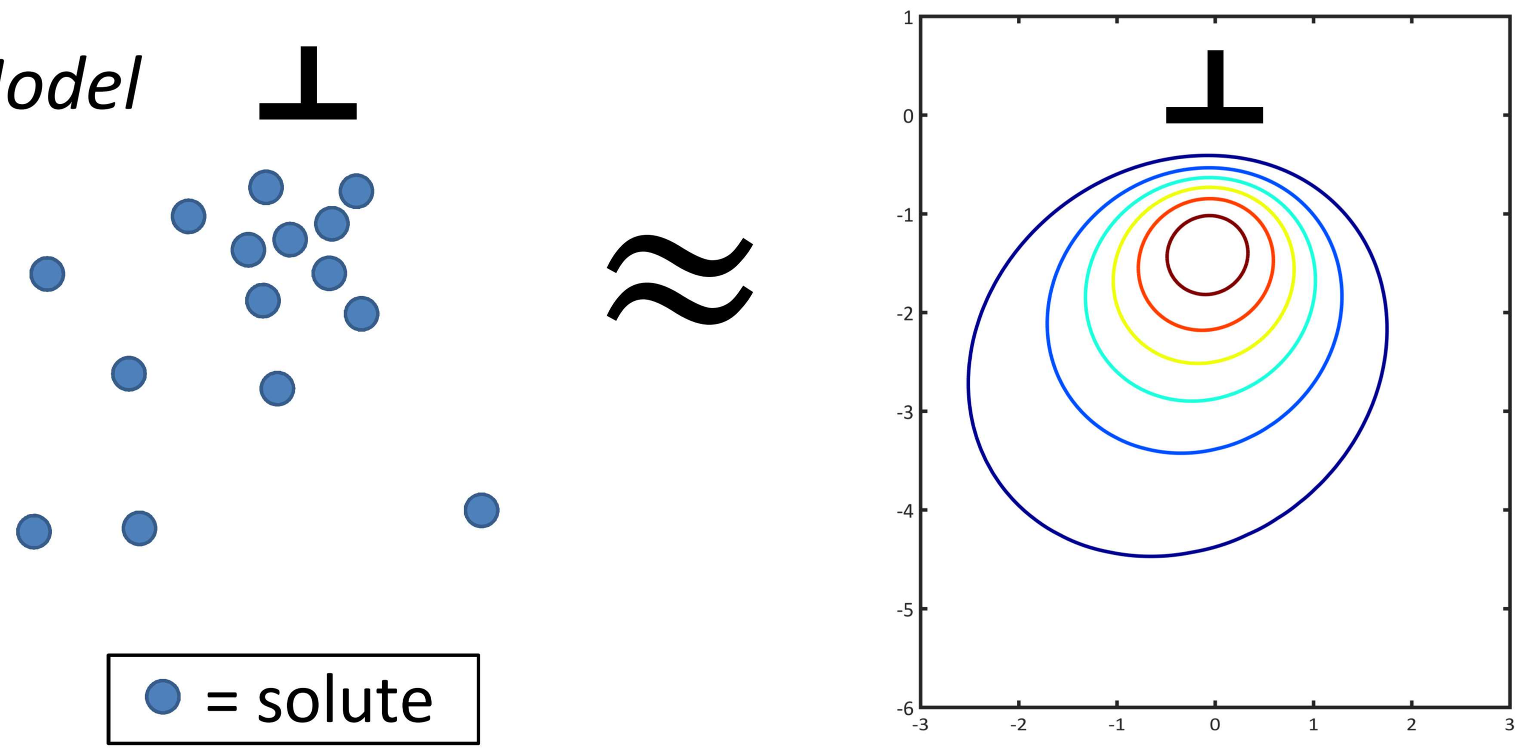
Introduction

Many mechanical properties of metals are the result of the motion of microscale defects called dislocations. In particular, the interaction of dislocations with solute atoms leads to *dynamic strain aging* (DSA), a phenomena in which material strength depends on the amount of time solutes have to travel to pinned dislocations. At equilibrium, solute atoms congregate beneath the dislocation lines, forming so-called *Cottrell atmospheres.*[1] Understanding the properties of alloys requires knowing how quickly these atmospheres form and the amount of solute drag the atmospheres exert on the dislocations.

Model



In our model, solute atoms are described by a continuous concentration field $c(\boldsymbol{x})$. The concentration field evolves in time according to the diffusion equation.[2]

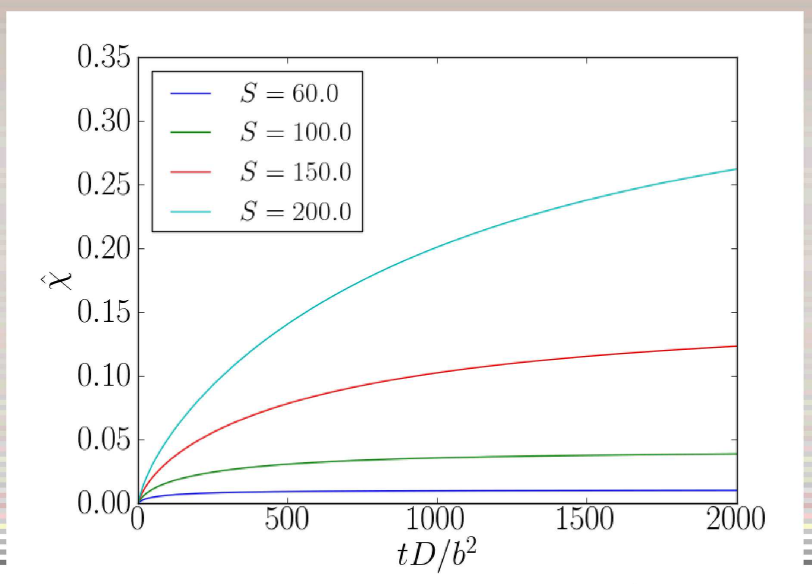
Diffusion Equation for Solutes

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

D: Diffusion constant; T: Temperature; μ: Chemical potential; $\boldsymbol{v}(t)$: Velocity of dislocation

Rate of Atmosphere Formation

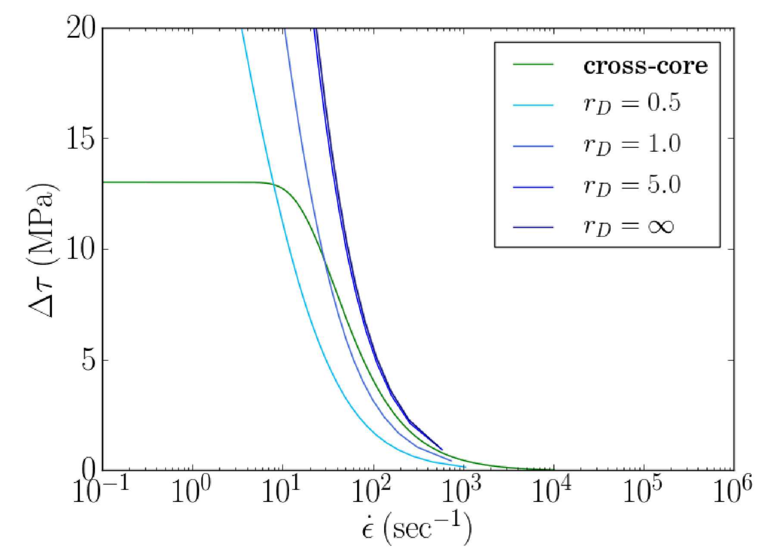
Simulations of atmosphere formation allow for accurate predictions of the timescale of dislocation-solute interactions. Our model agrees with the cross-core model[3] in predicting faster rates of formation than classical theories.



Atmosphere concentration $\hat{\chi}$ versus time for different atmosphere strengths S

Predicting Dynamic Strain Aging

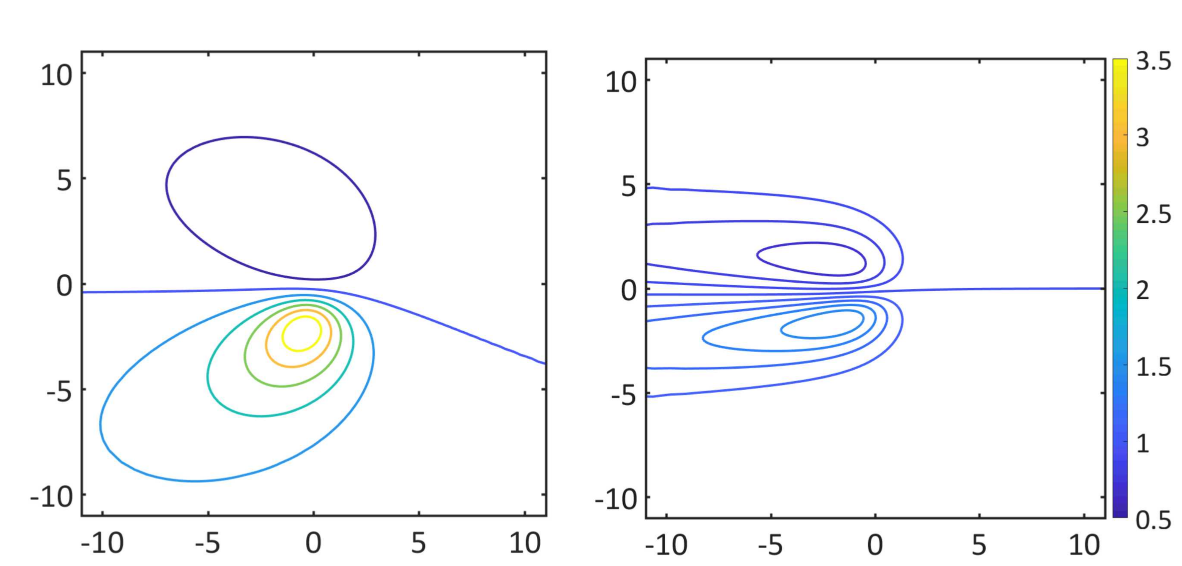
Our model can be used to predict the increase in material strength do to dynamic strain aging. Our calculations agree with existing literature models for high strain rates.



Predictions of dynamic strain aging for different values of the tunable "diffusivity radius" parameter r_D

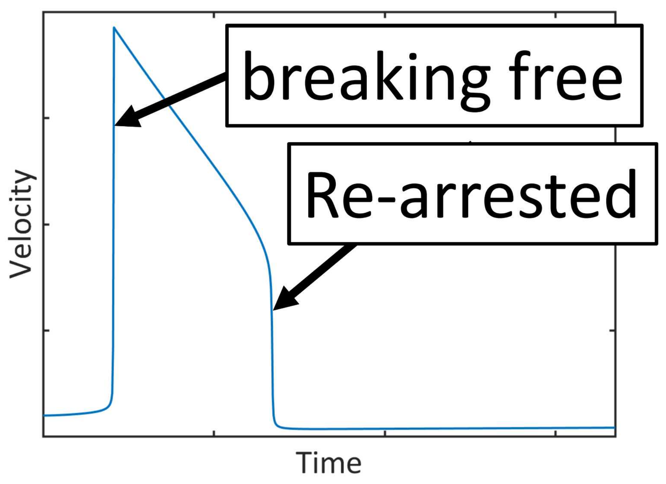
Mobile Dislocations

Our model also allows for the study of the interactions of mobile dislocations with their atmospheres. In particular, we are able to simulate dislocations breaking away from and being re-arrested by their atmospheres



arrested

broken free



Dislocation velocity jumps after breaking free of atmosphere and plummets after being rearrested.

Future Work

- Extending model to explain DSA at low strain rates
- More detailed simulations of effect of dislocation mobility and dislocation networks on DSA

References

[1] A.H. Cottrell and B.A. Bilby. Proc. Phys. Soc. A 62 (1949).

[2] R. B. Sills and W. Cai. Phil. Mag. 96 (2016).

[3] W. A. Curtin, D.L. Olmsted, & L.G. Hector. Nature Materials 5, 875 - 880 (2006)

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