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Dislocation-Solute Interactions:
Implications for Solute Embrittlement and Dynamic Strain Aging

Ryan B. Sills and Ethan N. Epperly

Sandia National Laboratories, Livermore, CA USA

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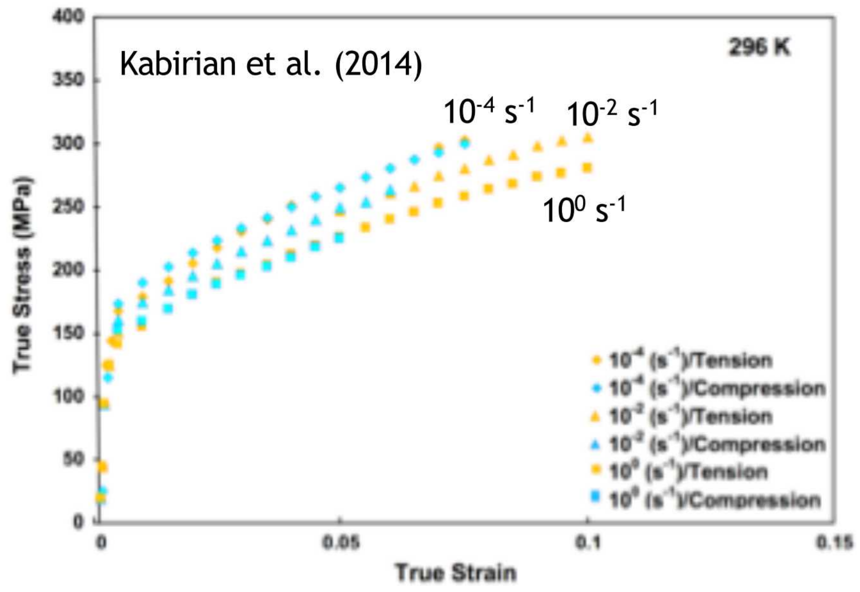
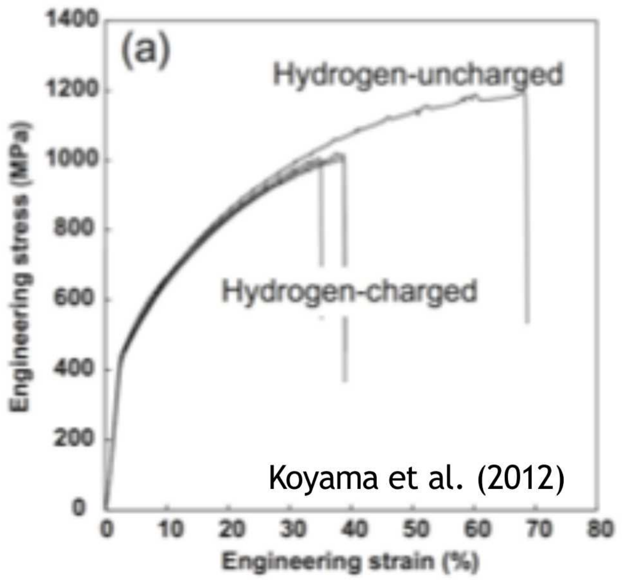
Solute embrittlement and dynamic strain aging

Solid solution systems are known to exhibit poor mechanical performance under certain temperature and strain rate conditions

A fundamental understanding is necessary to produce robust materials



Negative strain rate sensitivity in 5182 aluminum



Hydrogen embrittlement in an Fe-Mn-C TWIP steel

Believed to be governed by transient interactions between dislocations and mobile solutes

Goal of this research is to quantify those interactions and aid development of theories and material models

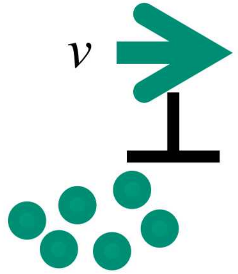
What governs the basic physics of dislocation-solute interactions?

Solutes diffuse towards and interact with dislocations

Two step process:

1. Atmosphere formation
2. Solute drag

Dynamic strain aging (DSA)



"Cottrell atmosphere"

Initial uniform background χ_0 diffuses towards dislocation leading to peak

We have been re-examining the continuum solution:

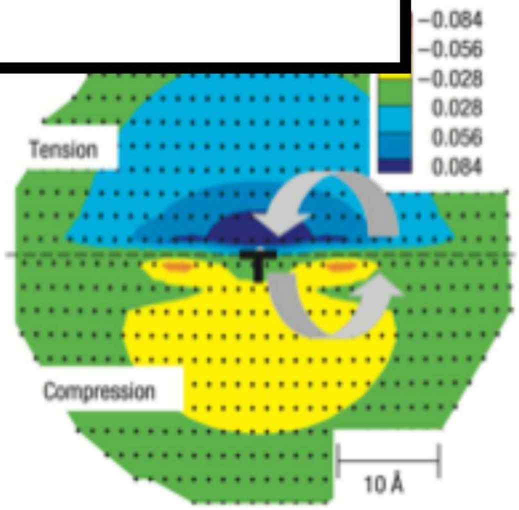
1) Rigorous numerical calculation of continuum theory prediction of atmosphere formation
2) Examination of drag forces with different transient time histories

$$\hat{\chi}(t) = \chi_0 + (\chi_{\mathrm{sat}} - \chi_0)\left\{1 - e^{-(t/t^*_{\mathrm{cl}})^n}\right\} \qquad n = 2/3$$

Curtin et al. (2006) pointed out that continuum theory predictions were too slow and too strong to explain experimentally observed phenomena

- Developed the *cross-core theory* to correct these inconsistencies

$$\hat{\chi}(t) = \chi_0 + (\chi_{\mathrm{sat}} - \chi_0)\left\{1 - e^{-(t/t^*_{\mathrm{cc}})^n}\right\} \qquad n = 1$$



Cross-core diffusion
Curtin et al. (2006)

Rigorous evaluation of continuum theory

Classical continuum theory calculations were all semi-analytical – are they correct?

We developed a numerical technique to solve for atmosphere evolution

- 2^{nd} order finite differences with non-uniform grid
- Implicit time integration scheme

Non-singular pressure field for edge dislocation (Cai et al., 2006)

Dislocation pressure field

Solute misfit

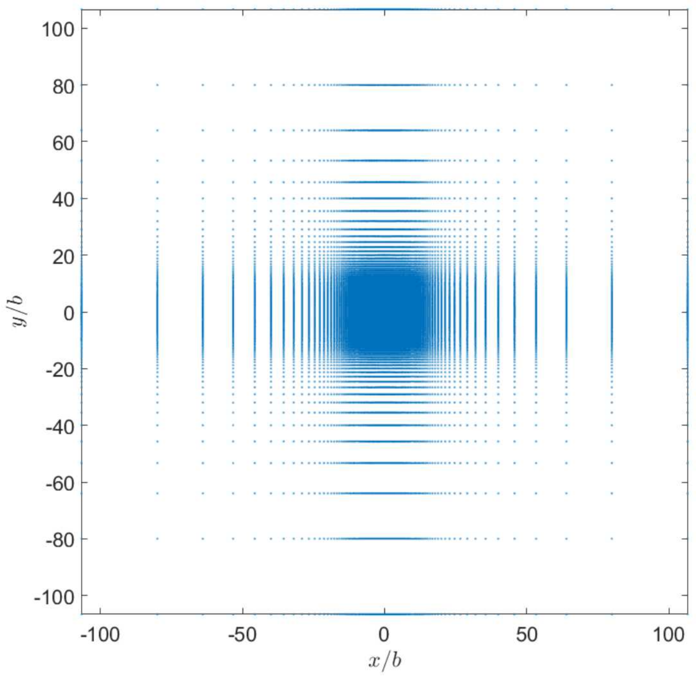
$$\mu_{\text{chem}}(t) = E_{\text{f}} + p_{\text{d}}\Delta V + k_{\text{B}}T\ln\left(\frac{\chi(t)}{1-\chi(t)}\right)$$

Enthalpic term

Entropic term

$$\frac{\partial\chi}{\partial t} = -\frac{1}{c_{\max}}\left(\nabla\cdot\mathbf{J}(t)\right)$$

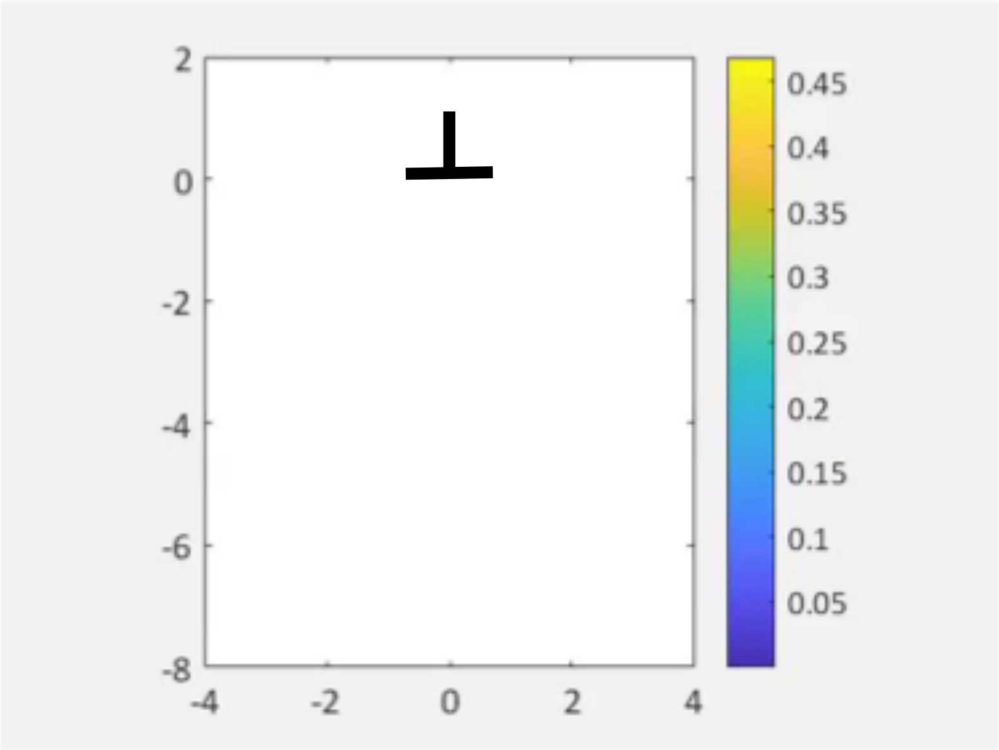
$$\mathbf{J}(t) = -\frac{D\chi(t)c_{\max}}{k_{\text{B}}T}\nabla\mu(t) - \chi(t)c_{\max}\mathbf{v}(t)$$



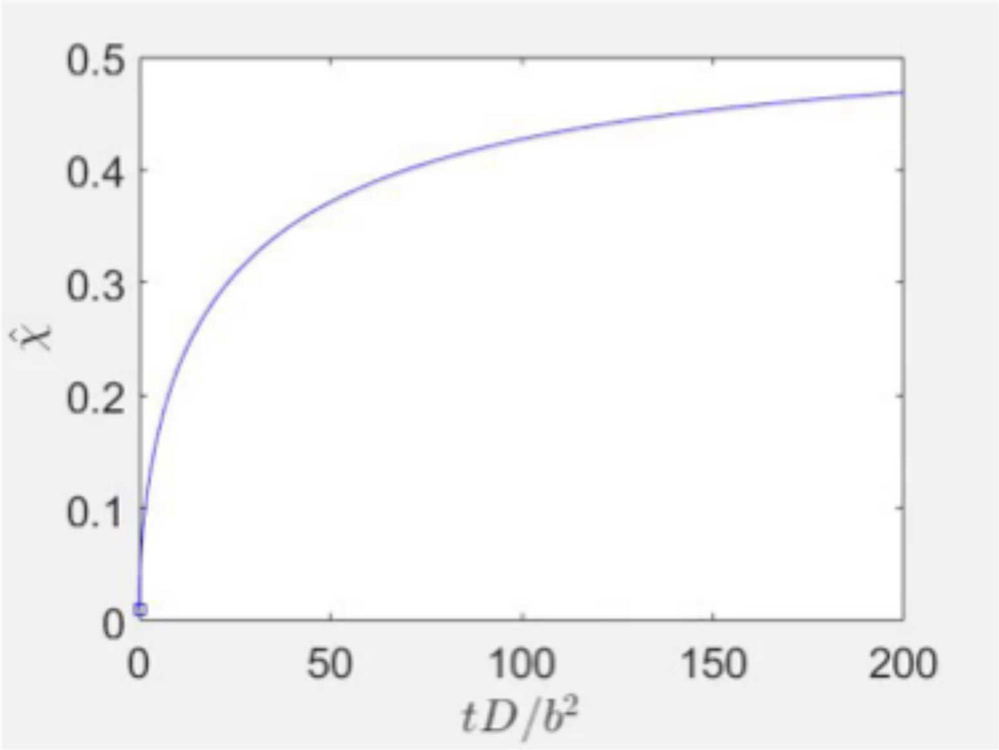
1000 x 1000 transformed grid

Dynamics of atmosphere formation

Initial condition: Uniform concentration χ_0



$$\hat{\chi}(t) = \max_{x,y}[\chi(t, \mathbf{x}, \mathbf{y})]$$



Dynamics of atmosphere formation

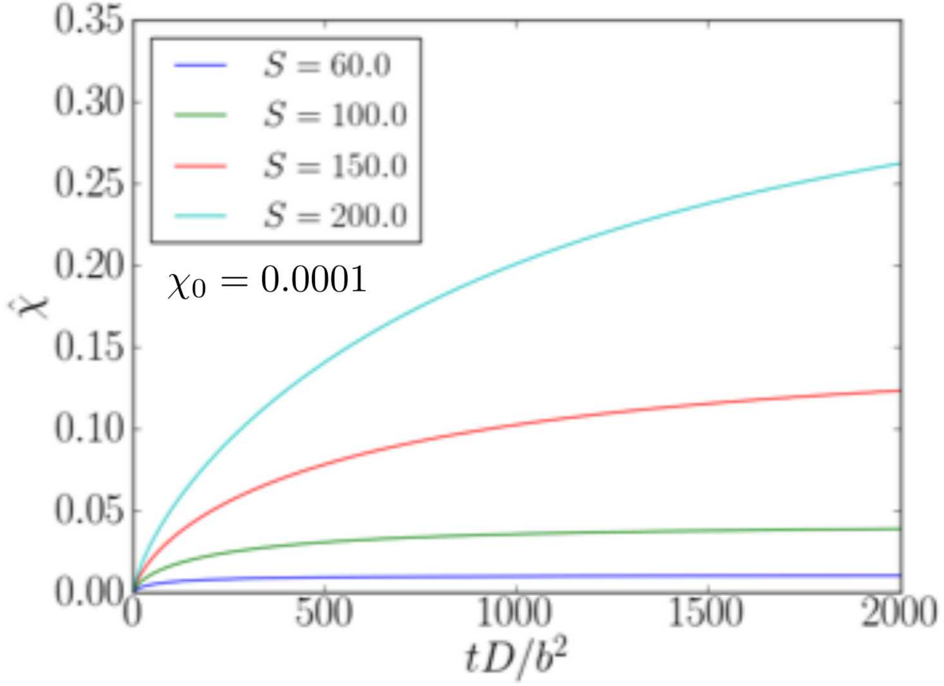
Important non-dimensional parameter:

$$S \equiv \left(\frac{\beta}{k_{\mathrm{B}}Tb}\right)^2$$

Atmosphere “strength” - ratio of enthalpy to entropy

$$p_{\mathrm{d}}\Delta V = \beta f(\mathbf{x}, \mathbf{y})$$

$$\beta \equiv \frac{\mu b}{3\pi}\left(\frac{1+\nu}{1-\nu}\right)\Delta V$$

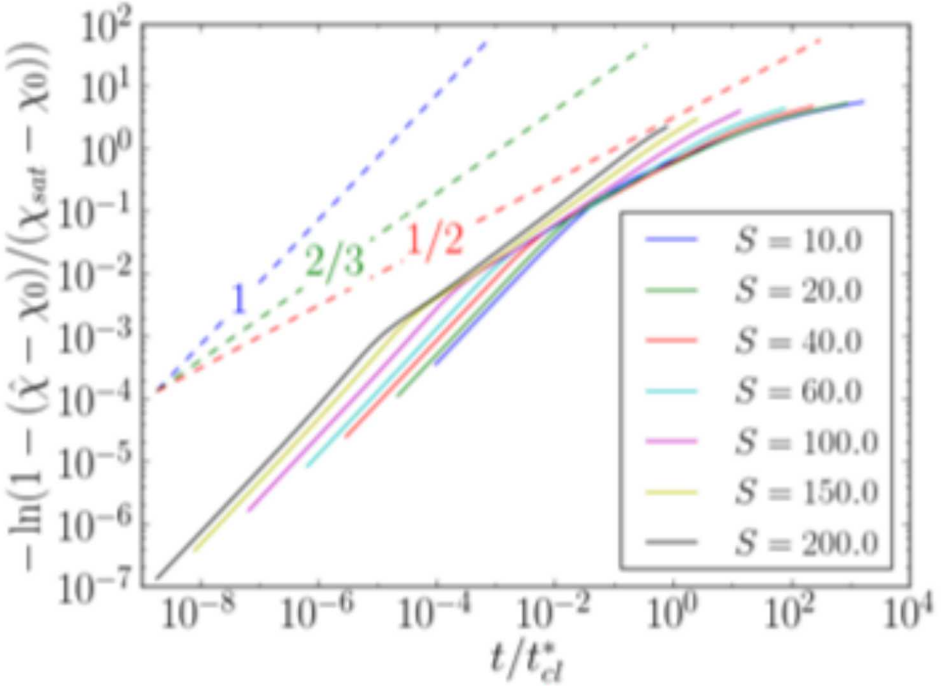


Behavior in "Cottrell-Louat space"

Always observe $n = 1$ at early times

- No region where $n = 2/3$ is observed

Dependence on S is NOT captured by the classical theory through t_{cl}^{*} (as it should be)



Classical time constant

$$\hat{\chi}(t) = \chi_0 + (\chi_{\mathrm{sat}} - \chi_0)\left\{1 - e^{-(t/t_{\mathrm{cl}}^{*})^{n}}\right\}$$

$$-\ln\left(1 - \frac{(\hat{\chi} - \chi_0)}{(\chi_{\mathrm{sat}} - \chi_0)}\right) = \left(\frac{t}{t_{\mathrm{cl}}^{*}}\right)^{n}$$

Classical continuum theory: $n = 2/3$

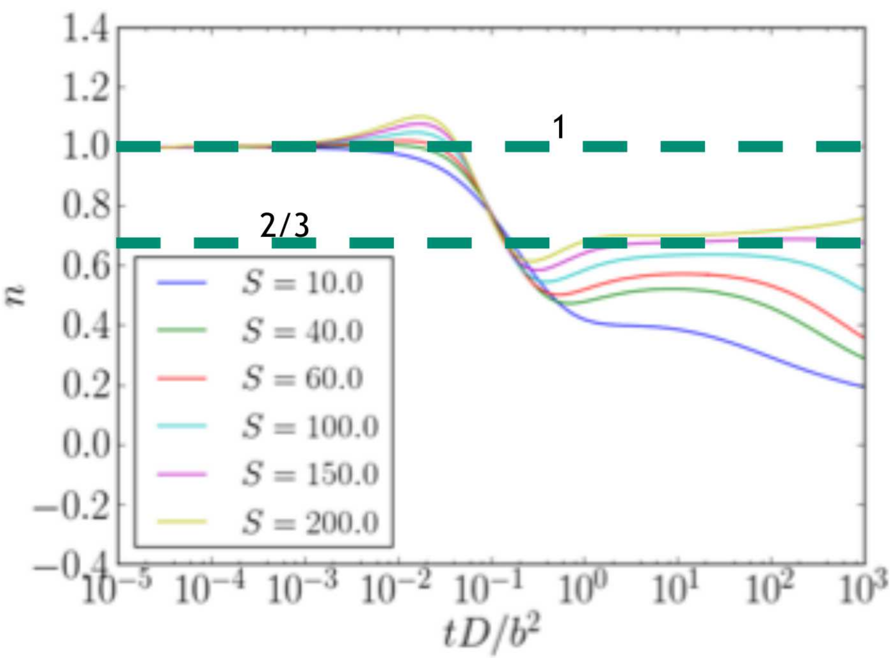
Cross-core theory: $n = 1$

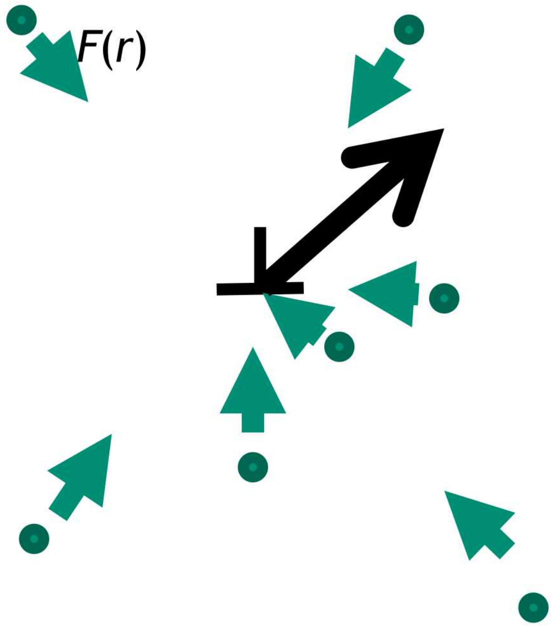
Evolution of *n*: Cross-core or not?

$n = 1$ was previously thought to be a hallmark of "…single-atomic-jump transport [cross-core diffusion] rather than bulk diffusion…" (Curtin et al., 2006)

- Our results indicate it is a hallmark of continuum theory!

Why did all of the classical works by Cottrell, Friedel, and colleagues get it wrong?





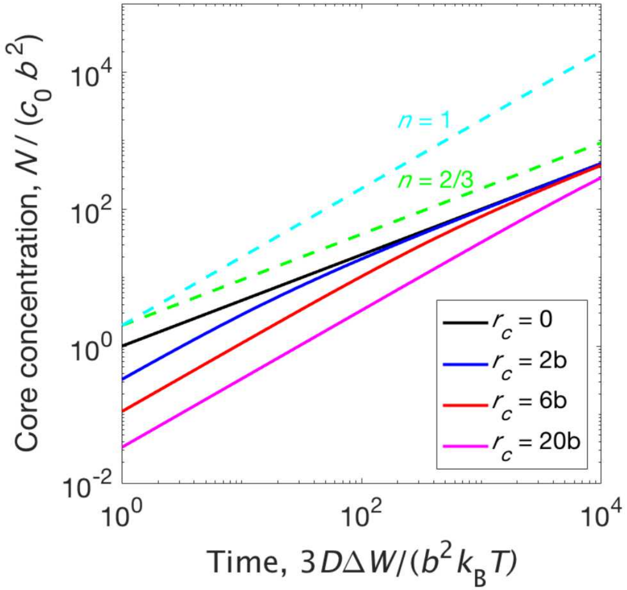
Following Friedel (1964):

$$\frac{dr}{dt} = \frac{D}{k_B T} F \qquad F \approx \frac{\Delta W b}{r^2}$$

Number of solutes that reach $r = 0$ by time t:

$$N = \pi c_0 \left(\frac{3 D \Delta W b}{k_B T} t \right)^{2/3}$$

Evolution of *n*: Cross-core or not?



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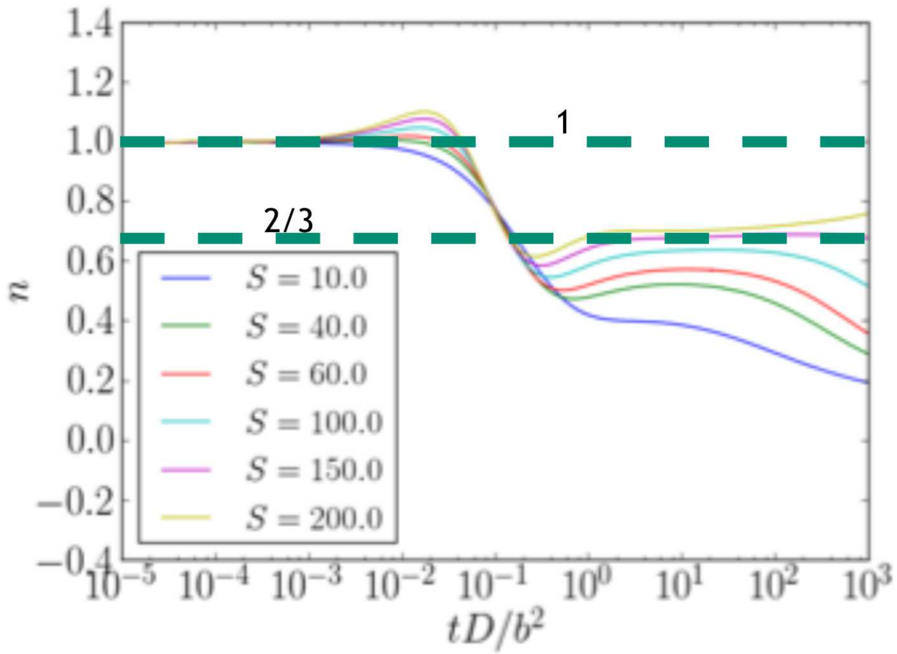
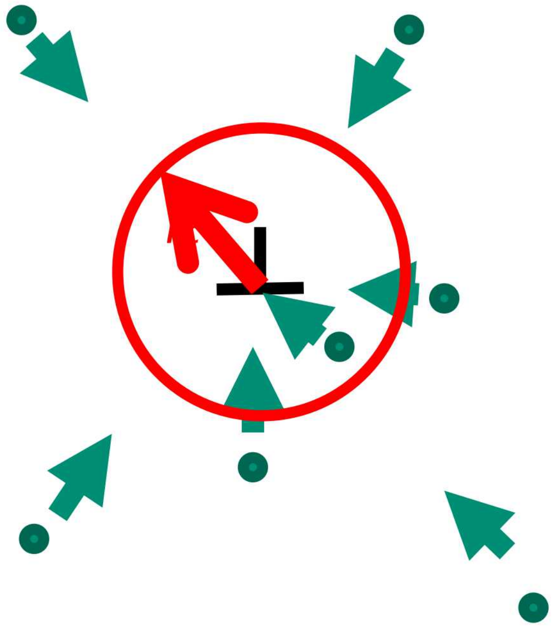




Following Friedel (1964):

$$\frac{dr}{dt} = \frac{D}{k_\mathrm{B}T}F \qquad F \approx \frac{\Delta W b}{r^2}$$

Number of solutes that reach $r = r_c$ by time t:

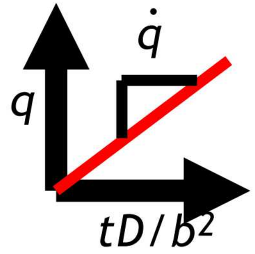
$$N = \pi c_0 \left[\left(r_c^3 + \frac{3D\Delta W b}{k_\mathrm{B}T} t \right)^{2/3} - r_c^2 \right]$$

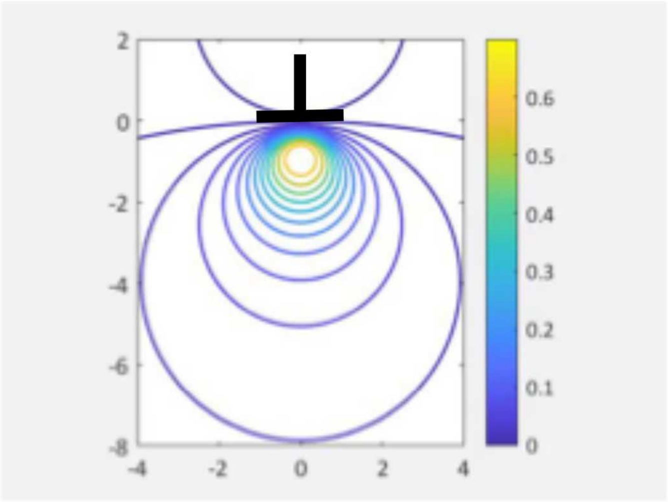
Cottrell atmospheres have a finite size!

Transient solute drag

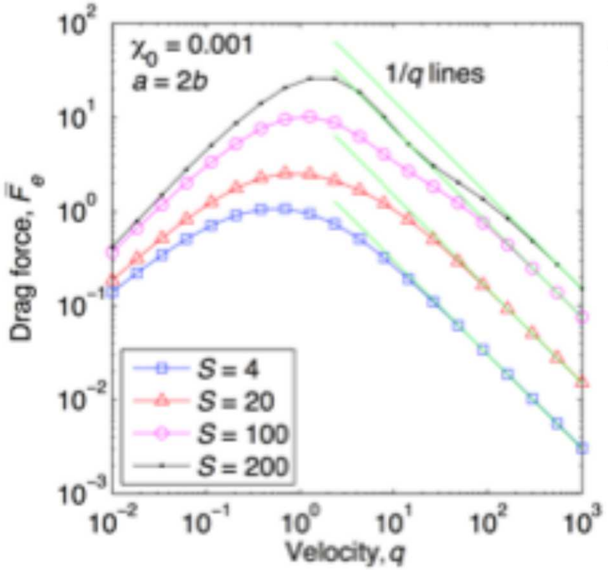
$$q \equiv \frac{v\beta}{4Dk_\mathrm{B}T}$$

Non-dimensional velocity

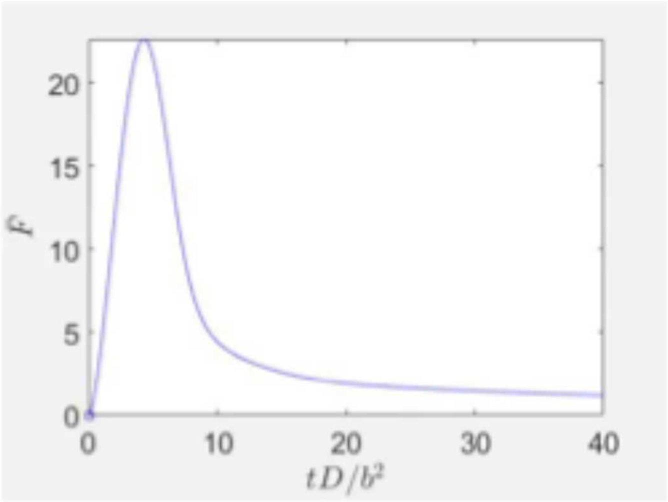




A number of researchers have considered drag forces due to steady state motion of a dislocation (Cottrell and Jaswon, 1949; Zhang and Curtin, 2008; Sills and Cai, 2016; …)



Sills and Cai (2016)

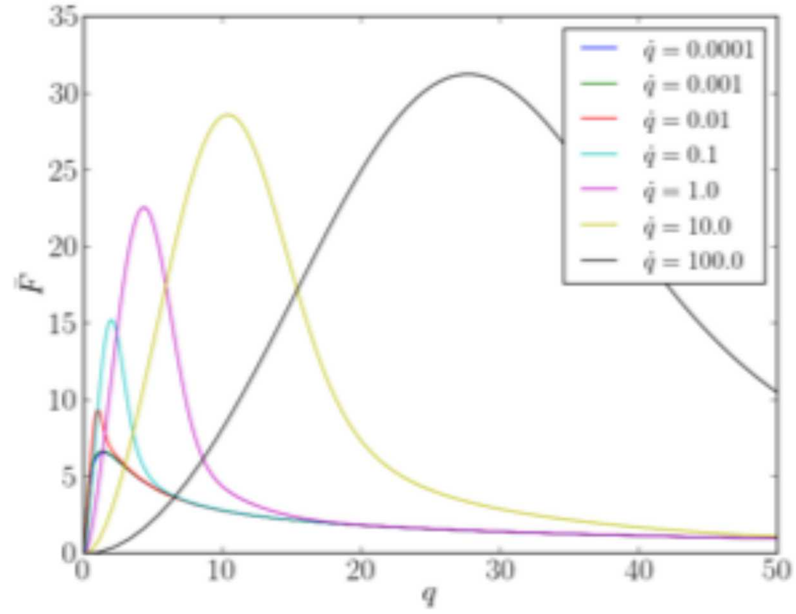


Constant Acceleration at Rate Velocity $\dot{q} = 1$

Transient drag forces less well studied

- *Dynamic strain aging is due to transient drag by a non-equilibrium atmosphere*

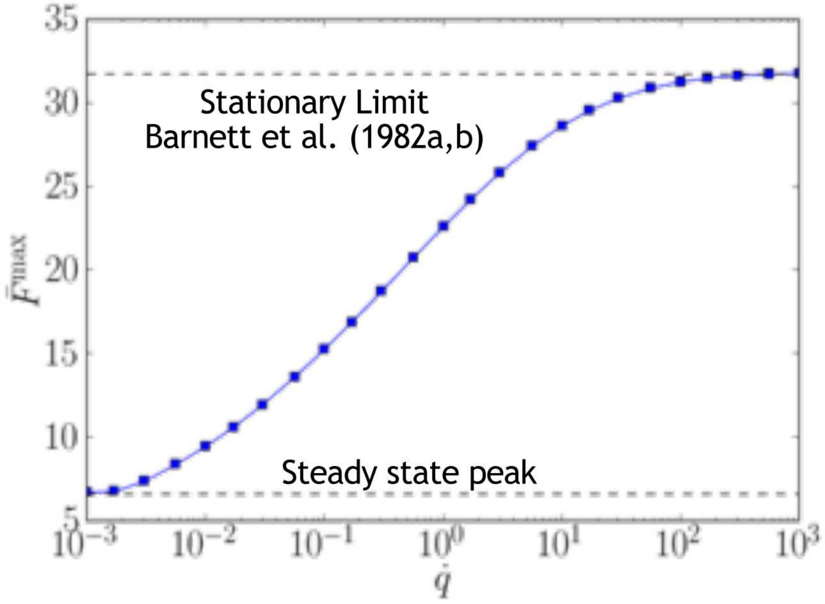
Drag forces depend sensitively on velocity history

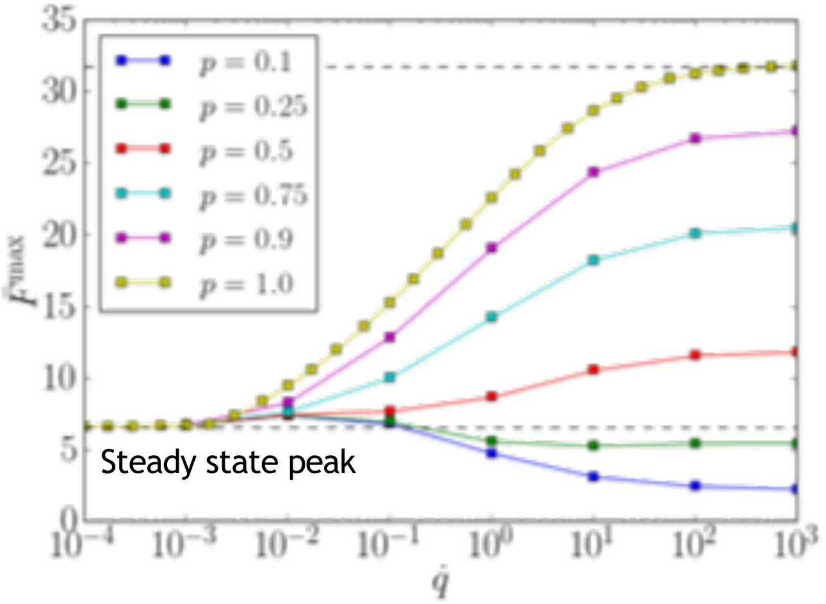


Steady state solution is well obeyed as long as $\dot{q} < 0.001$

Otherwise, overshoots with max force converging to the stationary limit studied by Barnett et al. (1982a,b)

Simulate DSA by starting with an atmosphere equilibrated to peak concentration $\hat{\chi} = \chi_0 + p\,(\chi_{\text{sat}} - \chi_0)$





Conclusions

Our results do not agree with the classical continuum theory

- No $n = 2/3$ scaling, not characterized by classical time constant

Instead, we recover $n = 1$ scaling previously attributed to cross-core diffusion

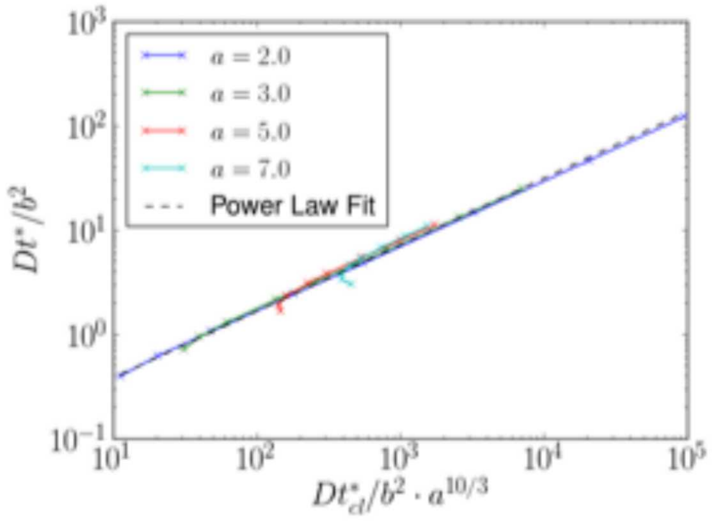
- Showed that previously theories made a bad assumption (neglect atmosphere size)

We observe that the peak drag force is sensitive to the velocity history and the amount of "aging" time

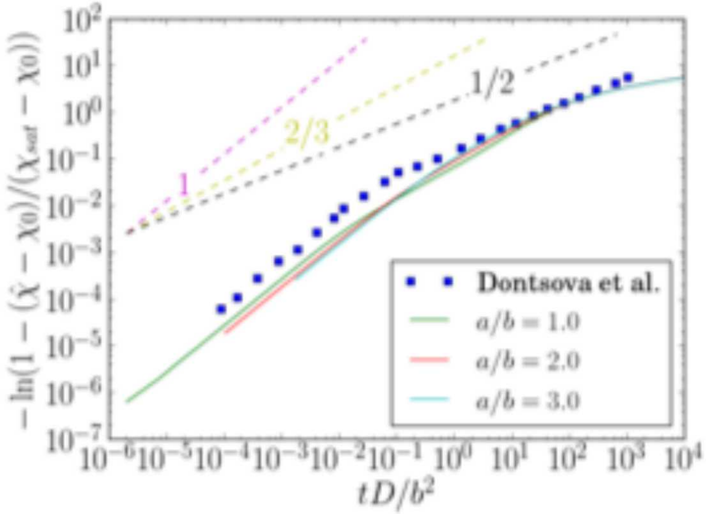
Maybe continuum theory is not so bad after all!

Next step: Comparison with static strain aging experiments

Manuscript is in preparation

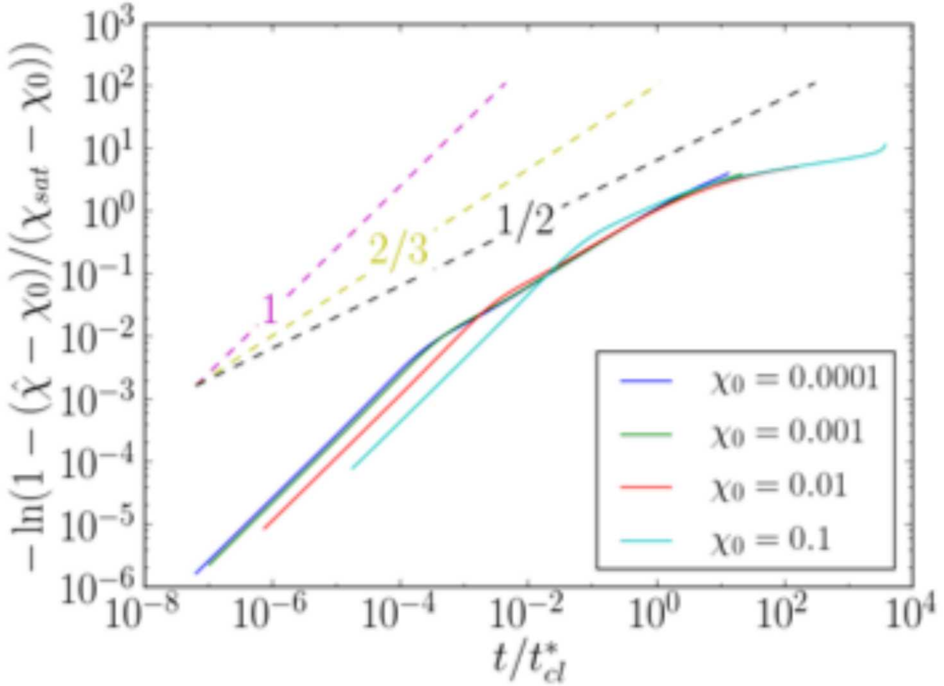


Relationship between our computed t^* and t^*_{cl}

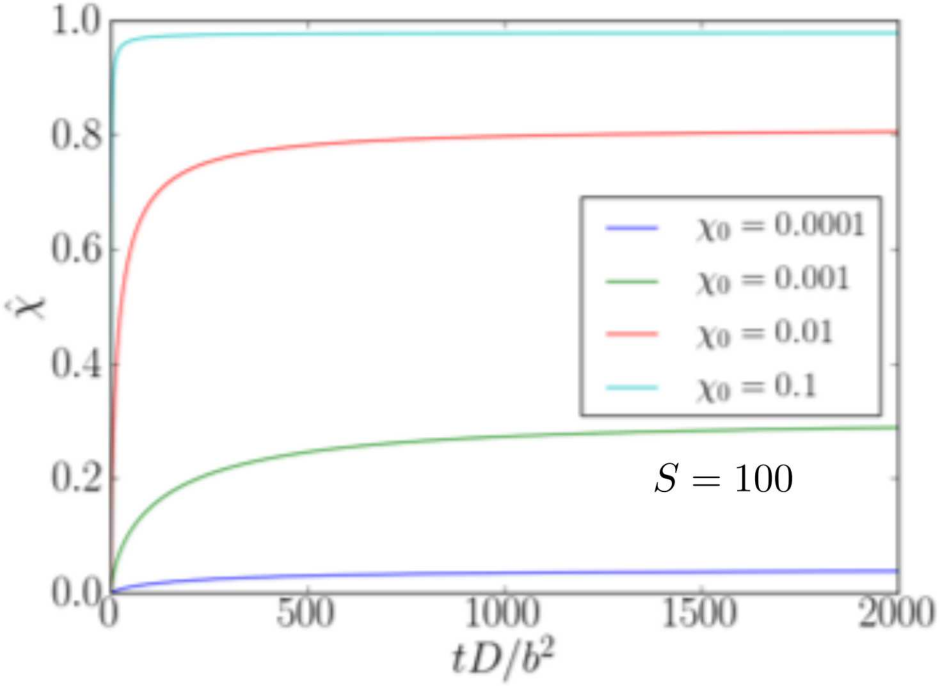


Comparison between continuum and diffusive molecular dynamics (Dontsova et al., 2015)

Back up

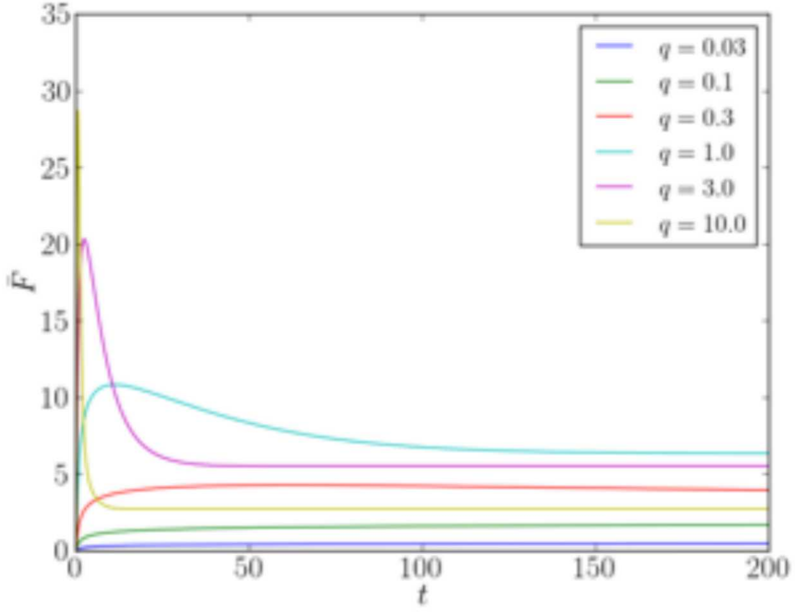


$-\ln(1-(\hat{\chi}-\chi_0)/(\chi_{sat}-\chi_0))$
t/t^*_{cl}
1
2/3
1/2
$\chi_0 = 0.0001$
$\chi_0 = 0.001$
$\chi_0 = 0.01$
$\chi_0 = 0.1$



$\hat{\chi}$
tD/b^2
$\chi_0 = 0.0001$
$\chi_0 = 0.001$
$\chi_0 = 0.01$
$\chi_0 = 0.1$
$S = 100$

Drag forces depend sensitively on velocity history

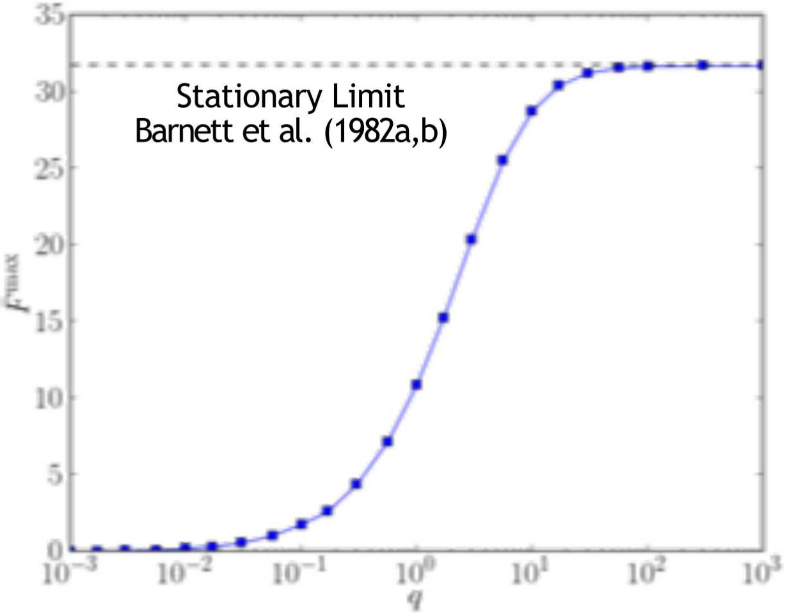


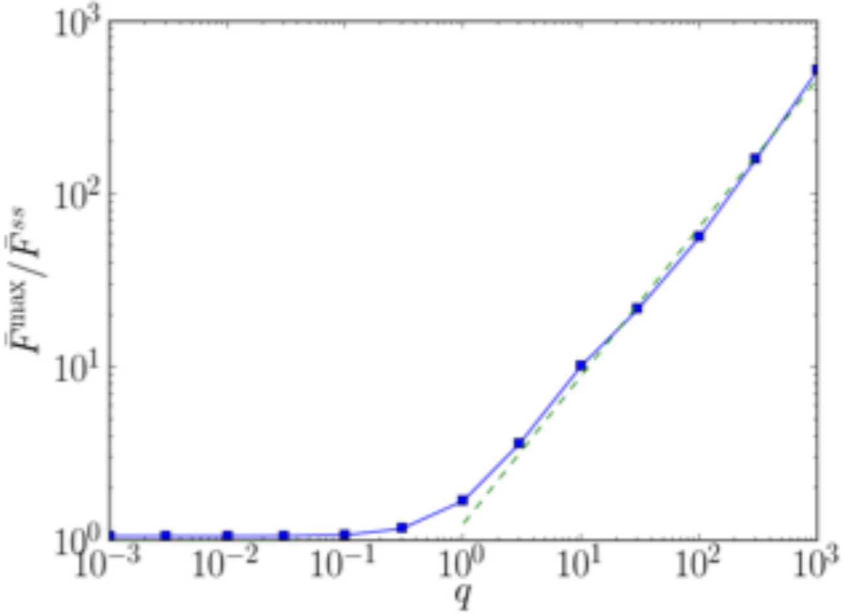
Monotonic force time histories for $q < 1$

Overshoots and decays back down for $q > 1$

Maximum force same as steady state for $q < 0.5$

Impulsive acceleration results





Transient solute drag

$$q \equiv \frac{v\beta}{4Dk_{\mathrm{B}}T}$$

Non-dimensional velocity

Cottrell atmospheres influence mechanical behavior by exerting drag forces on dislocations

$$F = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_{\max}\left[\chi\left(x', y'\right) - \chi_0\right] \Delta V\, F^{\mathrm{dila}}(x', y')\, dx'dy'$$

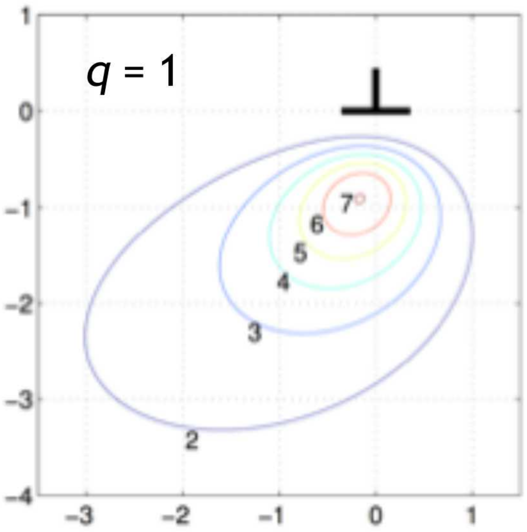
Drag force due to a solute of unit dilatation at (x',y')

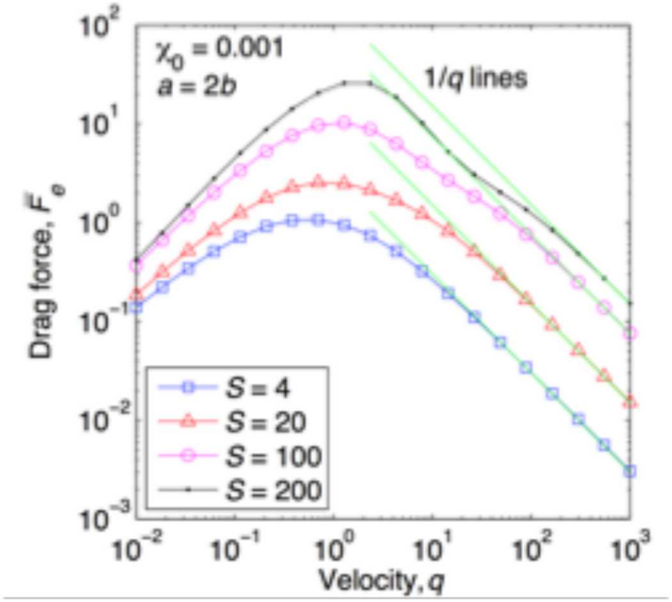
A number of researchers have considered drag forces due to steady state motion of a dislocation with an equilibrated atmosphere (Cottrell and Jaswon, 1949; Zhang and Curtin, 2008; Sills and Cai, 2016)

Transient drag forces less well studied

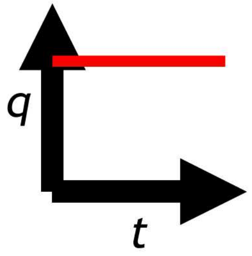
- *Dynamic strain aging is due to transient drag by a non-equilibrium atmosphere*

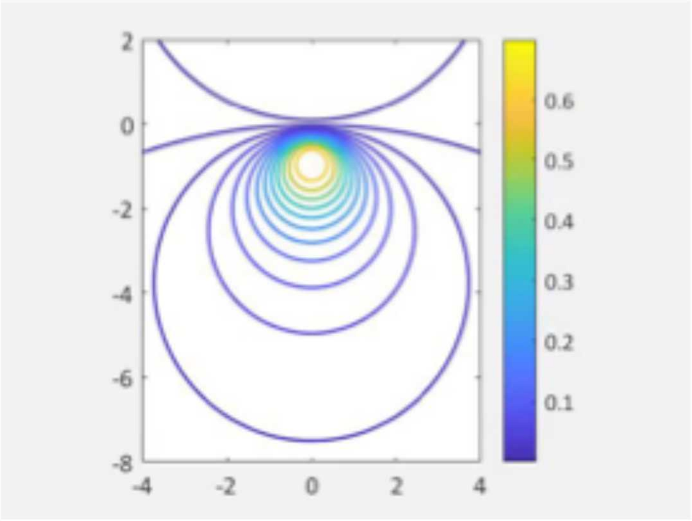
Sills and Cai (2016)

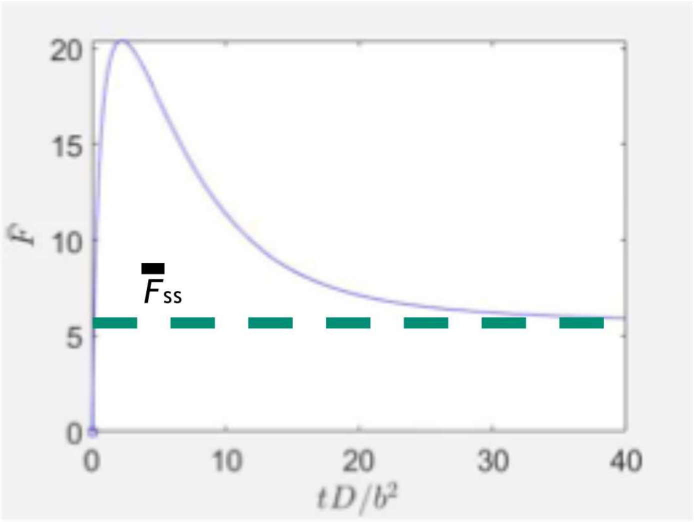




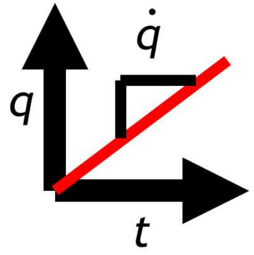
Two different velocity histories

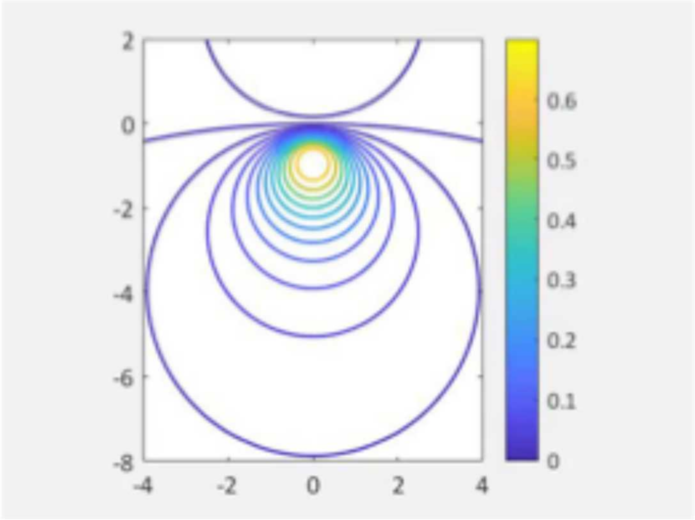


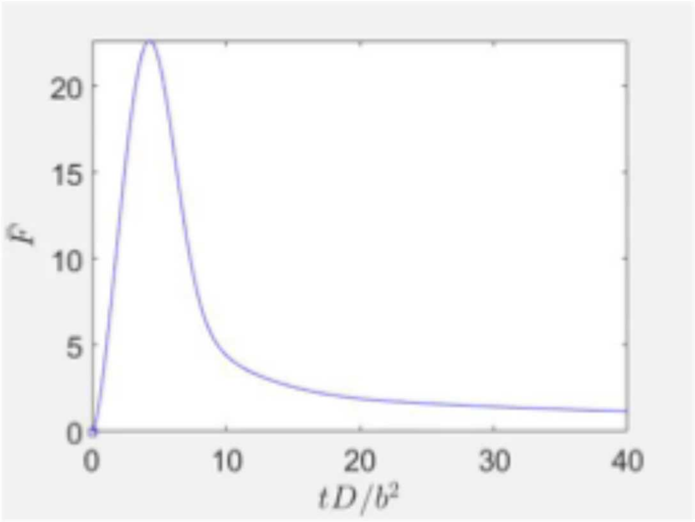




Impulsive Acceleration to Velocity *q* = *3*







Constant Acceleration at Rate Velocity $\dot{q}$ = *1*