Coupling

Stokes's creep and Herring's diffusion

at a small length scale

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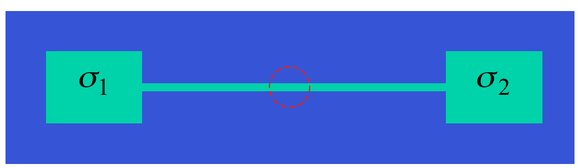
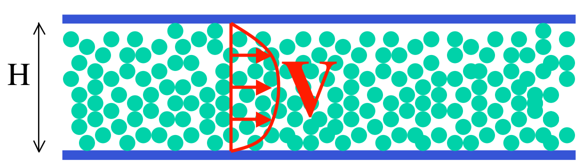
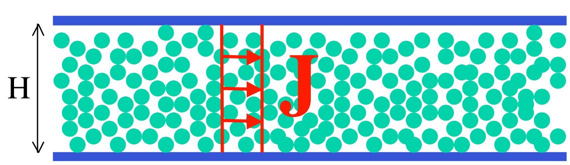
Stress gradient drives mass transport





$$q_{\text{creep}} = \frac{H^3}{12\eta} \nabla \sigma$$



$$q_{\text{diffuse}} = \frac{HD\Omega}{kT} \nabla \sigma$$

When does transition occur?

	Stokes's creep	Herring's diffusion
Kinematics	$d_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i})$ $v_{k,k} = 0$	$J_{k,k} = 0$
Kinetics	$\sigma_{ij} = s_{ij} + \sigma\delta_{ij}$, $s_{ij} = 2\eta d_{ij}$	$J_k = -\frac{D}{kT\Omega}\mu_{,k}$
Force balance	$\sigma_{ij,j} = 0$	?
Boundary conditions	Prescribe traction or velocity	Prescribe chemical potential $\mu = -\Omega\sigma_n$

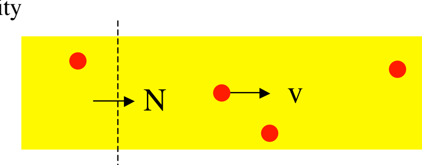
How to couple creep and self-diffusion?

Suo, Kubair, Evans, Clarke, Tolpygo
Acta Materialia 51, 959 (2003)

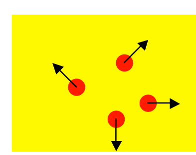
Kinematics

$$N_k = J_k + v_k / \Omega$$

net flux, diffusion flux, convection, marker velocity

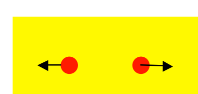


Net flux is divergence-free $J_{k,k} + v_{k,k}/\Omega = 0$



Strain-rate measures relative marker motion

$$d_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i})$$

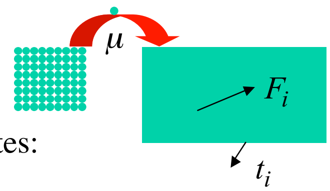


Diffusion-induced strain-rate
(isotropic placement rule)

$$d_{ij}^D = -\frac{\Omega}{3} J_{k,k}\delta_{ij}$$

Creep strain-rate $d_{ij}^C = \frac{1}{2}(v_{i,j} + v_{j,i}) - \frac{1}{3} v_{k,k}\delta_{ij}$

Energetics



Define driving forces as energy-conjugates:

$$\int \left(s_{ij} d_{ij}^{C} + f_i J_i\right) dV + \int \sigma \left(v_{k,k} + \Omega J_{k,k}\right) dV = \int F_i J_i dV + \int t_i v_i dA - \int \mu J_i n_i dA$$

power dissipation **kinematic constraint** **power supply**

$$-\int \left(s_{ij} + \sigma\delta_{ij}\right)_{,j} v_i dV + \int \left(\left(s_{ij} + \sigma\delta_{ij}\right) n_j - t_i\right) v_i dA + \int \left(f_i - F_i - \Omega\sigma_{,i}\right) J_i dV + \int \left(\Omega\sigma + \mu\right) J_i n_i dA = 0$$

$$\left(s_{ij} + \sigma\delta_{ij}\right)_{,j} = 0 \qquad \left(s_{ij} + \sigma\delta_{ij}\right) n_j = t_i$$

$$f_i = F_i + \Omega\sigma_{,i} \qquad \mu = -\Omega\sigma$$

Suo, JAM, in press

Kinetics

diffusion $$J_i = \frac{D f_i}{kT}$$

creep $$d_{ij}^{C} = \frac{s_{ij}}{2\eta}$$

Summary of equations for **v** and σ

$$\left[\eta\left(v_{i,j}+v_{j,i}-\frac{2}{3}v_{k,k}\delta_{ij}\right)\right]_{,j}+\sigma_{,i}=0$$

$$v_{k,k}=-\left(\frac{D}{kT}\left(F_k+\Omega\sigma_{,k}\right)\right)_{,k}$$

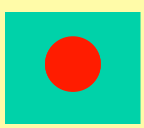
Characteristic length $\Lambda=\sqrt{\frac{\eta D\Omega}{kT}}$

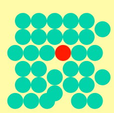
Suo, JAM, in press

Mechanistic pictures: self-diffusion and creep

$\Lambda=\sqrt{\frac{\eta D\Omega}{kT}}$

Stokes-Einstein

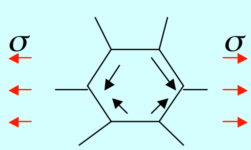




$D=\frac{kT}{6\pi a\eta}$ $\Lambda \sim a$

Nabarro-Herring

Coble



$\frac{1}{\eta}\sim\frac{D\Omega}{kTd_g^2}$

$\frac{1}{\eta}\sim\frac{D_b\delta_b\Omega}{kTd_g^3}$ $\Lambda \sim d_g$

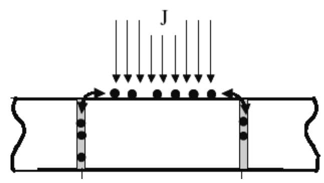
Needleman-Rice

Creep in grains,
Diffusion on grain boundaries

$\Lambda=\sqrt{\frac{\eta_* D\Omega}{kT}}$

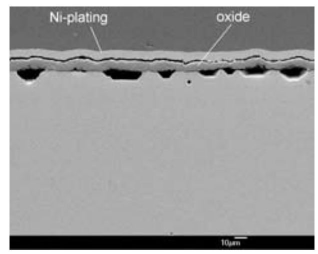
Injecting and emitting atoms

Deposition-induced compression
(chemical potential excess)



Chason et al. PRL 88, 156103 (2002)

Oxidation-induced tension: NiAl
(chemical potential deficit)



Suo, Kubair, Evans, Clarke, Tolpygo
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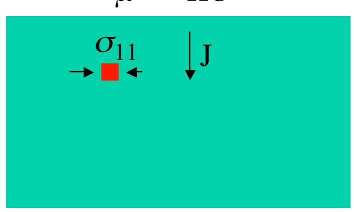
Thick substrate: stress generation

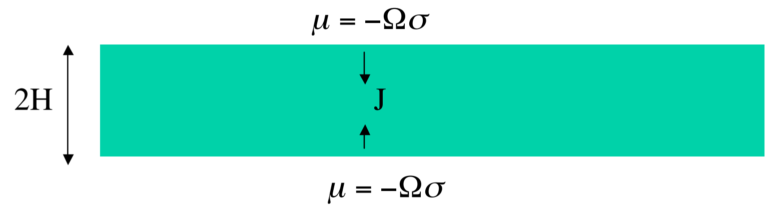
$$\mu = -\Omega\sigma$$



$$\sigma_{11}(x_3) = -\frac{3\mu}{2\Omega}\exp(x_3 / l)$$

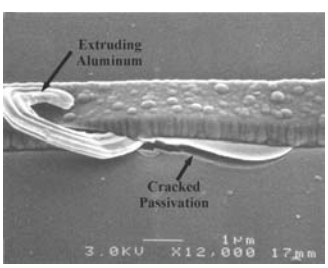
$$l = \sqrt{\frac{4D\eta\Omega}{3kT}}$$

Thin foil
lateral expansion/contraction

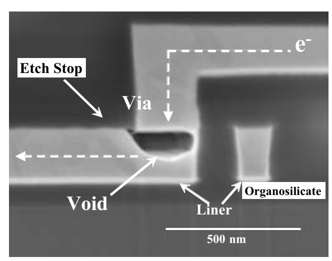


$$d_{11} = \left(\frac{\mu}{4\eta\Omega}\right)\frac{\sinh(H/l)}{(H/l)\cosh(H/l) - \sinh(H/l)}$$

Electromigration

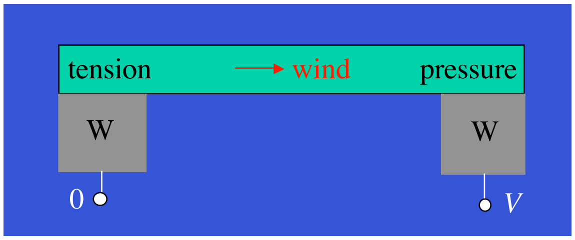


Chiras, Clarke
JAM 88, 6302 (2000)



He, Suo, Marieb, Maiz
Submitted

Electron wind vs. stress gradient

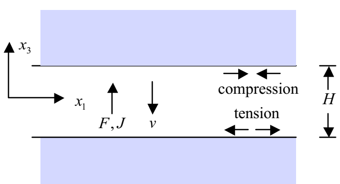


Electron wind drives diffusion $\frac{HDF}{kT\Omega}$

Stress gradient drives diffusion and creep $\frac{HD}{kT}\nabla\sigma + \frac{H^3}{12\eta}\nabla\sigma$

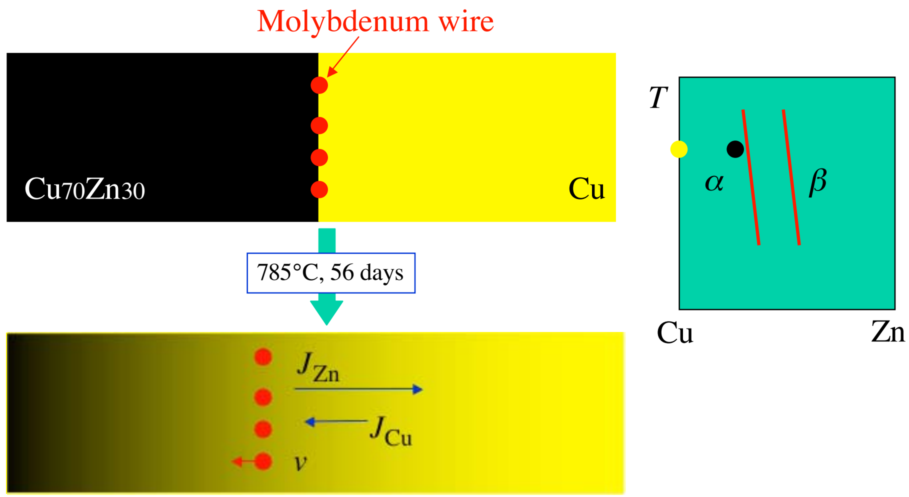
No net flow if $F = \left(1 + \frac{H^2}{12\Lambda^2}\right)\Omega\nabla\sigma$ (Blech condition generalized)

Electromigration through a foil



$$\sigma_{11} = -\frac{3Fl\sinh(x_3/l)}{2\Omega\cosh(H/2l)}$$

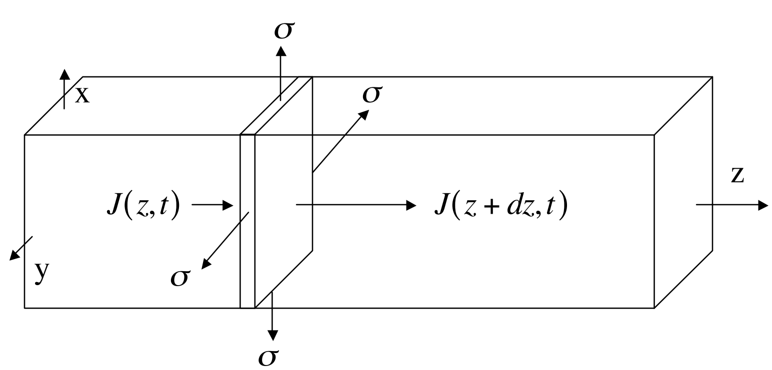
Nonreciprocal diffusion
The Kirkendall Effect



v = velocity of a marker relative to fixed space

Smigeleskas and Kirkendall, Trans. Am. Inst. Min. Engrs. **171**, 130 (1947)

Transverse constraint



Co-evolution of composition and stress

Number conservation

$$\frac{\partial C^A}{\partial t} + \left(J_i^A + C^A v_i\right)_{,i} = 0$$

diffusion kinetics

$$J_i^A = D^A\left[-\frac{\partial C^A}{\partial x_i} + \frac{c}{\phi kT}\frac{\partial \sigma_m}{\partial x_i}\right]$$

force balance

$$\sigma_{ij,j} = 0$$

mean stress

$$\sigma_m = \sigma_{kk}/3$$

deviatoric stress

$$s_{ij} = \sigma_{ij} - \sigma_m \delta_{ij}$$

effective shear stress

$$\tau_e = \sqrt{s_{ij}s_{ij}/2}$$

$$d_{ij} = d_{ij}^C + d_{ij}^D$$

total strain - rate

$$d_{ij} = \frac{1}{2}\left(v_{i,j} + v_{j,i}\right)$$

creep strain - rate

$$d_{ij}^C = f(\tau_e)\frac{s_{ij}}{2\tau_e}$$

dilatation strain - rate

$$d_{ij}^D = -\frac{\Omega}{3}\left(J_k^A + J_k^B\right)_{,k}\delta_{ij}$$

Summary

- Diffusion and creep are coupled
- Generate stress by

  excess chemical potential

  electron wind

  nonreciprocal diffusion

www.deas.harvard.edu/suo

Publication 135, 156