“DRIVING FORCES” ON MOVING DEFECTS:

DISLOCATIONS
and
INCLUSION/PHASE BOUNDARIES
With Inertia Effects

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by NSF

Energy-release rates (Driving forces) for moving defects: dislocations and inclusions

Dislocation: to create an incremental slip area

(-1 singularity in the stress)

Inclusion boundary: to create an incremental volume of eigens

(jump discontinuity in the stress)

Equation of motion, or evolution equation for moving defects

Dislocation dynamics DD with inertia effects

Self-force and effective mass of a dislocation in general motion

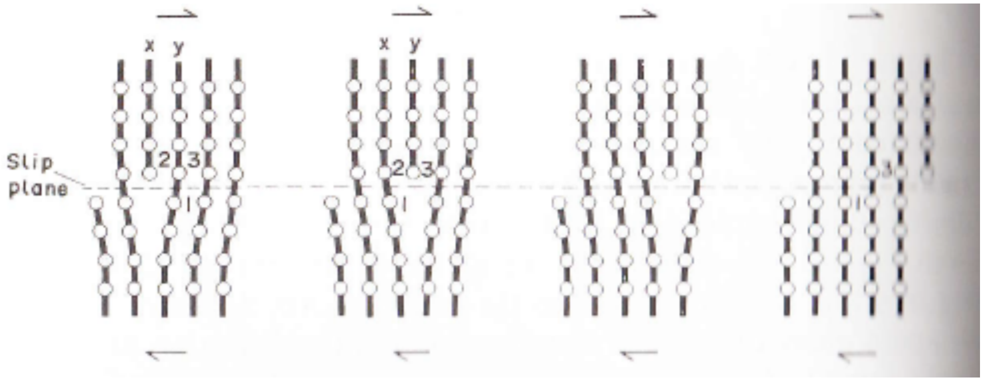
L.Ni & XM, *JMPS*, 2008

Can a dislocation accelerate through the shear-wave speed " barrier"? Self- force

XM & S. Huang, *JMPS*, 2008,
ibid, *APL*, 2009

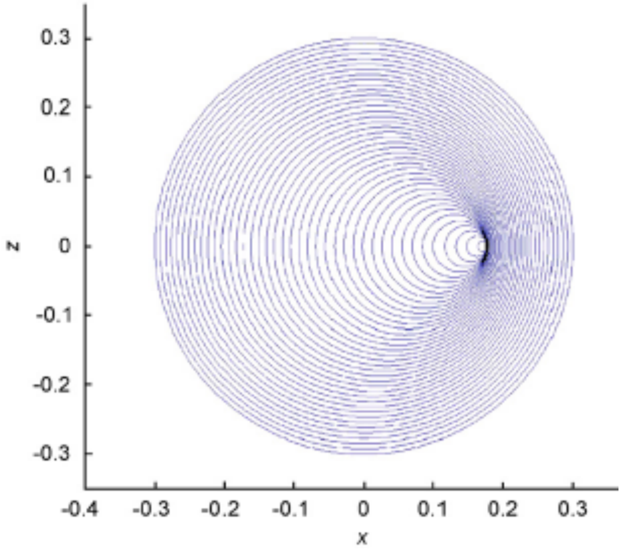
What is the effective mass of a moving dislocation?

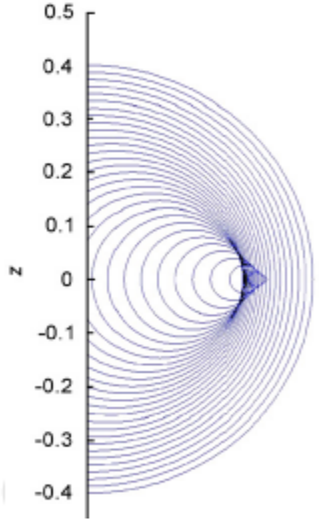
Can it accelerate through the shear-wave-speed barrier?

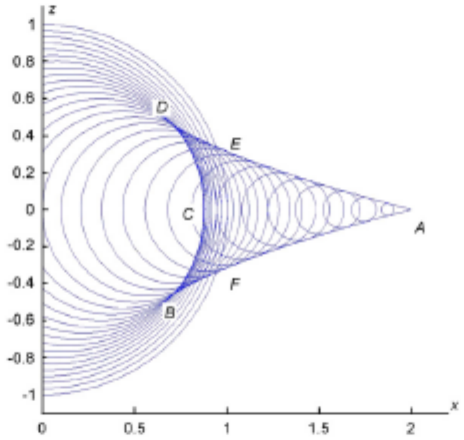


L.Ni & XM, *JMPS*, 2008

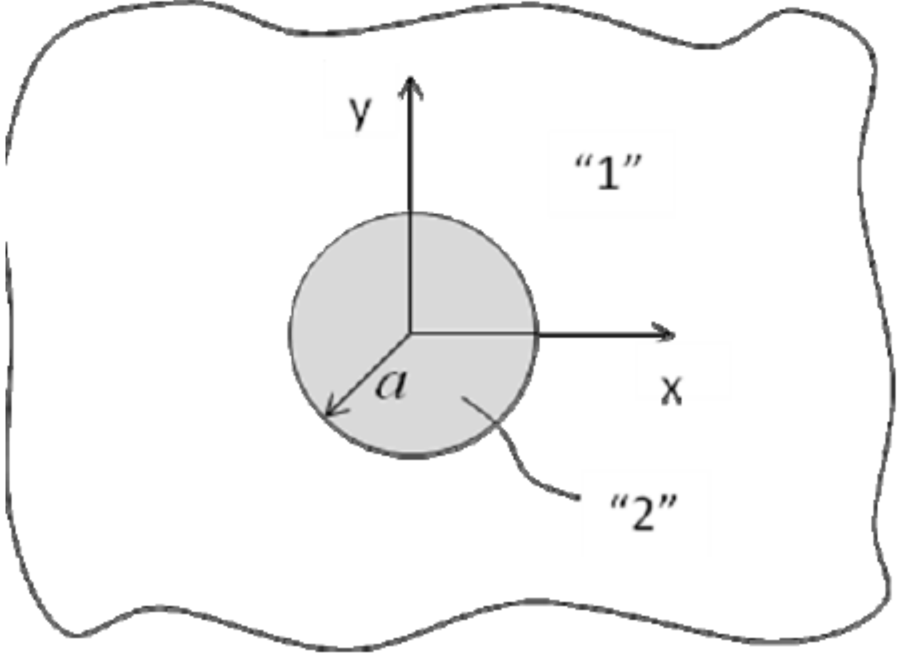
XM & S. Huang, *JMPS*, 2008,







EXPANDING ESHELBY INCLUSIONS



$$\sigma_{ij} = C_{ijkm}\left(\frac{\partial u_k}{\partial x_m} - \epsilon^*_{km}\right)$$

Dynamic Hadamard jump conditions

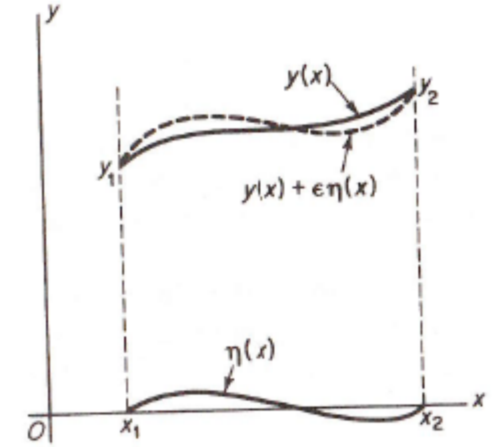
$$[[\dot{u}_i]] = -\dot{l}(t)[[\frac{\partial u_i}{\partial n}]] \qquad n_j[[\sigma_{ij}]] = -\dot{l}(t)[[\dot{u}_i]],$$

Dynamic Fields: Spherically expanding inclusion with dilatational eigenstrain in general motion

Plane half-space constrained inclusion/ inhomogeneity in general motion (general eigenstrain)

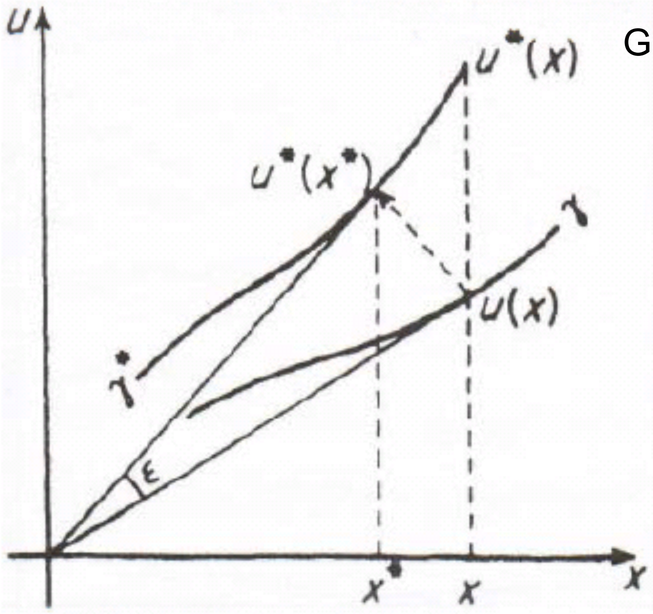
Energy release-rate to create incremental region of eigenstrain /driving force.

Variation of a functional defined on a variable region



$$I(\epsilon) = \int_{x_1}^{x_2} F(x, y + \epsilon\eta, y' + \epsilon\eta')\, dx,$$

Gelfand and Fomin



$$J[u] = \int \cdots \int_R F(x_1, \ldots, x_n, u, u_{x_1}, \ldots, u_{x_n})\, dx_1 \cdots dx_n,$$

$$J[u^*(x^*)] = \int_{R^*} F(x^*, u^*, \nabla^* u^*)\, dx^* \qquad J[u^*(x^*)] - J[u(x)].$$

Invariance for infinitesimal transformations, Noether, 1918

An interpretation of the configurational force

Noether

$$\Pi(u_i, u_{i,j}) = \int_\Omega W(x_i, u_i, u_{i,j}) dV$$

$$\text{new independent variables} \quad y_i = \hat{y}_i(x_i, \epsilon_i) \qquad u_i = \hat{u}_i(x_i, 0)$$

$$\text{new dependent variables} \quad v_i(y_i) = \hat{v}_i(x_i, \epsilon_i) \quad u_i = \hat{u}_i(x_i, 0)$$

$$y_i = x_i + \phi_i + O(\epsilon^2) \qquad v_i = u_i + \psi_i + O(\epsilon^2)$$

$$\delta\Pi = \int_\Omega \frac{d}{dx_i}\left(\frac{\partial W}{\partial u_{k,i}}\bar{\psi}_k + W\phi_i\right)dV + \int_\Omega \Psi_i \bar{\psi}_i dV$$

$$\bar{\psi}_k = \psi_k - u_{k,j}\phi_j \qquad \Psi_i = \frac{\partial W}{\partial u_i} - \frac{d}{dx_j}\frac{\partial W}{\partial u_{i,j}}$$

$\phi_i = \epsilon_i$ translation

$$\delta_x \Pi = \int_{\partial\Omega} (W\delta_{ij} - u_{k,j} p_{ki}) \epsilon_j n_i dA + \int_{\Omega} p_{ik,k} u_{i,j} \epsilon_j dV$$

$$F = \int_{\partial\Omega} E_{ij} \epsilon_j n_i dA \qquad E_{ij} = (W\delta_{ij} - u_{k,j} p_{ki})$$

Energy-momentum tensor

conjugate to ϵ_j *configurational force,*

$\delta_x \Pi$ is given by the flux F

J integral

Rice

if and only if the equilibrium condition is satisfied.

homogeneous and smooth $\frac{\partial W}{\partial x_i} = 0$ everywhere in Ω

$$\begin{aligned} \delta_x \Pi &= \int_{\Omega} (W\delta_{ij} - u_{k,j} p_{ki})_{,i} \epsilon_j dV + \int_{\Omega} p_{ik,k} u_{i,j} \epsilon_j dV \\ &= \int_{\Omega} (p_{ki} u_{k,ij} - u_{k,ji} p_{ki} - u_{k,j} p_{ki,i}) \epsilon_j dV + \int_{\Omega} p_{ik,k} u_{i,j} \epsilon_j dV \\ &= 0 \end{aligned}$$

the body remains infinitesimally close to equilibrium even after a small perturbation of the inhomogeneity position.

Gupta and Markenscoff.
Comptes Rendus, 2008

,

“Conservation Laws” for Elastodynamics

Noether’ s theorem
For Lagrangean
W-T,
Fletcher (1976):

$$\frac{\partial}{\partial x_j}\left[(W-T)\delta_{lj}-\sigma_{ij}u_{i,l}\right]+\frac{\partial}{\partial t}(\rho\dot{u}_i u_{i,l})=0$$

$$E_{ij}=\left((W-T)\delta_{ij}-u_{k,j}\frac{\partial W}{\partial u_{k,i}}\right)$$

Energy-momentum tensor

$$\Pi_L(u_{i,j},\dot{u}_i)=\int_{t_1}^{t_2}\int_{\Omega}(W(x_i,u_{i,j})-T(\dot{u}_i))dV\,dt,$$

$$y_\alpha=x_\alpha+\phi_\alpha+O(\varepsilon^2)\text{ and }v_i=u_i+\psi_i+O(\varepsilon^2)$$

Dynamic *J* integral

$$\begin{aligned}\delta_x\Pi_L = \quad & \varepsilon_j\int_{t_1}^{t_2}\int_{\partial\Omega}E_{ij}n_i\,dA\,dt+\varepsilon_j\int_{t_1}^{t_2}\int_{\Omega}\frac{d}{dt}(\rho u_{k,j}\dot{u}_k)dV\,dt\\ - \quad & \varepsilon_k\int_{t_1}^{t_2}\int_{\Omega}(-\sigma_{ij,j}+\rho\ddot{u}_i)u_{i,k}\,dV\,dt\end{aligned}$$

Gupta &XM, *J.Elast*. 2012

Transition from Lagrangean to Hamiltonian

$$\Pi_L(u_{i,j},\dot{u}_i)=\int_{t_1}^{t_2}\int_{\Omega}(W(x_i,u_{i,j})-T(\dot{u}_i))dV\,dt$$

$$\Pi_H(u_{i,j},\dot{u}_i)=\int_{t_1}^{t_2}\int_{\Omega}(W(x_i,u_{i,j})+T(\dot{u}_i))dV\,dt.$$

$$\begin{aligned}\delta_x\Pi_H = &\int_{t_1}^{t_2}\int_{\partial\Omega}E_{ij}\phi_j n_i\,dA\,dt+\int_{t_1}^{t_2}\int_{\Omega}(T\phi_{i,i}+\rho u_{k,j}\ddot{u}_k\phi_j)dV\,dt\\ &-\int_{t_1}^{t_2}\int_{\Omega}(-\sigma_{ij,j}+\rho\ddot{u}_i)u_{i,j}\phi_j\,dV\,dt.\end{aligned}$$

$\phi_i=\varepsilon_i$ (translational symmetry) $\phi_{i,i}=0$

$$\delta_x\Pi_L=\delta_x\Pi_H.$$

Divergence theorem

A.Gupta & XM, *J.Elast*, 2012

The equation of motion of a dislocation

Eshelby, 1953

"The dislocation is haunted by its past"

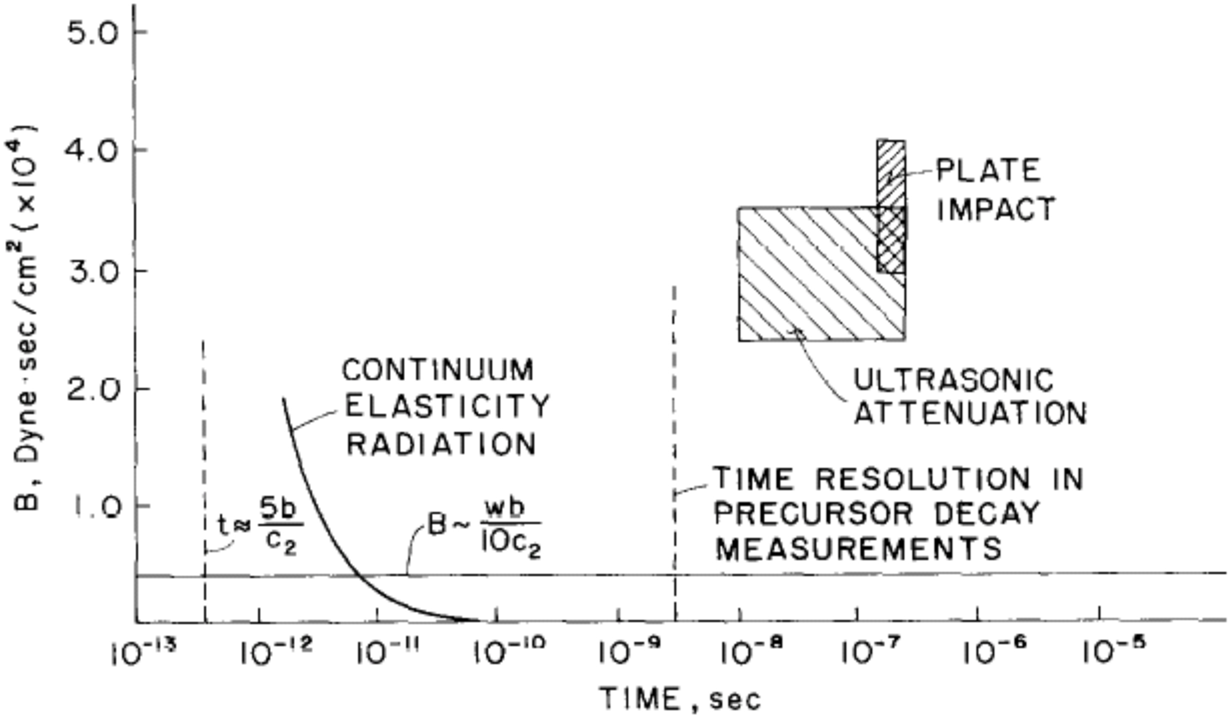
$$F_x = b p_{zy}{}^A = (1-\dot{\xi}^2/c^2)^{-\frac{3}{2}}(\rho b^2/4\pi)\{\ln f(t)\}\partial^2\xi/\partial t^2 + g(t)$$

Peach-Koehler force

Self-force (inertia)

the accelerating dislocation is continually catching up the radiation it has already emitted.

L. Ni & XM, *JMPS*, 2008



6. Comparison of the continuum elasticity drag force with values obtained from lattice dynamics estimates and from experiments.

Dislocation as Moving Elastic Singularity

Static dislocation (screw, edge): stress has
1/r singularity

Accelerating dislocation: ???? length scale $c_2^2/\dot{v}$,

Near field singularity: Logarithmic singularity depending on acceleration
Self-force and
effective mass

Gavazza and Barnett, *JMPS,* 1976, logarithmic singularity due to curvature of static loop

$$f_{\text{self}} = \frac{1}{\rho}\left\{E(\mathbf{t}) - \left[E(\mathbf{t}) + \frac{\partial^2}{\partial\alpha^2}(E(\mathbf{t}))\right]\ln\left(\frac{8\rho}{\varepsilon}\right) - \left[F(\alpha) + \frac{\partial^2 F}{\partial\alpha^2}\right]\right\} - J[\mathbf{L}, \mathbf{P}],$$

Solution for generally accelerating dislocation

For a Volterra screw dislocation starting from rest and moving non-uniformly(according to $x = l(t)$ or inversely $t = \eta(\xi)$), the solution has been obtained by Markenscoff(1980):

$$
\begin{aligned}
\frac{\partial u}{\partial z}(x,z,t) = &-\frac{\Delta u}{2\pi}\int_0^\infty \frac{(t-\eta(\xi))(x-\xi)^2 H(t-\eta(\xi)-rb)}{r^4[(t-\eta(\xi))^2-r^2b^2]^{\frac{1}{2}}}d\xi \\
&+\frac{\Delta u}{2\pi}z^2\frac{\partial}{\partial t}\int_0^\infty \frac{(t-\eta(\xi))^2 H(t-\eta(\xi)-rb)}{r^4[(t-\eta(\xi))^2-r^2b^2]^{\frac{1}{2}}}d\xi - \frac{\Delta u}{2\pi}\frac{x}{x^2+z^2} \qquad (1)
\end{aligned}
$$

where $r^2 = (x-\xi)^2 + z^2$, and Δu denotes the Burgers vector, b the shear wave slowness, which is valid for both subsonic and supersonic motion.

Edge Dislocation: Markenscoff and Clifton (*JMPS,* 1981)

Arch. Rat. Mech. Anal.
with C. Callias
Vol 102, p 275 (1988)

(New) Asymptotic Series

$$\int_0^\infty f(y,x)\,dx = \sum_{m=0}^{\infty} a_m \epsilon^m + \ln\epsilon \sum_{m=1}^{\infty} b_m \epsilon^m$$

$$y = \frac{\epsilon}{x}$$

$$\int_0^\infty \frac{dx}{x^n}\,\epsilon^n$$

$$a_0 = \int_0^\infty f(0,x)\,dx$$

$$\underset{m>0}{a_m} = -\frac{1}{m!\,(m-1)!}\int_0^\infty \ln x\,\frac{\partial^{2m} f(0,x)}{\partial y^m\,\partial x^m}\,dx + \underset{\sum_{1}^{m-1}\frac{1}{n}}{\underset{\downarrow}{c_m}}\,\frac{1}{m!\,(m-1)!}\,\frac{\partial^{2m-1} f(0,0)}{\partial y^m\,\partial x^{m-1}}$$

$$+\mathcal{L}_m(\varphi)\ \Big[\text{where}\ \ \mathcal{L}_m(\varphi) = \frac{1}{(m-1)!}\int_0^\infty d\xi\,\ln\xi\,\frac{\partial}{\partial\xi}\,\xi^m R_{m+1}\left(\frac{1}{\xi}\right)$$

$$R_{m+1}(y) = \varphi(y) - \sum_{k=0}^{m}\frac{1}{k!}\,\varphi^{(k)}(0)\,y^k\Big]$$

$$b_m = -\frac{1}{m!\,(m-1)!}\,\frac{\partial^{2m-1} f(0,0)}{\partial y^m\,\partial x^{m-1}}$$

Let f satisfy

(a) $f(y,x) \in C^\infty([0,\infty)\times[0,\infty))$,

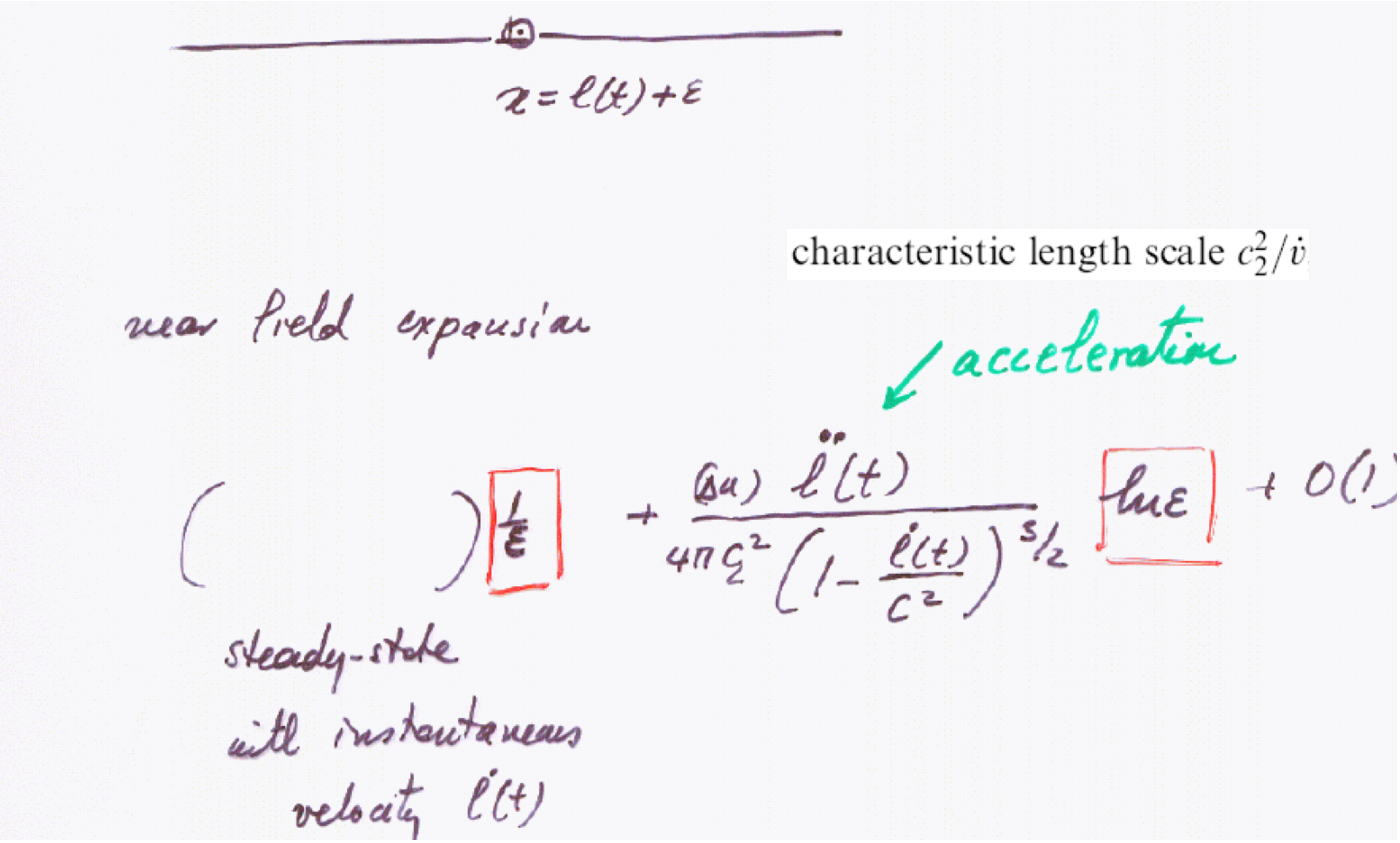
(b) $f(y,x)=0$ if $x > B$ for some $B>0$

(c) $|\partial_x^k f(y,x)| \leq y^k f_k(y)$ for all x, y,

$k=0,1,2,\dots$ where $f_k(y)$ are functions such that

$\int_0^s f_k\left(\frac{1}{x}\right) dx < \infty$ for each $s>0$

Near –field expansion around the current position of an accelerating dislocation



$x = \ell(t) + \varepsilon$

characteristic length scale $c_2^2/\dot{v}$

near field expansion

acceleration

$$\left(\qquad \right)\boxed{\frac{1}{\varepsilon}} + \frac{(\Delta u)\ \ddot{\ell}(t)}{4\pi c_2^2 \left(1 - \frac{\dot{\ell}(t)}{c^2}\right)^{3/2}} \boxed{\ln \varepsilon} + O(1)$$

steady-state
with instantaneous
velocity $\dot{\ell}(t)$

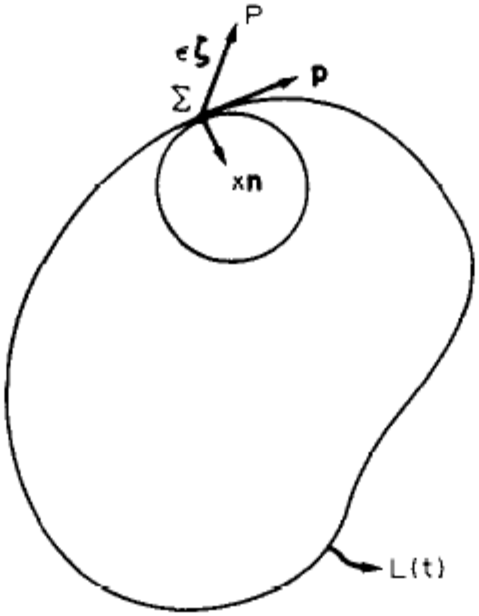
Callias and Markenscoff, *Arch Rat Mech Anal*, 1988

Near field of a moving dislocation loop

Logarithimc singularity associated with:

Acceleration of the tangent
Rotation of the tangent
Radius of curvature of osculating circle

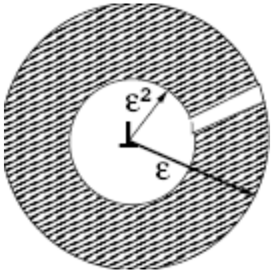
XM & L. Ni, *JMPS*,1990



$$U_{m,n} = \int_{-\infty}^{\infty} \oint_{L(t')} \varepsilon_{njh} C_{ijkl} G_{km,l}(x-x', t-t') b_i \, \mathrm{d}l_h \, \mathrm{d}t' + \int_{-\infty}^{\infty} \oint_{L(t')} \rho G_{im}(x-x', t-t') b_i \varepsilon_{nrs} V_r(x', t') \, \mathrm{d}l_s \, \mathrm{d}t',$$

The logarithmic singularity from the dynamic energy momentum tensor---as a field equation

$$\frac{\partial}{\partial t}\int_{V_{(\epsilon_0^2,\epsilon_0)}} \rho\dot{u}_i u_{i,1}\,dV = \int_{S_{\epsilon_0}} [(W-T)\delta_{1j} - u_{i,1}\sigma_{ij}]\,dS_j - \int_{S_{\epsilon_0^2}} [(W-T)\delta_{1j} - u_{i,1}\sigma_{ij}]\,dS_j.$$



$$\int_{V_{(\epsilon_0^2,\epsilon_0)}} \rho\dot{u}_i u_{i,1}\,dV = -\frac{\mu b^2}{4\pi c_2^2}\frac{v(t)}{\gamma}\ln(\epsilon_0/\epsilon_0^2) + O(\epsilon_0)$$

$$= \frac{\mu b^2}{4\pi c_2^2}\frac{v(t)}{\gamma}\ln(\epsilon_0) + O(\epsilon_0),$$

$$\gamma = \sqrt{1 - v^2(t)/c_2^2}$$

$$I_{\epsilon_0} - I_{\epsilon_0^2} = \mu b f_{32}(t)\ln(\epsilon_0/\epsilon_0^2) + O(\epsilon_0) = -\mu b f_{32}(t)\ln(\epsilon_0) + O(\epsilon_0).$$

$$f_{32}(t) = -\frac{b}{4\pi}\frac{\dot{v}(t)}{c_2^2\gamma^3},$$

Ni and Markenscoff, *MMS*, 2009,

Self-force on a generally moving dislocation from the dynamic *J* integral

Two options how to treat the divergence of the dynamic *J* integral for an accelerating dislocation

1) Smearing of the core (suggested by Eshelby)

Ramp-core: delta function as limit of delta sequence

2) Regularization based on the theory of distributions
(Gelfand &Shilov)

We show that they are equivalent to the leading order

Ni &XM, , *J. Mech. Phys. Sol*, **56**, pp1348-1379, 2008

Dislocation jumping from rest
to constant velocity

$$\dot{\mathscr{E}}^{\mathrm{s}}_{0} = -\frac{\mu b_x^2}{2\pi t}\left(\frac{1-(1-v_{\mathrm{d}}^2/c_2^2)^{\frac{1}{2}}}{(1-v_{\mathrm{d}}^2/c_2^2)^{\frac{1}{2}}}\right),$$

Clifton &XM, *JMPS*,1981,

Screw and edge dislocation accelerating through the shear-wave speed

Eshelby, 1956, “Supersonic motion is a formal possibility”

Gumbsch and Gao, *Science*,1999

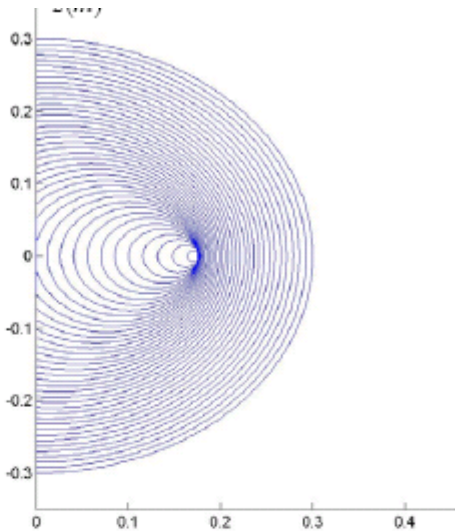
Dunham E.M. and Archuleta R.J. (2004) Evidence for a supershear transient during the 2002 Denali fault earthquake. *Bulletin of the Seismological Society of America*. Vol. 94, No. 6B, pp. S256-S268.

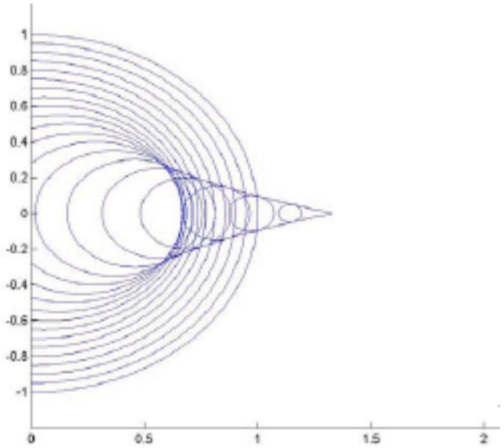
Olmsted D.L., Hector, L.G., Curtin W.A. and Clifton R. J. (2005) Atomistic simulations of dislocation mobility in Al, Ni and Al/Mg. *Modeling And Simulation in Engineering*. Vol. 13, No. 3, pp.371-388.

M. Bouchon, H. Karabulut, *Science* **320**, 1323(2008)

S. Das, *Science* **317**, 905 (2007)

Wavefronts as envelops of emitted wavelets

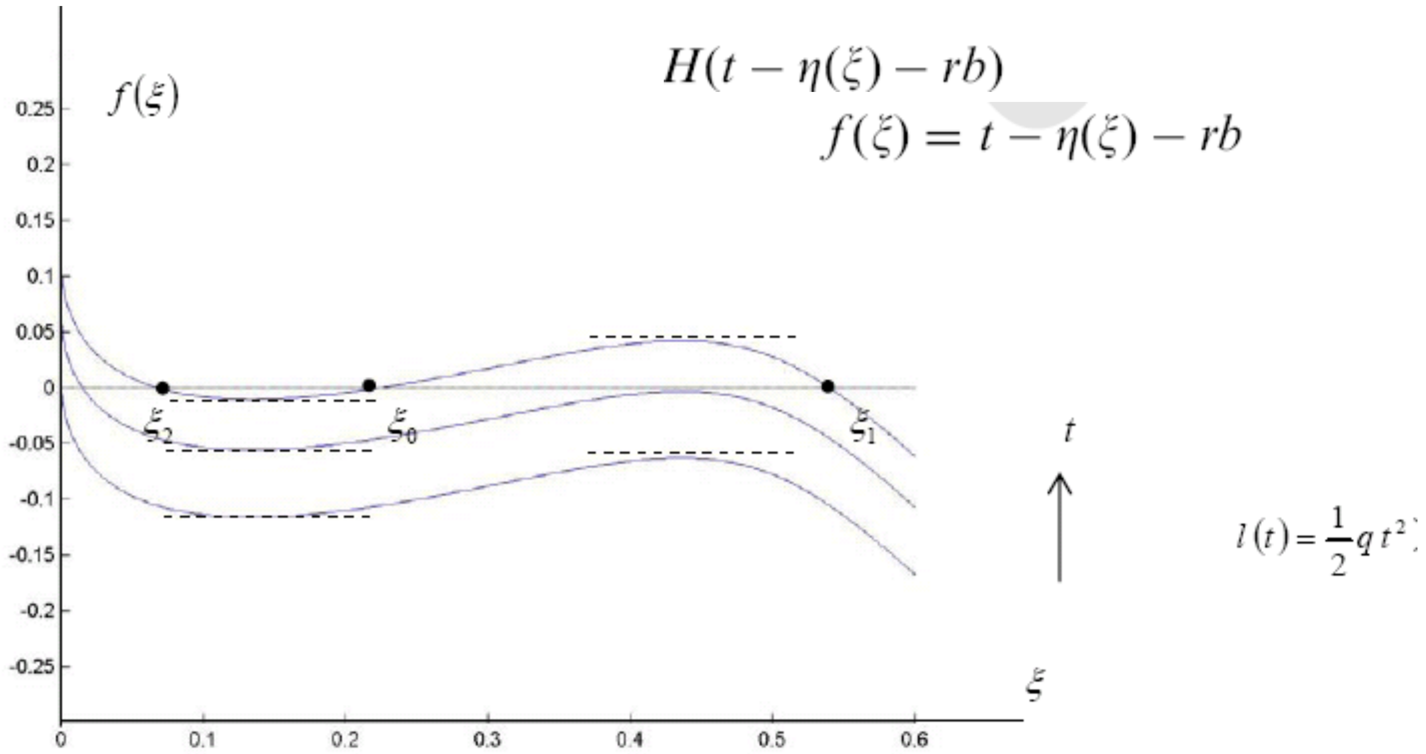




$$f\left(\xi^*\right) = t^* - \eta\left(\xi^*\right) - b\sqrt{\left(x-\xi^*\right)^2 + z^2} = 0$$

$$\frac{d}{d\xi}\left(t^* - \eta\left(\xi^*\right) - b\sqrt{\left(x-\xi^*\right)^2 + z^2}\right) = 0$$

The path intervals that contribute to the motion



$$H(t-\eta(\xi)-rb)$$

$$f(\xi)=t-\eta(\xi)-rb$$

$$l(t)=\frac{1}{2}qt^2$$

Figure 1 $f(\xi)=t-\sqrt{\dfrac{2\xi}{q}}-b\sqrt{(x-\xi)^2+z^2}$ with $q=4$, $b=1$, $x=0.5$, $z=0.1$.

Markenscoff and Huang, *JMPS,* 2008

Stress at forming Mach-front

$$\eta(\xi) = \eta(\xi^*) + \eta'(\xi^*)(\xi - \xi^*) + \frac{1}{2}\eta''(\xi^*)(\xi - \xi^*)^2 + o(\xi - \xi^*)^2$$

$$\eta'(\xi^*) = b.$$

$$\bar{A}\,\delta(t - t^*)$$

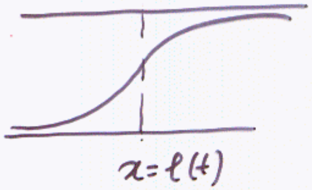
$$\bar{A} = \lim_{\xi_0,\xi_1 \to \xi^*} \frac{\Delta u}{2\pi} z^2 \frac{b^2}{[(x-\xi^*)^2 + z^2]\left|\eta''(\xi^*)(t - \eta(\xi^*))\right|^{\frac{1}{2}}} \int_{\xi_0}^{\xi_1} \frac{d\xi}{\left|(\xi - \xi^*)\right|}$$

$$= \lim_{\xi,\xi_0,\xi_1 \to \xi^*} O\left(\frac{\ln\left|(\xi - \xi^*)\right|\Big|_{\xi_0}^{\xi_1}}{\left|(\xi - \xi^*)\right|^{\frac{1}{2}}} \right)$$

X.M & S.Huang, *JMPS*, 2008

Self-force, X.M.& S.Huang *APL*, 2009

Ramp-core



ii) $\varepsilon = \varepsilon(t)$ variable core width

$$f_0(x) = \frac{1}{\pi} \arctan \frac{x}{\varepsilon} + \frac{1}{2}$$

$$f_1(x) = \frac{1}{\pi} \arctan \frac{x - \ell(t)}{\varepsilon(t)} + \frac{1}{2}$$

$$f_3(x,t) = \frac{\partial}{\partial t} f_1(x,t) = -\frac{1}{\pi} \frac{(x - \ell(t))\,\varepsilon'(t) + \varepsilon(t)\,\ell'(t)}{\varepsilon^2(t) + (x - \ell(t))^2}$$

$$\frac{\partial u}{\partial z}(x,z,t) = \frac{\Delta u}{2\pi} \frac{\partial}{\partial t} \Big\{ \Big[\int_{-\infty}^{\infty} d\xi \int_0^{\infty} d\omega \, H(t - \omega - \hat{r} b)$$

$$\cdot F(t-\omega, x-\xi) * \frac{1}{\pi} \frac{(\xi - \ell(t))\,\varepsilon'(\omega)\,\ell'(\omega)}{\varepsilon^2(\omega) + (\xi - \ell(\omega))^2} \Big] \Big\}$$

Markenscoff & Ni, J.M.P.S (2001)

Ramp-core dislocation accelerating through the shear-wave speed

$$\frac{\partial u(x,z,t)}{\partial z}=\frac{B}{2\pi}\frac{\partial}{\partial t}\left\{\int_{-\infty}^{\infty}d\xi\left[\int_{\zeta_0}^{\zeta_1}d\zeta H\left(t-\eta(\zeta^*)-\sqrt{(x-\xi-\zeta^*)^2+z^2}\,b\right)\right.\right.$$

$$\left(\frac{(t^*-\eta(\zeta^*))^2 z^2}{\left[(x-\xi-\zeta^*)^2+z^2\right]^2\sqrt{-b^2\xi^2+2b^2(x-\zeta^*)\xi-(t-\eta(\zeta^*))\eta''(\zeta^*)(\zeta-\zeta^*)^2}}\right.$$

$$\left.\left.\left.-\frac{(x-\xi-\zeta^*)^2\sqrt{-b^2\xi^2+2b^2(x-\zeta^*)\xi-(t-\eta(\zeta^*))\eta''(\zeta^*)(\zeta-\zeta^*)^2}}{\left[(x-\xi-\zeta^*)^2+z^2\right]^2}\right)\right]\frac{1}{\pi}\frac{\varepsilon}{\varepsilon^2+\xi^2}d\xi\right\}$$

Convolution first, wave-front limit next, singularity smoothed out

For a ramp-core dislocation the coefficient of the delta function
for the stress at the forming Mach front will be finite.

SELF_FORCE (dynamic J)

Markenscoff ,X.& S.Huang, *JMPS*,vol 56,pp2225-2239, 2008

Self-Force on a Dislocation Accelerating/ Decelerating through the shear wave-speed

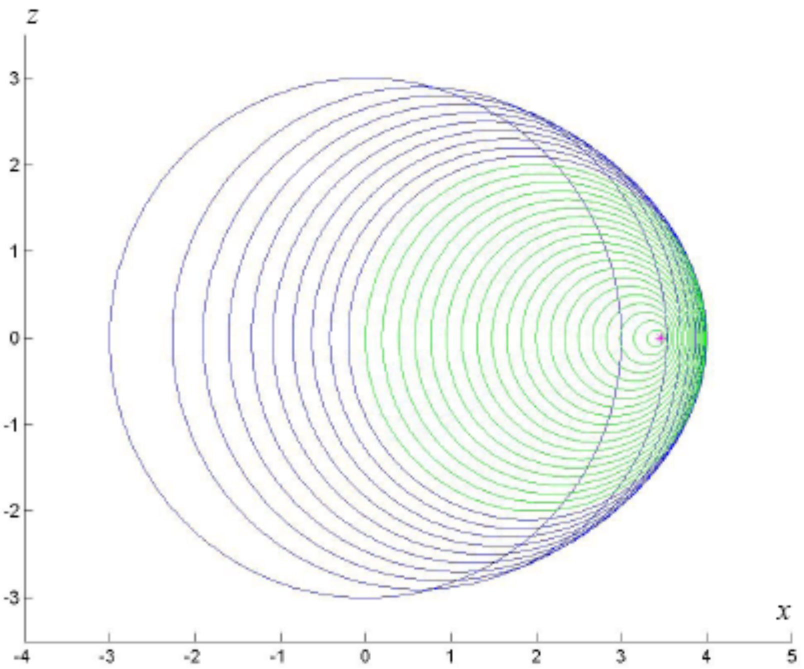


Figure 2: Detachment of the Mach cone from the decelerating dislocation

The red * refers to the current position of the dislocation moving with $x = 2t^{\frac{1}{2}}$ at time t=3. The dislocation motion transits from supersonic to subsonic at time t=1. The blue circles refer to the wavelets let off by the dislocation before t=1. The green circles refer to the wavelets let off after t=1. The ratio of the dislocation velocity at time t=3 versus the shear wave speed is $\dot{l}(t = 3.0)/c_2 = 0.5774$.

$$
\begin{aligned}
F_l(t) = {} & \lim_{z \to 0, x \to l(t^*)} \mu \frac{b}{2\pi} \frac{1}{|\ddot{l}(t^*)|^{1/2}} \\
& \times \int_{-\infty}^{\infty} \frac{z^2}{\{[x - l(t^*) - \xi]^2 + z^2\}^{5/4}} \ln[x - l(t^*) - \xi] \\
& \times \frac{\varepsilon}{\varepsilon^2 + \xi^2} d\xi \times \delta(t - t^*),
\end{aligned}
$$

Markenscoff and Huang, *APL* , 2009

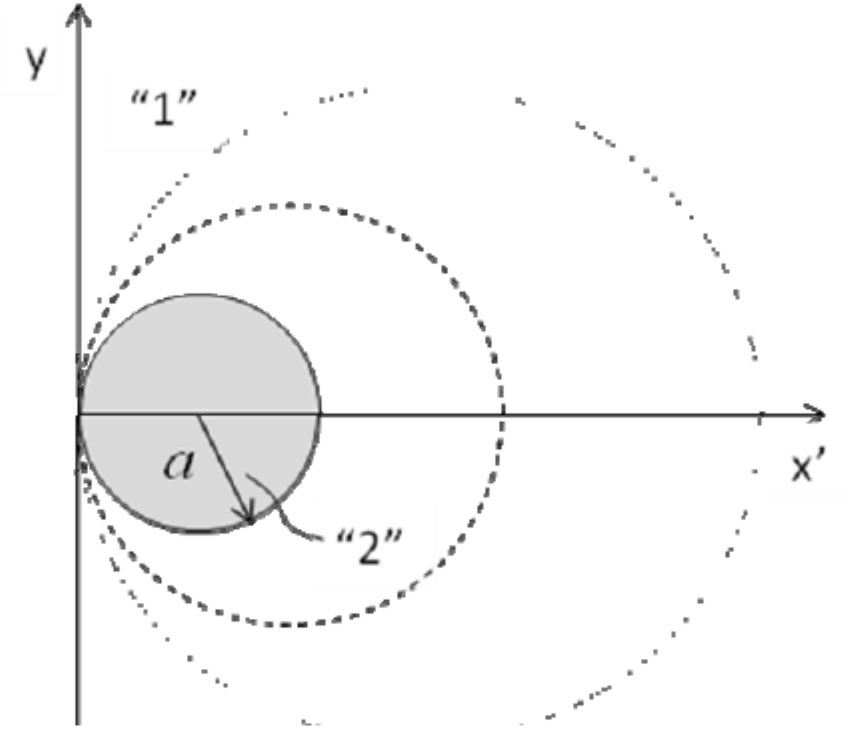
Dundurs &XM, *IJSS*, 2009

Plane boundary as a limit of a circular/spherical inclusion/ inhomogeneity

$$x' \rightarrow x-a$$

$$y \rightarrow y$$

$$r^2 \rightarrow (x-a)^2 + y^2$$



$$\sigma_{xx}^{(1)} = -2\mathrm{K}e\left\{-\frac{a^2}{(x-a)^2+y^2} + \frac{2a^2(x-a)^2}{\left[(x-a)^2+y^2\right]^2}\right\}$$

$$\sigma_{xy}^{(1)} = -2\mathrm{K}e\frac{2xya^2}{\left[(x-a)^2+y^2\right]^2}$$

$$\sigma_{yy}^{(1)} = -2\mathrm{K}e\left\{\frac{a^2}{(x-a)^2+y^2} - \frac{2a^2(x-a)^2}{\left[(x-a)^2+y^2\right]^2}\right\}$$

$$\sigma_{xx}^{(2)} = \sigma_{yy}^{(2)} = -2\mathrm{K}e, \quad \sigma_{xy}^{(2)} = 0$$

Limit $a \rightarrow \infty$, $\frac{a^2}{(x-a)^2+y^2} \rightarrow 1, \quad \frac{a^2(x-a)^2}{\left[(x-a)^2+y^2\right]^2} \rightarrow 1$

$$\sigma_{xx}^{(1)} = \sigma_{xx}^{(2)} = -2\mathrm{K}e$$

$$\sigma_{xy}^{(1)} = \sigma_{xy}^{(2)} = 0$$

$$\sigma_{yy}^{(1)} = -\sigma_{yy}^{(2)} = 2\mathrm{K}e$$

Eshelby solution + Hill jump conditions

$$[\sigma_{ij}] \equiv \sigma_{ij}(\mathrm{out}) - \sigma_{ij}(\mathrm{in}) = C_{ijkl}\{[u_{k,l}] - [\epsilon^*_{kl}]\}$$

$$= C_{ijkl}\{-C_{pqmn}\epsilon^*_{mn}n_q n_l N_{kp}(\boldsymbol{n})/D(\boldsymbol{n}) + \epsilon^*_{kl}\}$$

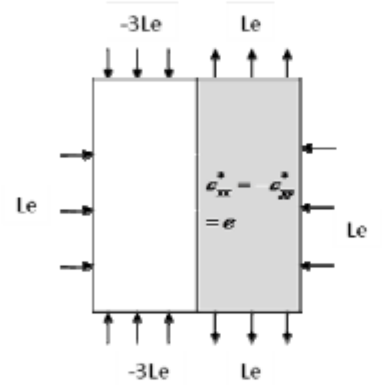
Superposed tractions at infinity

Pure shear eigenstrain

$$\sigma_{xx}^{(1)} = \sigma_{xx}^{(2)} = -Le$$

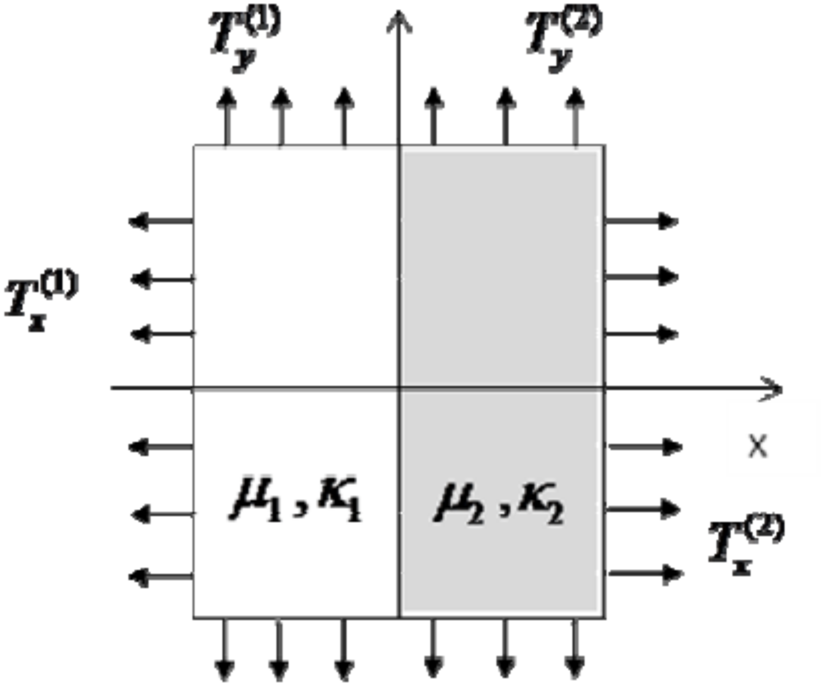
$$\sigma_{xy}^{(1)} = \sigma_{xy}^{(2)} = 0$$

$$\sigma_{yy}^{(1)} = -3Le,\ \sigma_{yy}^{(2)} = Le \qquad \text{with} \quad L = \frac{2\mu_2}{\Gamma\kappa_1 + 1}$$



Rogue states!

$$(1-\alpha)T_y^{(2)} = (1+\alpha)T_y^{(1)} - 2(\alpha - 2\beta)T_x$$



$$F_x = \frac{1}{2}(\sigma_{xx}^{(1)} + \sigma_{xx}^{(2)})\varepsilon_{xx}^{*} + \frac{1}{2}(\sigma_{yy}^{(1)} + \sigma_{yy}^{(2)})\varepsilon_{yy}^{*}$$

$$= \frac{1}{2}(-2Le)e + \frac{1}{2}(-3Le + Le)(-e) = -Le^2 + Le^2 = 0$$

$$W^* = \tfrac{1}{2}\int_D \sigma_{ij}^0 u_{i,j}^0 \,\mathrm{d}D - \tfrac{1}{2}\int_\Omega \sigma_{ij}\epsilon_{ij}^{*} \,\mathrm{d}D.$$

Increase the energy

Strips with eigenstrain meeting a free surface

Cancel tractions by Boussisnesq/Cerruti

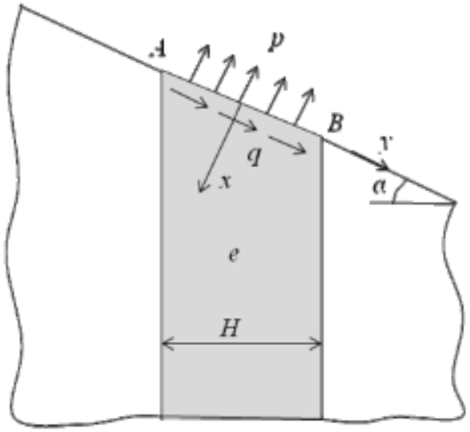
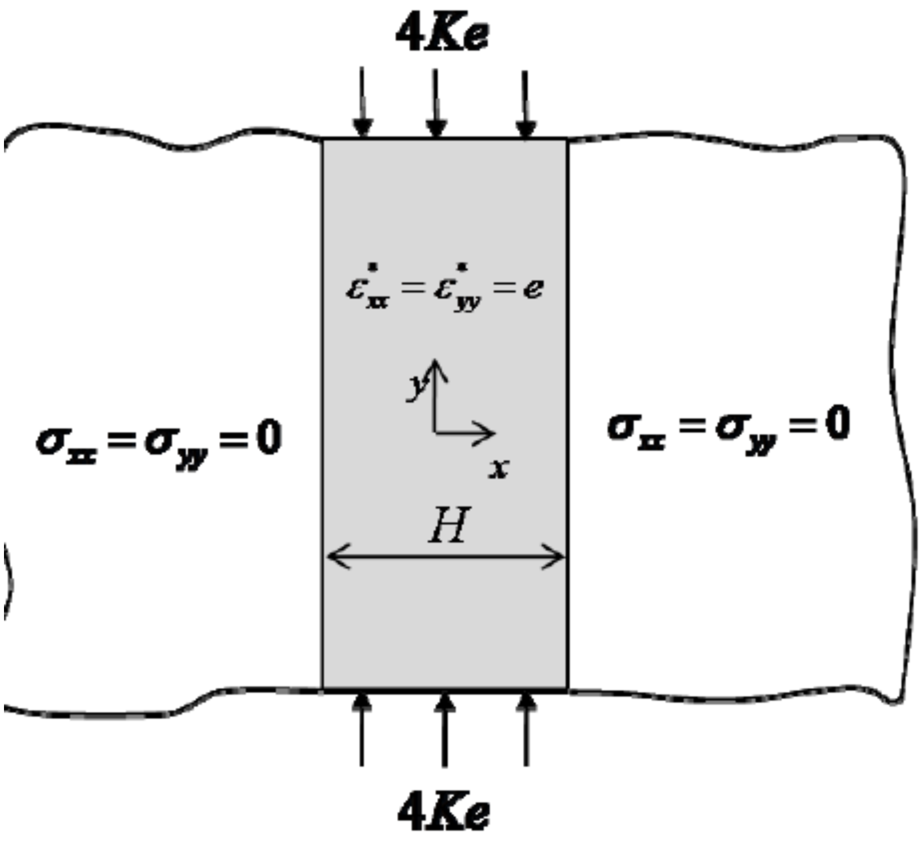
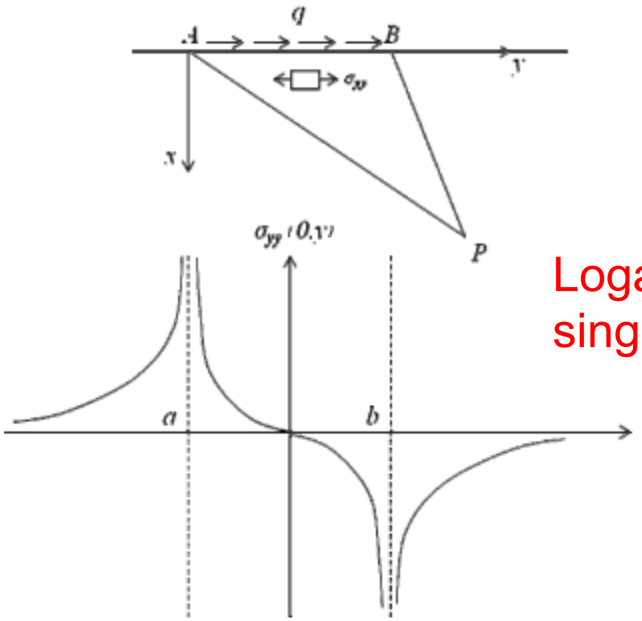


Figure 6. Strip meeting a free surface

inclusion





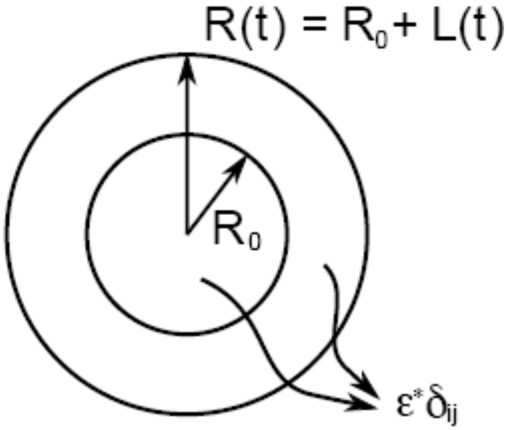
Logarithmic singularity

A dynamically expanding spherical Eshelby Inclusion

$$u_i(\boldsymbol{x},t) = \int_{-\infty}^{\infty} dt' \int_{S(t)} c_{jklm}\delta_{lm}\epsilon^* n_k(\boldsymbol{x'})G_{ij}(\boldsymbol{x}-\boldsymbol{x'},t-t')dS,$$

Willis, 1965

$$G_{km}(\bar{r}_i,\bar{t}) = \frac{1}{4\pi\rho}\left\{\frac{\bar{t}}{\bar{r}^2}[\frac{3\bar{r}_k\bar{r}_m}{\bar{r}^3} - \frac{\delta_{km}}{\bar{r}}]H(\bar{t}-\frac{\bar{r}}{a})H(\frac{\bar{r}}{b}-\bar{t}) + \frac{\bar{r}_k\bar{r}_m}{\bar{r}^3}[\frac{\delta(\bar{t}-\bar{r}/a)}{a^2} - \frac{\delta(\bar{t}-\bar{r}/b)}{b^2}] + \frac{\delta_{km}\delta(\bar{t}-\bar{r}/b)}{b^2}\right\},$$



$$u_r(r,t) = \frac{3\lambda+2\mu}{2\rho a}\left[\int_{-\infty}^{0}\frac{R_0}{r}\epsilon^*\cos\theta_0(t-t')f_0(t-t')dt' + \int_{0}^{\infty}\frac{R(t')}{r}\epsilon^*\cos\theta_{t'}(t-t')f_{t'}(t-t')dt'\right],$$

$$f_s(t-t') = \begin{cases} 0, & a(t-t') < |r-R(s)| \\ 1, & |r-R(s)| \le a(t-t') \le r+R(s) \\ 0, & r+R(s) < a(t-t'). \end{cases}$$

$$\cos\theta_s(t-t') = \begin{cases} 1, & \\ \frac{r^2+R^2(s)-a^2(t-t')^2}{2rR(s)}, & |r-R(s)| \le a(t-t') \le r+R(s), \\ -1, & r+R(s) < a(t-t'), \end{cases}$$

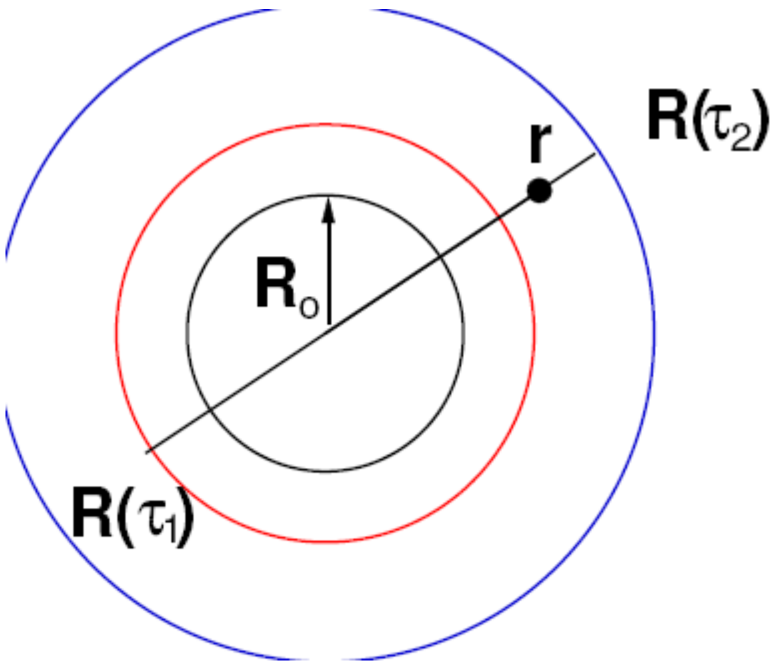
$$
\begin{aligned}
u_r(r,t) = & -\frac{R_0^3(3\lambda+2\mu)\epsilon^*}{3r(\lambda_2\mu)}H(r-R_0-at) + \frac{r(3\lambda+2\mu)\epsilon^*}{3(\lambda+2\mu)}H(R_0-r-at) \\
& + u_r^{II}(r,t)H(at-|r-R_0|)H(r+R_0-at) \\
& + u_r^{III}(r,t)H(at-r-R_0), \qquad (2.5)
\end{aligned}
$$

where u_r^{II} and u_r^{III} are given by

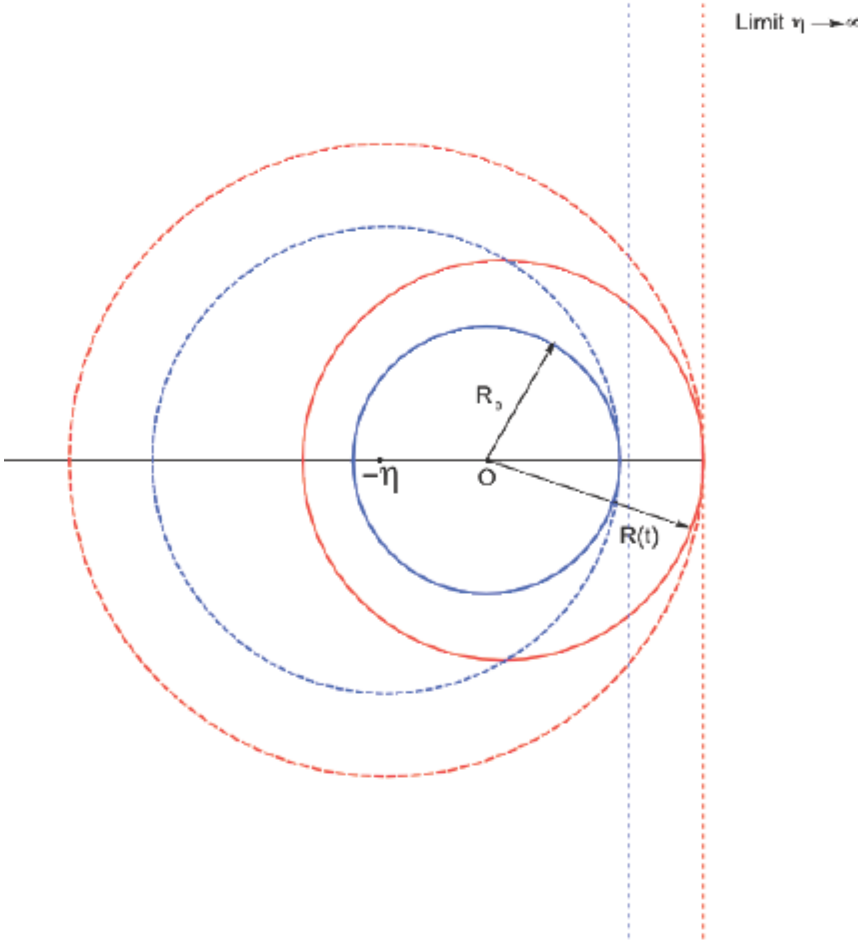
Hadamard jumps

$$
\begin{aligned}
u_r(r,t) = & \frac{a(3\lambda+2\mu)\epsilon^*}{4(\lambda+2\mu)r^2}\int_t^{\frac{r+R_0}{a}}(r^2+R_0^2-a^2s^2)ds \\
& + \frac{a(3\lambda+2\mu)\epsilon^*}{4(\lambda+2\mu)r^2}\int_0^{\tau_2}[r^2+R^2(t')-a^2(t-t')^2]dt' \\
& = \frac{(3\lambda+2\mu)\epsilon^*}{4\rho a^2r^2}\left\{a(r^2+R_0^2)(\tau_2-t)+\frac{1}{3}[2(r^3+R_0^3)+a^3(t-\tau_2)^3]\right. \\
& \left. + \int_0^{\tau_2} a[2R_0l(t')+l^2(t')]dt'\right\},
\end{aligned}
$$

$$
\begin{aligned}
u_r^{III}(r,t) = & \frac{(3\lambda+2\mu)\epsilon^*}{4\rho ar^2}\int_{\tau_1}^{\tau_2}[r^2+R^2(t')-a^2(t-t')^2]dt' \\
= & \frac{(3\lambda+2\mu)\epsilon^*}{4\rho ar^2}\{(r^2+R_0^2)(\tau_2-\tau_1) \\
& + \frac{a^2}{3}[(t-\tau_2)^3-(t-\tau_1)^3] + \int_{\tau_1}^{\tau_2}[2R_0l(t')+l^2(t')]dt'\}
\end{aligned}
$$

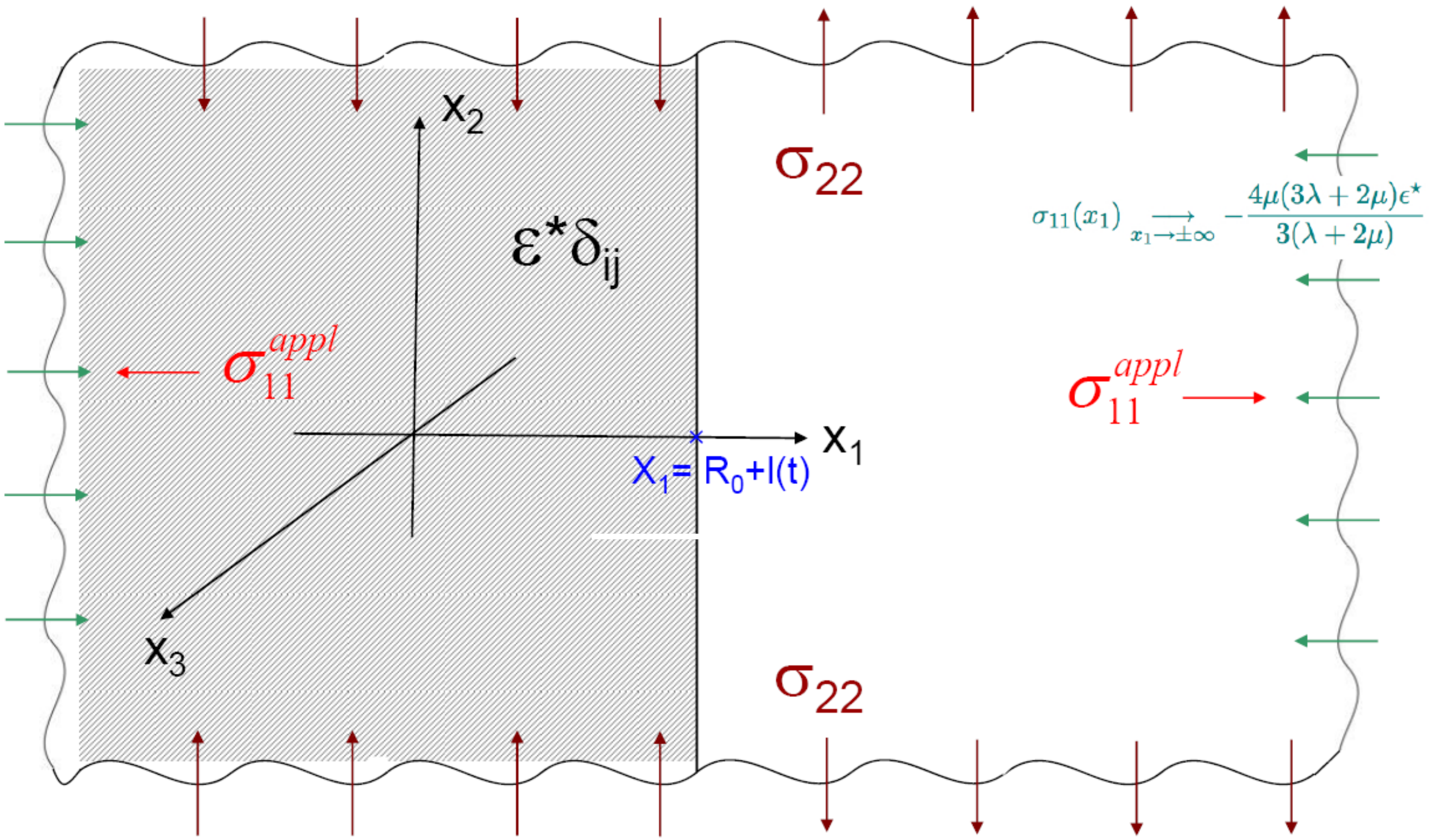


Limiting procedure to obtain plane moving phase boundary



$$Q_s(R_0, R(t), r; t) \Longrightarrow Q_s(R_0+\eta, R(t)+\eta, r+\eta; t).$$

$$Q_p(R_0, R(t), x_1; t) = \lim_{\eta\to\infty} Q_s(R_0+\eta, R(t)+\eta, x_1+\eta; t).$$



$$\sigma_{11}(x_1) \underset{x_1 \to \pm\infty}{\longrightarrow} -\frac{4\mu(3\lambda+2\mu)\epsilon^\star}{3(\lambda+2\mu)}$$

$$(\sigma_{22})_P = (\sigma_{33})_P = -H(R_0 + l(t) - x_1)\left[\frac{4\mu(3\lambda+2\mu)\epsilon^\star}{3(\lambda+2\mu)} + \frac{\lambda(3\lambda+2\mu)\epsilon^\star}{2(\lambda+2\mu)}\frac{\dot{l}(\tau_2)}{a+\dot{l}(\tau_2)}H(at - |x_1 - R_0|)\right]$$

$$+H(x_1 - (R_0 + l(t)))\left[\frac{2\mu(3\lambda+2\mu)\epsilon^\star}{3(\lambda+2\mu)} - \frac{\lambda(3\lambda+2\mu)\epsilon^\star}{2(\lambda+2\mu)}\frac{\dot{l}(\tau_2)}{a-\dot{l}(\tau_2)}H(at - |x_1 - R_0|)\right]$$

Unique, with initial condition the minimum energy one

Energy-release rate for a moving phase boundary

Dynamic *J* integral equivalent to energy-release-rate for jump discontinuity

Freund, 1972

$$\dot{\mathcal{E}} = \lim_{\epsilon \to 0} \int_{S_\epsilon} [n_j \sigma_{ij} \dot{u}_i + v_n (W + T)] dS$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (n_j [[\sigma_{ij} \dot{u}_i]] + \dot{l}[[W]] + \dot{l}[[T]]) dx_2 dx_3,$$

$$n_j [[\sigma_{ij}]] = -\dot{l}(t) [[\dot{u}_i]].$$

$$[[\dot{u}_i]] = -\dot{l}(t) [[\frac{\partial u_i}{\partial n}]].$$

$$\dot{\mathcal{E}} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} -\dot{l}(t) ([[W]] - < \sigma_{ij} > [[\frac{\partial u_i}{\partial x_j}]]) dx_2 dx_3.$$

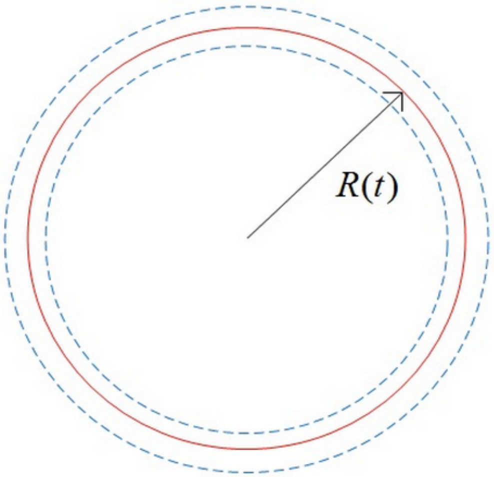
$$f = [[W]] - < \sigma_{ij} > [[\partial u_i / \partial x_j]].$$

Self-Force on a Dynamically Expanding Spherical Inclusion

$$f = [[W]] - < \sigma_{ij} > [[\partial u_i / \partial x_j]],$$

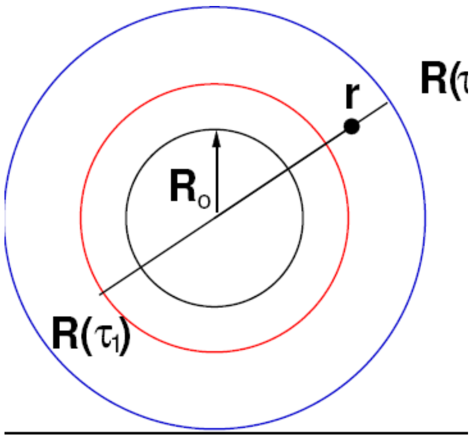
$$f = -\langle \sigma_{km} \rangle [\![\varepsilon^*_{km}]\!]$$

$$= -\frac{2\mu(3\lambda+2\mu)^2\epsilon^{*2}}{(\lambda+2\mu)} - \frac{(3\lambda+2\mu)^2\epsilon^{*2}}{2(\lambda+2\mu)}[\frac{a\dot{l}(t)}{(a^2-\dot{l}^2(t))}]$$
$$+H(at-(R(t)+R_0))\frac{\epsilon^{*2}(3\lambda+2\mu)^2}{2(\lambda+2\mu)}[\frac{R(\tau_1)}{R(\tau_2)}(\frac{\dot{l}(\tau_1)}{a+\dot{l}(\tau_1)})]|_{r=R(t)}$$



$$a(t-\tau_2) = |r - R(\tau_2)|$$

XM & L.Ni, *JMPS*, 2010



Static term coincides with Gavazza (1977),
Eshelby (1977)

SELF- FORCE ON MOVING PLANE BOUNDARY

(limit from the sphere)

$$\dot{\mathcal{E}} = \lim_{S_d \to 0} \int_{S_d} [n_j \sigma_{ij} \dot{u}_i + v_n (W + T)] dS.$$

$$f = \mathcal{E}/\dot{l}(t) = [[W]] - < \sigma_{ij} > [[\frac{\partial u_i}{\partial x_j}]]$$

$$f = - < \sigma_{km} > [[\epsilon^*_{km}]];$$

$$\begin{aligned} f_p &= (< \sigma^0_{11} + \sigma^0_{22} + \sigma^0_{33} >)_p \epsilon^* - \frac{3}{2}(3\lambda + 2\mu)\epsilon^{*2} \\ &= \lim_{\eta \to \infty} (< \sigma^0_{11} + \sigma^0_{22} + \sigma^0_{33} >)_S |_{(R_0+\eta, R(t)+\eta)} \epsilon^* - \frac{3}{2}(3\lambda + 2\mu)\epsilon^{*2} \\ &= \lim_{\eta \to \infty} f_s(R(t) + \eta) \\ &= -\frac{2\mu(3\lambda + 2\mu)\epsilon^{*2}}{(\lambda + 2\mu)} - \frac{(3\lambda + 2\mu)^2 \epsilon^{*2}}{2(\lambda + 2\mu)} [\frac{a\dot{l}(t)}{a^2 - \dot{l}^2(t)}]. \end{aligned}$$

Self-force

Static, Eshelby,
Gavazza,1977

inertia

Markenscoff and Ni, *J.M.P.S.*, 2010

EQUATION OF MOTION OF AN INCLUSION BOUNDARY
("kinetic relation")

$$f = -\langle \sigma_{km} \rangle [\![\varepsilon^*_{km}]\!]$$

Peach-Koehler force

$$< \sigma^{appl}_{k\ell} > [[\varepsilon^*_{k\ell}(\mathbf{x}, t)]]$$

Superpose *external loading*---all interaction terms in driving force

Noether's theorem (N&S,
Also in non-linear elasticity)

dynamic

total $J = 0$

A plane boundary with dilatational eigenstrain and superposed applied tension

$$-\frac{2\mu(3\lambda+2\mu)\varepsilon^{*2}}{(\lambda+2\mu)} - \frac{(3\lambda+2\mu)^2\varepsilon^{*2}}{2(\lambda+2\mu)}\left[\frac{a\dot{\ell}(t)}{a^2-\dot{\ell}^2(t)}\right] + \sigma^a_{11}\varepsilon^* = \begin{cases} 0 & \\ F(\dot{l}(t)) & \text{(dissipation)} \end{cases}$$

surface energies

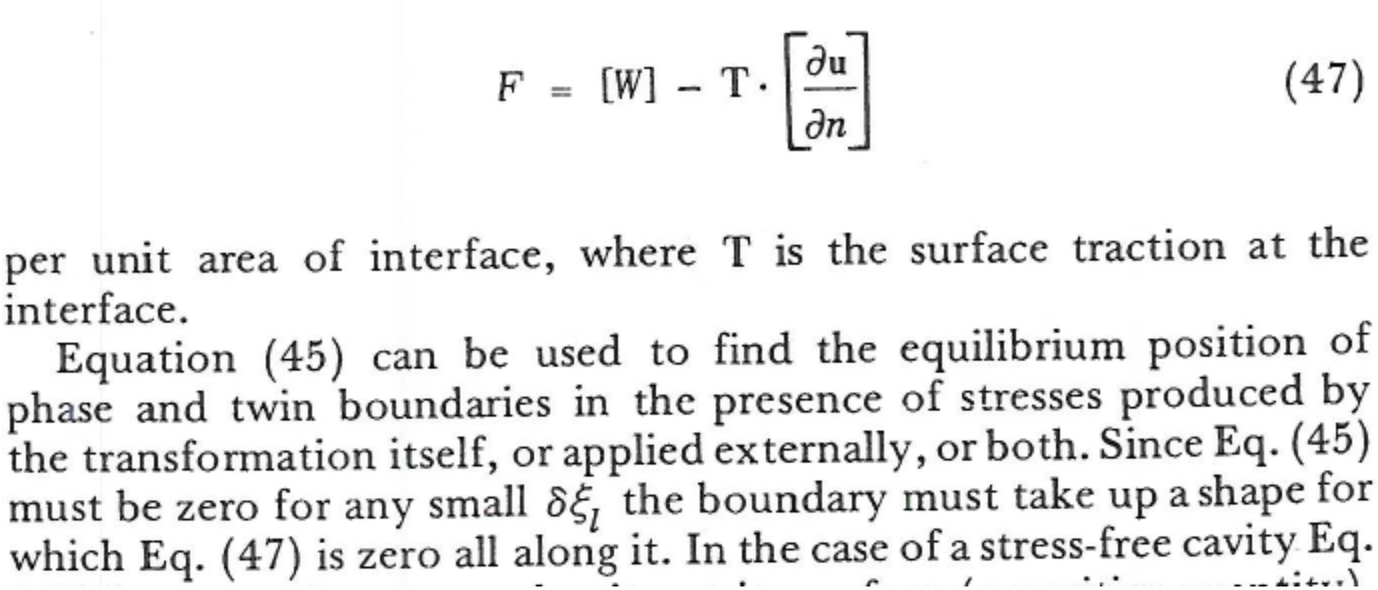
Self-force

Peach-Koehler

$$\frac{\partial \sigma^a_{11}}{\partial \dot{l}} = \frac{(3\lambda+2\mu)^2\epsilon^*}{2(\lambda+2\mu)}\left[\frac{a(a^2+\dot{l}^2(t))}{(a^2-\dot{l}^2(t))^2}\right].$$

Equilibrium position of phase boundary

“Eshelby principle”



$$F = [W] - \mathbf{T} \cdot \left[\frac{\partial \mathbf{u}}{\partial n}\right] \tag{47}$$

per unit area of interface, where T is the surface traction at the interface.

Equation (45) can be used to find the equilibrium position of phase and twin boundaries in the presence of stresses produced by the transformation itself, or applied externally, or both. Since Eq. (45) must be zero for any small $\delta\xi_l$ the boundary must take up a shape for which Eq. (47) is zero all along it. In the case of a stress-free cavity Eq.

Eshelby, 1970

In the physical cases described, and in others, the boundary may be capable of migrating through the material (growth of martensitic plates, change in the form of a cavity by volume or surface diffusion, and so on). In Fig. 3 migration has made S develop a shallow blister, changing it to S'. The migration may be specified by erecting a small vector $\delta\xi_i$ at each point of S. It is then a sensible question to ask what is the change in the total energy of the system as a result of the migration. The answer is that

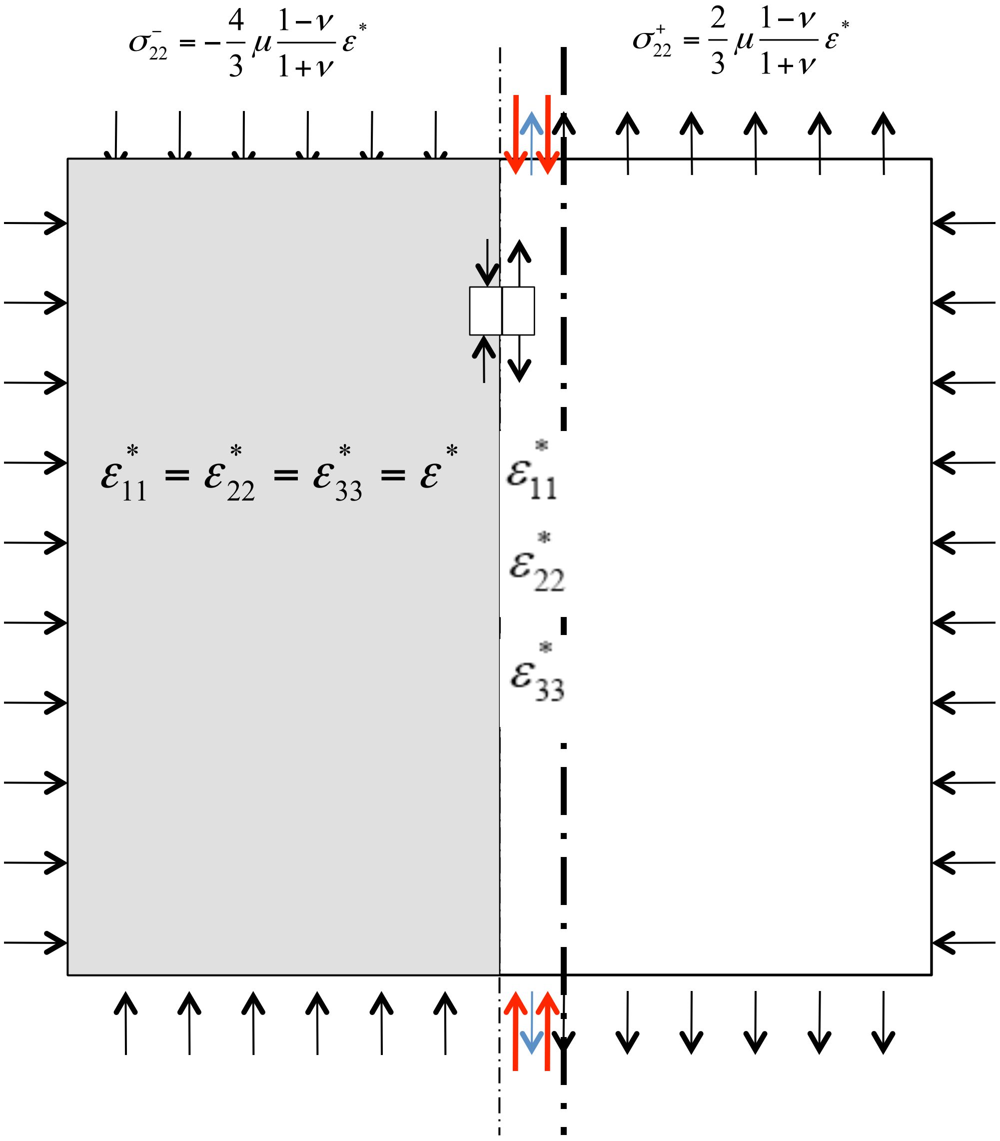
This expression only gives the change in the elastic energy and the energy of the loading mechanism. If it is to be applied to phase changes we must also include the "chemical" energy, the work required to transform the material which disappeared from A into the material which appeared in B, say

$$\int \delta\xi_l (W_0^B - W_0^A)\, dS_l \tag{44}$$

where $W_0^B - W_0^A$ is the work required to transform a mass of unstressed A into an equal mass of unstressed B, the mass occupying

$W^A(0) - W^B(0) = W_o^A - W_o^B$. The addition of a constant to W does not, of course, alter Eq. (18), because the extra term is proportional to $\int dS_l$ and so is zero for a closed surface being, by Gauss' theorem, the volume integral of the gradient of unity. It appears that the value

Generate new region of eigenstrain



$$\sigma_{22}^{-} = -\frac{4}{3}\mu\frac{1-\nu}{1+\nu}\varepsilon^{*}$$

$$\sigma_{22}^{+} = \frac{2}{3}\mu\frac{1-\nu}{1+\nu}\varepsilon^{*}$$

$$\varepsilon_{11}^{*} = \varepsilon_{22}^{*} = \varepsilon_{33}^{*} = \varepsilon^{*}$$

ε_{11}^{*}

ε_{22}^{*}

ε_{33}^{*}

$$\sigma_{11} = -\frac{4}{3}\mu\frac{1-\nu}{1+\nu}\varepsilon^{*}$$

Total driving force=0

$$-\frac{2\mu(3\lambda+2\mu)\epsilon^{*2}}{(\lambda+2\mu)} + \sigma_{11}^{a}\epsilon^{*} = 0,$$

$$\sigma_{11}^{a} = -\frac{2\mu(3\lambda+2\mu)\epsilon^{*}}{(\lambda+2\mu)}$$

determines $\varepsilon_{11}^{*} = \varepsilon^{*}$

$$\varepsilon_{ij} - \varepsilon_{ij}^{*} = (\sigma_{ij} - \delta_{ij}\sigma_{kk}\frac{\nu}{1+\nu})/2\mu$$

Interface condition : $\sigma_{11}^{-} = \sigma_{11}^{+}$

$\varepsilon_{22}^{-} = \varepsilon_{22}^{+}$

$\varepsilon_{33}^{-} = \varepsilon_{33}^{+}$

$\varepsilon_{33}^{*} = \varepsilon_{22}^{*} = \varepsilon^{*}$, ε_{11}^{*} undertermined

Limit of Spherical inclusion

Eshelby inside+ Hill jump conditions outside

XM, *Int. J. Fr, 2010*

Driving force on a plane boundary of a half-space inclusion with *general* eigenstrain

Self-force

$$f = f_o - \frac{1}{2}\frac{\left[(\lambda+2\mu)\varepsilon_{11}^{*} + \lambda(\varepsilon_{22}^{*}+\varepsilon_{33}^{*})\right]^2}{(\lambda+2\mu)}\frac{c_1\dot{\ell}(t)}{c_1^2-\dot{\ell}^2(t)} - \frac{2\mu c_2\dot{\ell}(t)}{c_2^2-\dot{\ell}^2(t)}\left[(\varepsilon_{12}^{*})^2+(\varepsilon_{13}^{*})^2\right]$$

$$\begin{aligned} f_0 &= \varepsilon_{11}^{\star}\sigma_{11}^{0} + \frac{1}{2}\varepsilon_{22}^{\star}({\sigma_{22}^{0}}^{(\mathrm{in})} + {\sigma_{22}^{0}}^{(\mathrm{ex})}) + \frac{1}{2}\varepsilon_{33}^{\star}({\sigma_{33}^{0}}^{(\mathrm{in})} + {\sigma_{33}^{0}}^{(\mathrm{ex})}) \\ &+ 2\sigma_{12}^{0}\varepsilon_{12}^{\star} + 2\varepsilon_{13}^{\star}\sigma_{13}^{0} + \varepsilon_{23}^{\star}({\sigma_{23}^{0}}^{(\mathrm{in})} + {\sigma_{23}^{0}}^{(\mathrm{ex})}) \\ &= -\frac{32\mu(\lambda+\mu)}{15(\lambda+2\mu)}(\varepsilon_{11}^{\star})^2 - \frac{2\mu(\lambda+\mu)}{15(\lambda+2\mu)}\left((\varepsilon_{22}^{\star})^2 + (\varepsilon_{33}^{\star})^2\right) - \frac{4\mu(7\lambda+2\mu)}{15(\lambda+2\mu)}\varepsilon_{11}^{\star}(\varepsilon_{22}^{\star}+\varepsilon_{33}^{\star}) \\ &+ \frac{2\mu(\lambda-4\mu)}{15(\lambda+2\mu)}\varepsilon_{22}^{\star}\varepsilon_{33}^{\star} - \frac{4\mu(9\lambda+14\mu)}{15(\lambda+2\mu)}\left((\varepsilon_{12}^{\star})^2 + (\varepsilon_{13}^{\star})^2\right) - \frac{2\mu(3\lambda-2\mu)}{15(\lambda+2\mu)}(\varepsilon_{23}^{\star})^2 \qquad (75) \end{aligned}$$

Superpose external loading--- all interaction terms in driving force

Peach-Koehler force

$$< \sigma_{k\ell}^{appl} > [[\varepsilon_{k\ell}^{*}(\mathbf{x},t)]]$$

XM &L.Ni, *Q.A.M,* 2011

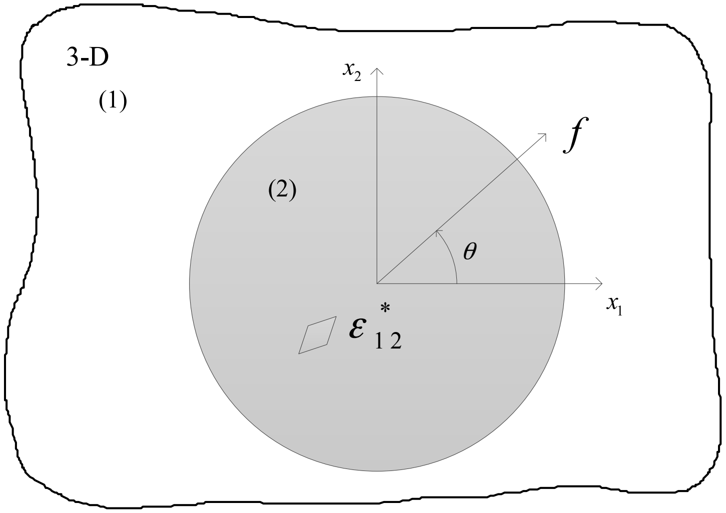
Propagation of the rotation for a plane boundary with shear eigenstrain

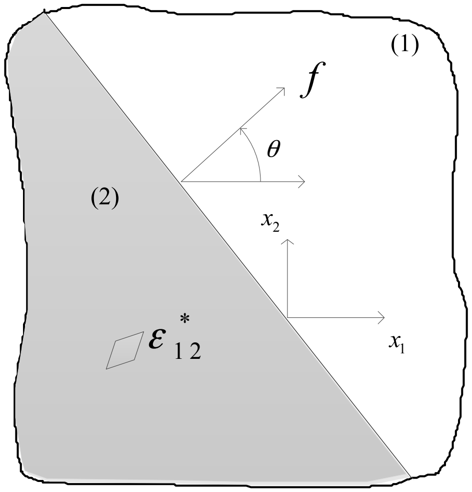
$$\omega_{\ell m} = \frac{1}{2}\left(\frac{\partial u_\ell}{\partial x_m} - \frac{\partial u_m}{\partial x_\ell}\right)$$

$\omega^0_{12} = \varepsilon^\star_{21} H(x_1 - R_0).$

$$\begin{aligned}\omega_{12} = \varepsilon^\star_{21} H\left(x_1 - R(t)\right) + \frac{\varepsilon^\star_{21}}{2}&\left[\frac{\ell(\tau_2)}{\dot{\ell}(\tau_2) + c_2} H\left(R(t) - x_1\right)\right.\\ &\left.+ \frac{\dot{\ell}(\tau_2)}{c_2 - \dot{\ell}(\tau_2)} H\left(x_1 - R(t)\right)\right] H\left(t - \frac{|x_1 - R_0|}{c_2}\right)\end{aligned}$$

$$[[\omega_{12}]] = \varepsilon^\star_{12}\frac{c_2^2 + \dot{\ell}^2(t)}{c_2^2 - \dot{\ell}^2(t)}$$

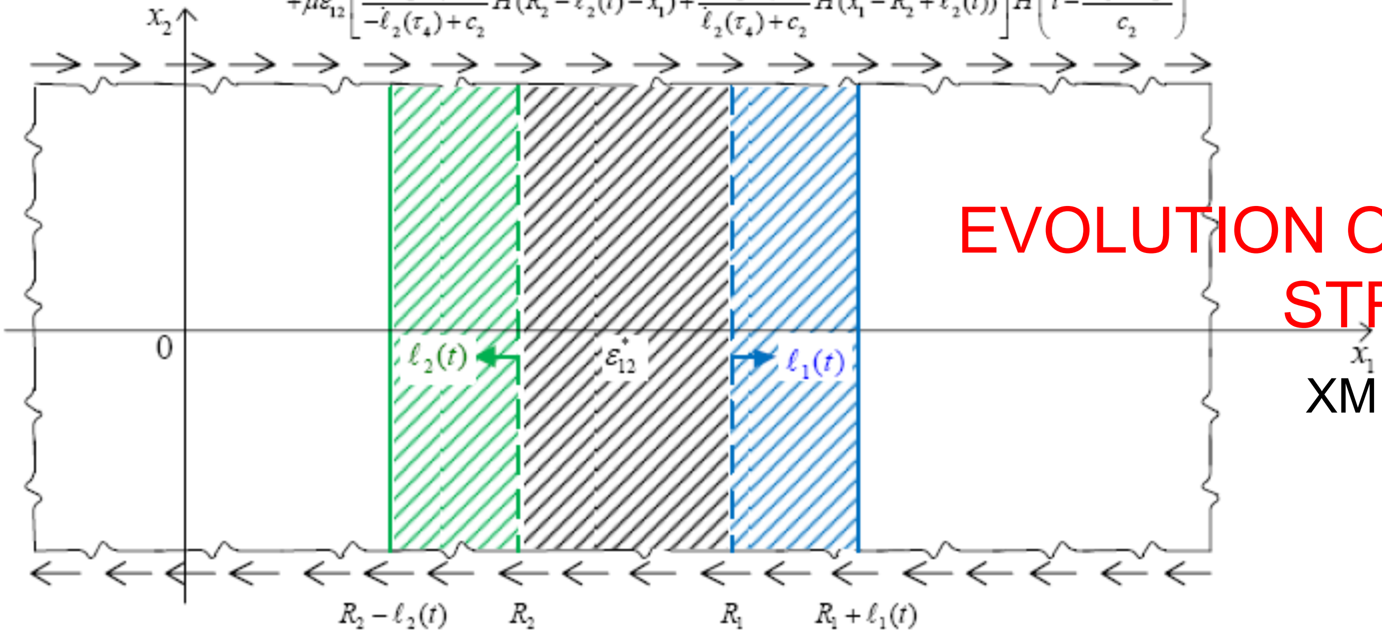




3D $$f(\theta) = -2\mu\left[\frac{7-5\nu}{15(1-\nu)} - \frac{1-\cos 4\theta}{8(1-\nu)}\right]\varepsilon_{12}^*$$

2D $$f(\theta) = -\frac{2\mu_2\varepsilon_{12}^*(1+\cos 4\theta)}{1+\Gamma\kappa_1}$$ $$f = 0 \quad \theta = 45^\circ$$

$$\sigma_{21}=\sigma_{12}=-\mu\varepsilon_{12}^{*}\left[\frac{\dot{\ell}_1(\tau_3)}{\dot{\ell}_1(\tau_3)+c_2}H(R_1+\ell_1(t)-x_1)-\frac{\dot{\ell}_1(\tau_3)}{\dot{\ell}_1(\tau_3)-c_2}H(x_1-R_1-\ell_1(t))\right]H\left(t-\frac{|x_1-R_1|}{c_2}\right)$$
$$+\mu\varepsilon_{12}^{*}\left[\frac{\dot{\ell}_2(\tau_4)}{-\dot{\ell}_2(\tau_4)+c_2}H(R_2-\ell_2(t)-x_1)+\frac{\dot{\ell}_2(\tau_4)}{\dot{\ell}_2(\tau_4)+c_2}H(x_1-R_2+\ell_2(t))\right]H\left(t-\frac{|x_1-R_2|}{c_2}\right)$$



EVOLUTION OF EXPANDING STRIPS

XM & L.Ni, *I.J.E.S.*, 2012

$$\begin{aligned}
f &= -\langle\sigma_{km}\rangle\left[\left[\varepsilon_{km}^{*}\right]\right]=\langle\sigma_{km}\rangle\varepsilon_{km}^{*}\\
&= -\frac{2\mu}{\lambda+2\mu}\left[(\lambda+\mu)\left((\varepsilon_{22}^{*})^2+(\varepsilon_{33}^{*})^2\right)+\mu\varepsilon_{22}^{*}\varepsilon_{33}^{*}+(\lambda+2\mu)(\varepsilon_{23}^{*})^2\right]\\
&\quad-\frac{\left[(\lambda+2\mu)\varepsilon_{11}^{*}+\lambda(\varepsilon_{22}^{*}+\varepsilon_{33}^{*})\right]^2}{2(\lambda+2\mu)}\left[\frac{c_1\dot{\ell}_1(t)}{c_1^2-\dot{\ell}_1^2(t)}+\frac{\dot{\ell}_2(\hat{\tau}_1)}{c_1+\dot{\ell}_2(\hat{\tau}_1)}H(c_1t+R_2-R_1-\ell_1(t))\right]\\
&\quad-2\mu\left[(\varepsilon_{12}^{*})^2+(\varepsilon_{13}^{*})^2\right]\left[\frac{c_2\dot{\ell}_1(t)}{c_2^2-\dot{\ell}_1^2(t)}+\frac{\dot{\ell}_2(\hat{\tau}_2)}{c_2+\dot{\ell}_2(\hat{\tau}_2)}H(c_2t+R_2-R_1-\ell_1(t))\right],
\end{aligned}$$

Modeling

:

Yang,S-Y., Escobar,J. and Clifton, R.J. (2009)
“Computational models for Stress-Induced Martensitic Transformations in NiTi”sss,
Math. Mech. Sol., 14, 220-257. (D. M. Barnett volume)

Expanding inhomogeneity boundaries with eigenstrain

Eshelby’s equivalent inclusion method

$$\varepsilon_{ij}^{**equiv} = \varepsilon_{ij}^{*equiv} + \varepsilon_{ij}^{*}$$

$$C_{ijmn}\varepsilon^{**}_{mn} - \Delta C_{ijmn}\varepsilon_{mn}(\mathbf{x}, t; l(\tau), \varepsilon^{**}_{kl}) = C^{*}_{ijmn}\varepsilon^{*}_{mn} + \sigma^{appl}_{ij} - C^{*}_{ijmn}\varepsilon^{appl}_{mn}$$

Statics, self-similar motion: $\varepsilon_{mn} = S_{mnpq}\varepsilon^{**}_{pq}$

$$c_i(t-\tau_i) = |x_1 - R_0 - \ell(\tau_i)|$$

$$\varepsilon_{12} = \varepsilon^{0}_{12} - \frac{1}{2}\left[\varepsilon^{*}_{12}\frac{\dot{\ell}(\tau_2)}{\dot{\ell}(\tau_2)+c_2}H(R(t)-x_1) - \varepsilon^{*}_{12}\frac{\dot{\ell}(\tau_2)}{\dot{\ell}(\tau_2)-c_2}H(x_1-R(t))\right] \times H\left(t - \frac{|x_1 - R_0|}{c_2}\right).$$

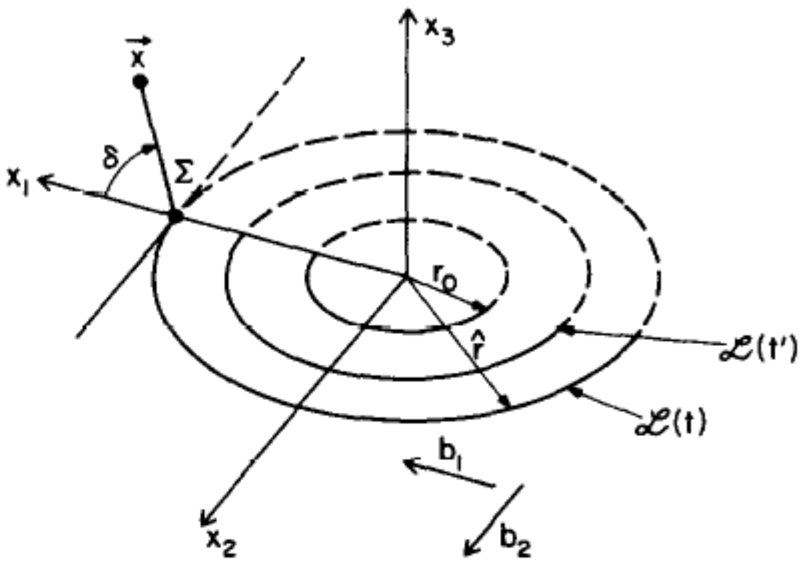
Obtained for spherical and plane
Inclusion moving boundaries

$$u_i(\mathbf{x},t) = \int_{-\infty}^{+\infty} dt' \int_{V(t)} C_{jk\ell m}\varepsilon^{**equiv}_{\ell m}(\mathbf{x}', t'; \dot{l}(t'))\frac{\partial G_{ij}(\mathbf{x}-\mathbf{x}', t-t')}{\partial x_k}dV'$$

Radiated fields as the eigenstrain expands and the material constants change

Near field of an expanding loop with acceleration

Arbitrarily moving dislocation loop



$$U_{2,3}(P) = \left[\frac{b_2 c_2}{2\pi} \frac{\sqrt{c_2^2 - v^2}\cos\delta}{(c_2^2 - v^2\sin^2\delta)}\right]\frac{1}{\varepsilon} + \left[\frac{b_2 c_2}{4\pi}\frac{a}{(c_2^2 - v^2)^{3/2}} - \frac{b_2}{4\pi c_2}\frac{c_2^2 - 2c_1^2}{(c_2^2 - v^2)^{1/2}\hat{r}}\right]\ln\varepsilon$$

Logarithmic singularity associated with current radius of curvature

Limiting fields: plane phase boundary

$$a(t-\tau_2) = |x_1 - R_0 - l(\tau_2)|.$$

$$(\sigma_{11})_p = -\frac{4\mu(3\lambda+2\mu)\epsilon^*}{3(\lambda+2\mu)}$$
$$-\frac{(3\lambda+2\mu)\epsilon^*}{2}\left(\frac{\dot{l}(\tau_2)}{a+\dot{l}(\tau_2)}\right)H(at-|x_1-R_0|))H(R_0+l(t)-x_1)$$
$$-\frac{(3\lambda+2\mu)\epsilon^*}{2}\left(\frac{\dot{l}(\tau_2)}{a-\dot{l}(\tau_2)}\right)H(at-|x_1-R_0|)H(x_1-(R_0+l(t))).$$

$$(\sigma_{22})_p = (\sigma_{33})_p = -\frac{4\mu(3\lambda+2\mu)\epsilon^*}{3(\lambda+2\mu)}H(R_0+l(t)-x_1)$$
$$+\frac{2\mu(3\lambda+2\mu)\epsilon^*}{3(\lambda+2\mu)}H(x_1-(R_0+l(t)))$$
$$-\frac{\lambda(3\lambda+2\mu)\epsilon^*}{2(\lambda+2\mu)}\left(\frac{\dot{l}(\tau_2)}{a+\dot{l}(\tau_2)}\right)H(at-|x_1-R_0|)H(R_0+l(t)-x_1)$$
$$-\frac{\lambda(3\lambda+2\mu)\epsilon^*}{2(\lambda+2\mu)}\left(\frac{\dot{l}(\tau_2)}{a-\dot{l}(\tau_2)}\right)H(at-|x_1-R_0|)H(x_1-(R_0+l(t))).$$

Jumps across moving phase bndry

$$(\sigma_{22})_p = (\sigma_{33})_p = -\frac{4\mu(3\lambda+2\mu)\epsilon^*}{3(\lambda+2\mu)}H(R_0+l(t)-x_1)$$
$$+\frac{2\mu(3\lambda+2\mu)\epsilon^*}{3(\lambda+2\mu)}H(x_1-(R_0+l(t)))$$

Static: Eshelby inside+ Hill jump conditions

Radiated fields of a plane boundary of a half-space inclusion with general eigenstrain

$$u_\ell(\mathbf{x},t)=\int_{-\infty}^{+\infty}dt'\int_D C_{jk\ell m}\varepsilon^{*}_{\ell m}(\mathbf{x},t)\frac{\partial}{\partial x_k}G_{ij}(\mathbf{x}-\mathbf{x}',t-t')dV'$$

Willis, 1965

$$\varepsilon^{*}_{\ell m}(\mathbf{x},t)=\varepsilon^{*}_{\ell m}H(R_o+\ell(t)-x_1)$$

Initial condition:
Three-dimensional fields of the Eshelby limiting half-space inclusion
(Unique minimum energy solution)
Superposed dynamic 1-D problem (unique)

X.M. & L.Ni,*Q.A.M.*,2011

Example: A moving plane inhomogeneity boundary with shear eigenstrain

$$\varepsilon_{ij}^{**} = \varepsilon_{ij}^{*inhom} + \varepsilon_{ij}^{*}.$$

$$\varepsilon_{12}^{**} = \{2(\mu - \mu^*)\varepsilon_{12}^{appl} + 2\mu^*\varepsilon_{12}^*\} \Big/ \left\{4(\mu^* - \mu)\left[S_{1212} - \frac{1}{2}\frac{\dot{l}(\tau_2)}{\dot{l}(\tau_2) + c_2}\right] + 2\mu\right\},$$

$$f_2(\tau_2) = c_2(t - \tau_2) - |x_1 - R_o - \ell(\tau_2)| = 0.$$

DRIVING FORCE

$$f = -\langle \sigma_{km} \rangle [[\varepsilon_{km}^{**}(\mathbf{x}, t)]]$$

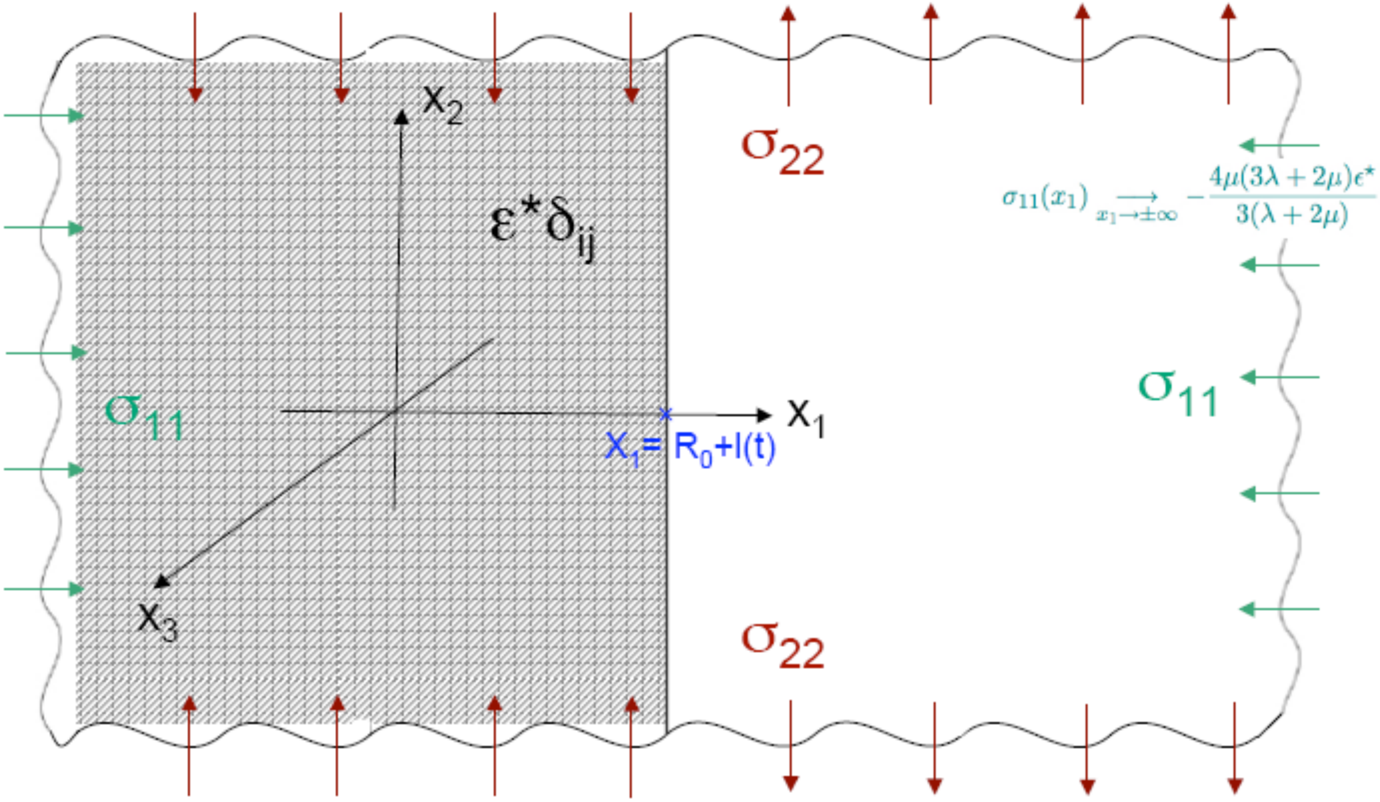
$$f^{self} + \langle \sigma_{k\ell}^{appl.} \rangle \varepsilon_{k\ell}^{**}(\mathbf{x}, t)$$

’

Peach-Koehler force—
coupling terms with motion

XM, *J. Elast*, Carlson volume, 2011

Moving plane phase boundary with dilatational eigenstrain



$$\sigma_{11}(x_1) \underset{x_1 \to \pm\infty}{\longrightarrow} -\frac{4\mu(3\lambda+2\mu)\epsilon^\star}{3(\lambda+2\mu)}$$

$$(\sigma_{22})_P = (\sigma_{33})_P = -H(R_0 + l(t) - x_1)\left[\frac{4\mu(3\lambda+2\mu)\epsilon^\star}{3(\lambda+2\mu)} + \frac{\lambda(3\lambda+2\mu)\epsilon^\star}{2(\lambda+2\mu)}\frac{\dot{l}(\tau_2)}{a+\dot{l}(\tau_2)}H(at - |x_1 - R_0|)\right]$$

$$+H(x_1 - (R_0 + l(t)))\left[\frac{2\mu(3\lambda+2\mu)\epsilon^\star}{3(\lambda+2\mu)} - \frac{\lambda(3\lambda+2\mu)\epsilon^\star}{2(\lambda+2\mu)}\frac{\dot{l}(\tau_2)}{a-\dot{l}(\tau_2)}H(at - |x_1 - R_0|)\right]$$

Ramp-core (delta –sequence) accelerating dislocation through the shear wave-speed barrier

The governing equation

$$\left(\frac{\partial^2 u_y}{\partial x^2}+\frac{\partial^2 u_y}{\partial z^2}\right)=b^2\frac{\partial^2 u_y}{\partial t^2}$$

with boundary condition

$$u_y(x,0,t)=\begin{cases}\dfrac{B}{2}H_\varepsilon(x), & t<0\\ \dfrac{B}{2}H_\varepsilon(x-l(t)), & t\geq 0\end{cases}$$

$$\frac{1}{\pi}\arctan\left(\frac{x}{\varepsilon(0)}\right)+\frac{1}{2},$$

$$=\frac{1}{\pi}\arctan\left(\frac{x-l(t)}{\varepsilon(t)}\right)+\frac{1}{2}$$

Variable core

$$\frac{\partial u(x,z,t)}{\partial z}=\frac{B}{2\pi}\frac{\partial}{\partial t}\left\{\int_0^\infty d\zeta\left[H(t-\eta(\zeta)-\hat{r}b)F(t-\eta(\zeta),x-\zeta)\right]*\frac{1}{\pi}\frac{\varepsilon}{\varepsilon^2+x^2}\right\}$$

where

$$F(t-\eta(\zeta),x-\zeta)=\frac{(t-\eta(\zeta))^2z^2}{\hat{r}^4\sqrt{(t-\eta(\zeta))^2-\hat{r}^2b^2}}-\frac{(x-\zeta)^2\sqrt{(t-\eta(\zeta))^2-\hat{r}^2b^2}}{\hat{r}^4}$$

$$\hat{r}=\left[(x-\zeta)^2+z^2\right]^{\frac{1}{2}}.$$

Steady-state: Peierls-Nabarro

Markenscoff and Ni, *JMPS*, 49, pp 1603-1619, 2001

Markenscoff & Huang, *JMPS*, 2008

Equilibrium position of inhomogeneity strip

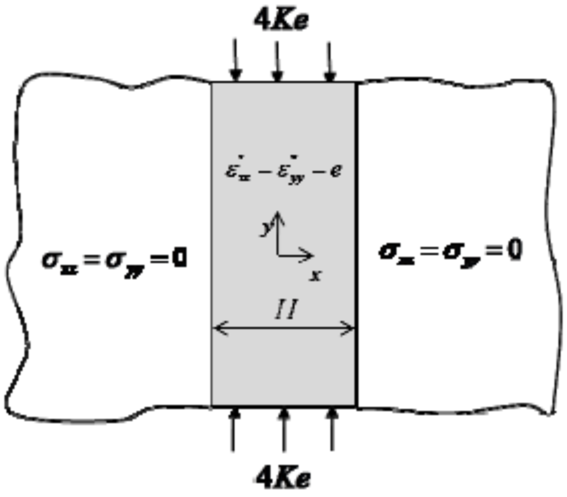


Figure 5(a) Strip with volumetric eigenstrain in an infinite solid

Equivalent eigenstrain, Eshelby

material 2 by material 1 with initial eigenstrain “e”

$$\varepsilon_{equivalent} = \frac{\mu_2\kappa_1 - \mu_2 - \mu_1\kappa_2 + \mu_1}{2\mu_2 + \mu_1\kappa_2 - \mu_1} e$$

(Kun Zhou)

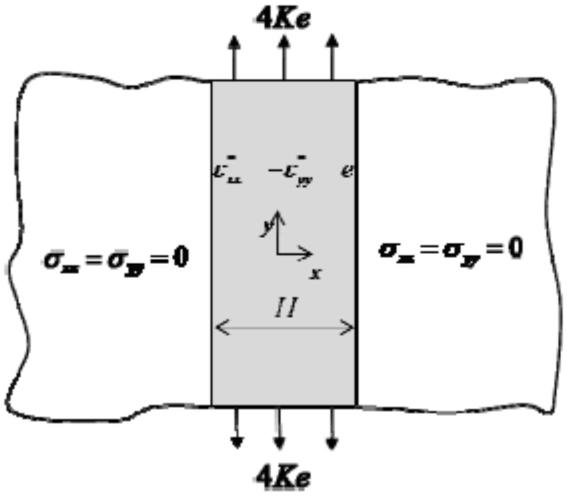


Figure 5(b) Strip with pure shear eigenstrain in an infinite solid

Tractions at infinity with equivalent eigenstrain

Equilibrium position with equivalent eigenstrain in Eshelby force.

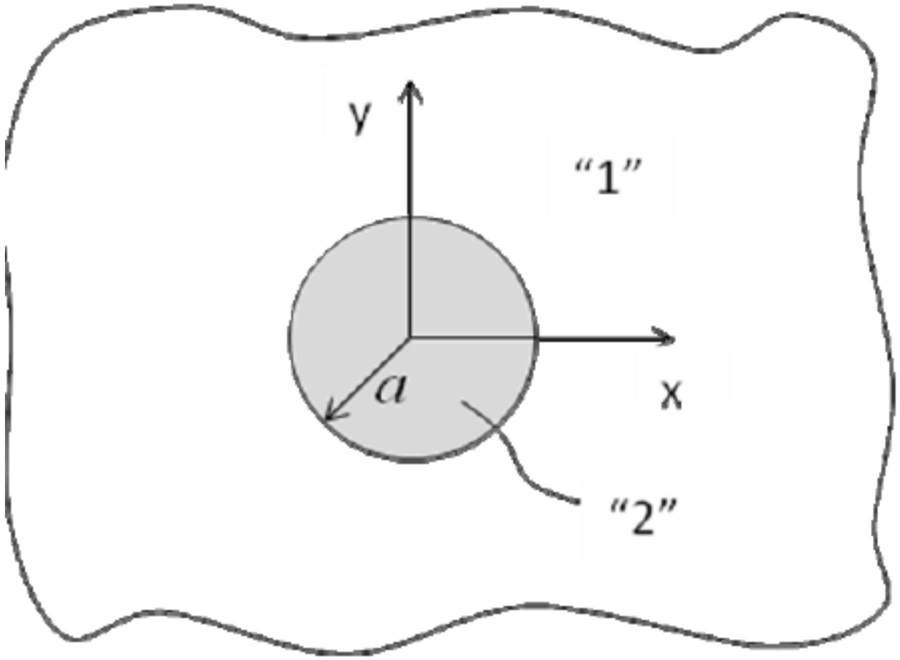
COMPUTE NUMERICALLY ANY FINITE # of STRIPS

Driving forces on circular inhomogeneities

Eshelby $$F = [\![W]\!] - \mathbf{T} \cdot \left[\!\!\left[\frac{\partial \mathbf{u}}{\partial n} \right]\!\!\right]$$

$$F_k = \frac{1}{2}(\sigma_{ij}^{out} + \sigma_{ij}^{in})\varepsilon_{ij}^{*} n_k$$

$$\sigma_{ij}^{(i)} = C_{ijkl}(\varepsilon_{kl}^{(i)} - \varepsilon_{kl}^{*}),$$



$$F_r \begin{array}{l} = -2\mathrm{K}e^2 \qquad \varepsilon_{xx}^{*} = \varepsilon_{yy}^{*} = \eta_1 \equiv e \\ = -2e^2 L \sin^2 2\theta \qquad \varepsilon_{xx}^{*} = -\varepsilon_{yy}^{*} = e \end{array}$$

$$L = \frac{2\mu_2}{\Gamma\kappa_1 + 1} \qquad \mathrm{K} = \frac{2\mu_2}{2\Gamma + \kappa_2 - 1}, \ \Gamma = \frac{\mu_2}{\mu_1}$$

With John Dundurs, *IJSS*, 2009

$$\delta_x \Pi = \int_\Omega B_{i,i} dV - \int_\Omega \Psi_i u_{i,j} \phi_j dV$$

$\bar{\psi}_k = -u_{k,j}\phi_j$

$$B_i = \left(W\delta_{ij} - u_{k,j}\frac{\partial W}{\partial u_{k,i}} \right)\phi_j \qquad F = \int_\Omega B_{i,i} dV$$

$\Psi_i \equiv 0$ represent the Euler-Lagrange equations

"$\delta_x \Pi = F$ if and only if $\Psi_i = 0$"

Near-field expansion of radiated fields

Steady-state motion:

$$\begin{aligned} u_{3,1} &= -\frac{b}{2\pi}\frac{\gamma\,\sin\theta}{\cos^2\theta+\gamma^2\sin^2\theta}\frac{1}{\epsilon}+\text{h.o.t.}, \\ u_{3,2} &= \frac{b}{2\pi}\frac{\gamma\,\cos\theta}{\cos^2\theta+\gamma^2\sin^2\theta}\frac{1}{\epsilon}+\text{h.o.t.}, \\ u_{3,t} &= \frac{b}{2\pi}\frac{v(t)\gamma\,\sin\theta}{\cos^2\theta+\gamma^2\sin^2\theta}\frac{1}{\epsilon}+\text{h.o.t.}, \end{aligned}$$

Accelerating motion:

$$u_{3,1} = u^0_{3,1} + f_{31}(\theta,t)\ln\epsilon + g_{31}(\theta,t) + h.o.t.,$$

$$u_{3,2} = u^0_{3,2} + f_{32}(\theta,t)\ln\epsilon + g_{32}(\theta,t) + h.o.t.,$$

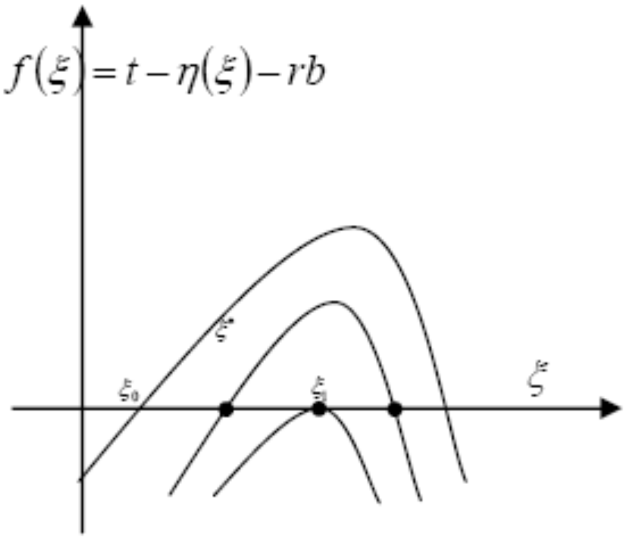
$$u_{3,t} = u^0_{3,t} + f_{3t}(\theta,t)\ln\epsilon + g_{3t}(\theta,t) + h.o.t.,$$

Stress at Mach Wave fronts

$$\eta(\xi) = \eta(\xi^*) + \eta'(\xi^*)(\xi - \xi^*) + o(\xi - \xi^*)$$

$$(t-\eta(\xi))^2 - r^2b^2 = (t-t^*)^2 + [(\eta'(\xi^*))^2 - b^2](\xi-\xi^*)^2 + 2(t^*-\eta(\xi^*))(t-t^*)$$
$$-[2\eta'(\xi^*)(t^*-\eta(\xi^*)) - 2b^2(x-\xi^*)](\xi-\xi^*) - 2\eta'(\xi^*)(t-t^*)(\xi-\xi^*) + o((\xi-\xi^*),(t-t^*))$$

$$\frac{\Delta u}{2\pi} z^2 \frac{\partial}{\partial t} \int_{\xi_0}^{\xi_1} \frac{(t^*-\eta(\xi^*))^2 H(t-t^*)\,d\xi}{[(x-\xi^*)^2+z^2]^2 (b^2-\eta'(\xi^*)^2)^{\frac{1}{2}} \sqrt{(\xi-\xi_0)(\xi_1-\xi)}}$$



$$A\delta(t-t^*)$$

with

$$A = \lim_{\xi_0,\xi_1\to\xi^*} \frac{\Delta u}{2\pi} z^2 \frac{(t^*-\eta(\xi^*))^2}{[(x-\xi^*)^2+z^2]^2 (b^2-\eta'(\xi^*)^2)^{\frac{1}{2}}} \int_{\xi_0}^{\xi_1} \frac{d\xi}{\sqrt{(\xi-\xi_0)(\xi_1-\xi)}}$$

Self-force of a generally moving screw dislocation

$$
\begin{aligned}
F_1 = & -\frac{\mu b^2 \dot{v}}{4\pi c_2^2 \gamma^3} \ln q + \frac{\mu b^2 \dot{v}}{4\pi c_2^2 \gamma^3} \left[\ln(\gamma(1+\gamma)/2) - \frac{4 + \beta^4 - \beta^2(7+2\gamma)}{(1+\gamma)^2} \right] \\
& + \mu b g_{32}(0,t) + \text{h.o.t.}
\end{aligned}
$$

$0 < q \ll 1$ is a fixed number,

$$
\begin{aligned}
g_{32}(0,t) = \frac{b}{2\pi} \Bigg\{ & \frac{c\dot{v}(t)}{2(c^2 - v^2(t))^{3/2}} \left[1 + \ln\left(\frac{cv}{2(c^2 - v^2)} \right) \right] \\
& + \frac{\dot{v}}{2c(c-v)^4} \left[4c^2(c-2v) + v^2(2c-v) \right] \ln\left(\frac{c + \sqrt{c^2 - v^2}}{v} \right) + \frac{\dot{v}(c^2+v^2)}{2v(c-v)^2\sqrt{c^2-v^2}} + \frac{1}{l(t)} \\
& + \int_0^{\eta(\omega)} \frac{c(t-\tau) l(\tau)\, \mathrm{d}\tau}{(l(t)-l(\tau))^2 [c^2(t-\tau)^2 - (l(t)-l(\tau))^2]^{1/2}} + \int_{\eta(\omega)}^{t} \frac{\ln(l(t)-l(\tau)) K(t,\tau,v(\tau))\, \mathrm{d}\tau}{[c^2(t-\tau)^2 - (l(t)-l(\tau))^2]^{5/2}} \\
& + \frac{c(t-\eta(\omega))}{(l(t)-\omega)[c^2(t-\eta(\omega))^2 - (l(t)-\omega)^2]^{\frac{1}{2}}} \\
& + \frac{c \ln(l(t)-\omega) [(t-\eta(\omega)) v(\eta(\omega)) - (l(t)-\omega)] (l(t)-\omega)}{v(\eta(\omega)) [c^2(t-\eta(\omega))^2 - (l(t)-\omega)^2]^{3/2}} \Bigg\},
\end{aligned}
$$

$$F^{\text{in}} = \frac{\mathrm{d}}{\mathrm{d}t}(m_e v),$$

and given by

$$m_e = \frac{1}{v} \int_0^t F^{\text{in}}\, \mathrm{d}t,$$

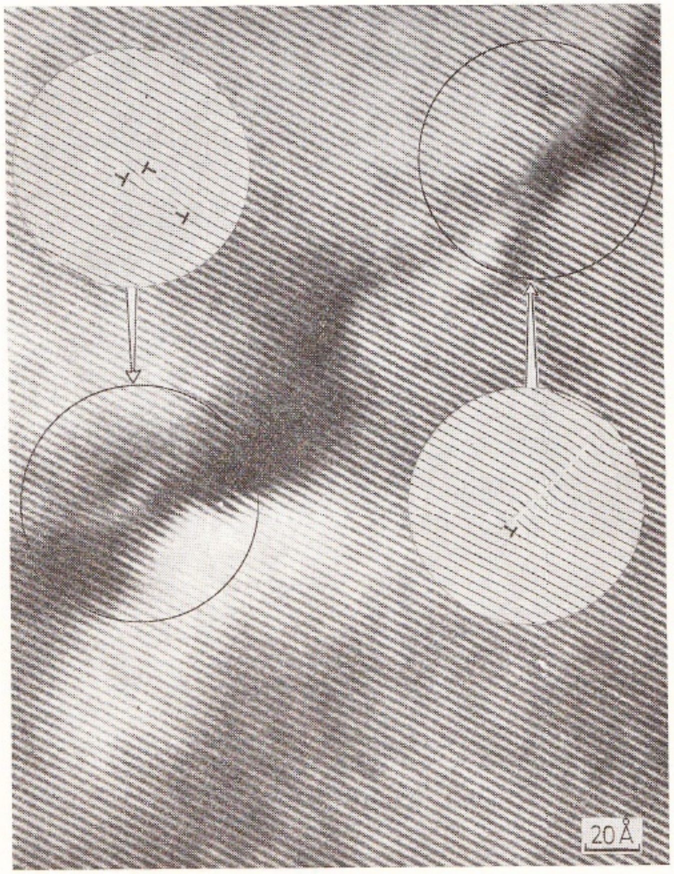


FIG. 1.8. Electronmicrograph resolving the lattice of germanium directly. The distance of the resolved (111) planes is 3.27 Å. At the left lower part of the picture three dislocations can be seen relatively close to each other. The encircled sketch shows their exact positions [V. A. Philips and J. A. Hugo, *Acta Met.* **18** (1970) 123]

- SELF_FORCE and EFFECTIVE MASS OF A MOVING DISLOCATION

- THE DYNAMIC J INTEGRAL and THE GENERALIZATION OF ESHELBY’S THOUGHT EXPERIMENT FOR DYNAMICS

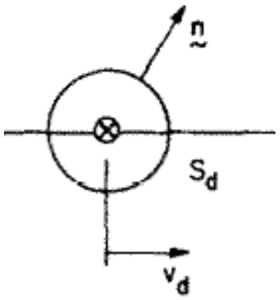
- THE SELF FORCE OF A MOVING PHASE BOUNDARY

- A DISLOCATION ACCELERATING THROUGH THE SHEAR WAVE SPEED BARRIER

. A VARIABLE CORE MODEL AND THE PEIERLS STRESS

Self-force of an accelerating dislocation

Jumping from rest



$$\dot{\mathscr{E}}^{s}_{0} - \frac{-\mu b_x^2}{2\pi t}\left\{\frac{12-8\alpha^2}{\beta^2(1-\alpha^2)^{\frac{1}{2}}} - \frac{(2-\beta^2)(6-7\beta^2)}{\beta^2(1-\beta^2)^{\frac{3}{2}}} - 2\left(1-\frac{\alpha^2}{\beta^2}\right)\right\} \tag{47}$$

of the self-stress field as $S_{\mathrm{d}} \rightarrow 0$. The total energy flux into the core of the dislocation is

$$\dot{\mathscr{E}}^{s}_{0} = \dot{\mathscr{E}}^{s}_{0} + \sigma^{a}_{xz} b_x v_{\mathrm{d}}, \tag{48}$$

Clifton , R.J.&X.M, *JMPS*, 1981

Surface-Independent dynamic J integral

$$F_l = \int_V \frac{\partial}{\partial t}[\rho \dot{u}_i u_{i,l}]\,\mathrm{d}V + \int_S [(W-T)\delta_{lj} - u_{i,l}\sigma_{ij}]\,\mathrm{d}S_j.$$

The dynamic J-integral is surface-independent, which means that for any two volumes V_1 and V_2 $V_2 \supset V_1$, both containing the same elastic inhomogeneity,

$$\int_{V_2} \frac{\partial}{\partial t}[\rho \dot{u}_i u_{i,l}]\,\mathrm{d}V + \int_{\partial V_2} [(W-T)\delta_{lj} - u_{i,l}\sigma_{ij}]\,\mathrm{d}S_j$$
$$= \int_{V_1} \frac{\partial}{\partial t}[\rho \dot{u}_i u_{i,l}]\,\mathrm{d}V + \int_{\partial V_1} [(W-T)\delta_{lj} - u_{i,l}\sigma_{ij}]\,\mathrm{d}S_j.$$

Transition from subsonic to supersonic motion

Forming Mach cone

$$f(\xi^*) = t - \eta(\xi^*) - \sqrt{(x-\xi^*)^2 + z^2}\,b = 0$$

$$\frac{d}{d\xi}\left(t - \eta(\xi^*) - \sqrt{(x-\xi^*)^2 + z^2}\,b\right) = 0$$

$$f(\xi^*) = t^* - \sqrt{\frac{2\xi^*}{a}} - \sqrt{(x-\xi^*)^2 + z^2}\,b = 0$$

$$\frac{d}{d\xi} f(\xi^*) = -\sqrt{\frac{2}{a}}\frac{1}{\sqrt{\xi^*}}\frac{1}{2} + \frac{(x-\xi^*)b}{\sqrt{(x-\xi^*)^2 + z^2}} = 0$$

solve for ξ^* and obtain

$$\theta^3 - \frac{(1+qb^2x)\cdot\theta}{qb^2} + \frac{\sqrt{\frac{q}{2}}t^*}{qb^2} = 0$$

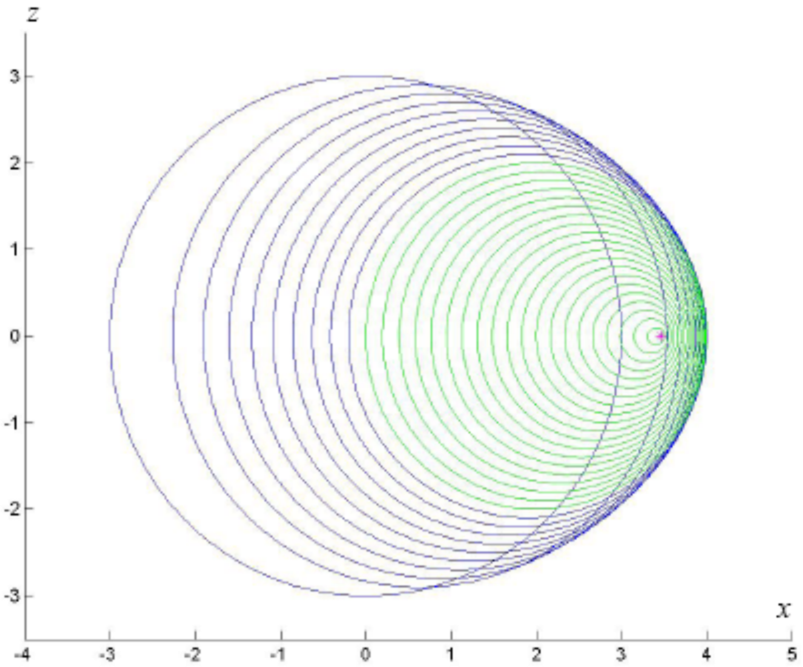
where $\theta \equiv \sqrt{\xi^*}$.

Double root of a cubic

$$D = Q^3 + R^2 = -\frac{1}{27}\left(x^3 + 3x^2\frac{1}{ab^2} + 3x\frac{1}{a^2b^4} + \frac{1}{a^3b^6}\right) + \frac{1}{8a}\frac{t^2}{b^4} \qquad (8)$$

For $D = 0$, a cubic equation has a real double root, which corresponds to the transition point for the cubic equation from containing two complex conjugate roots to two real

Self-Force on a Dislocation Accelerating/ Decelerating through the shear wave-speed



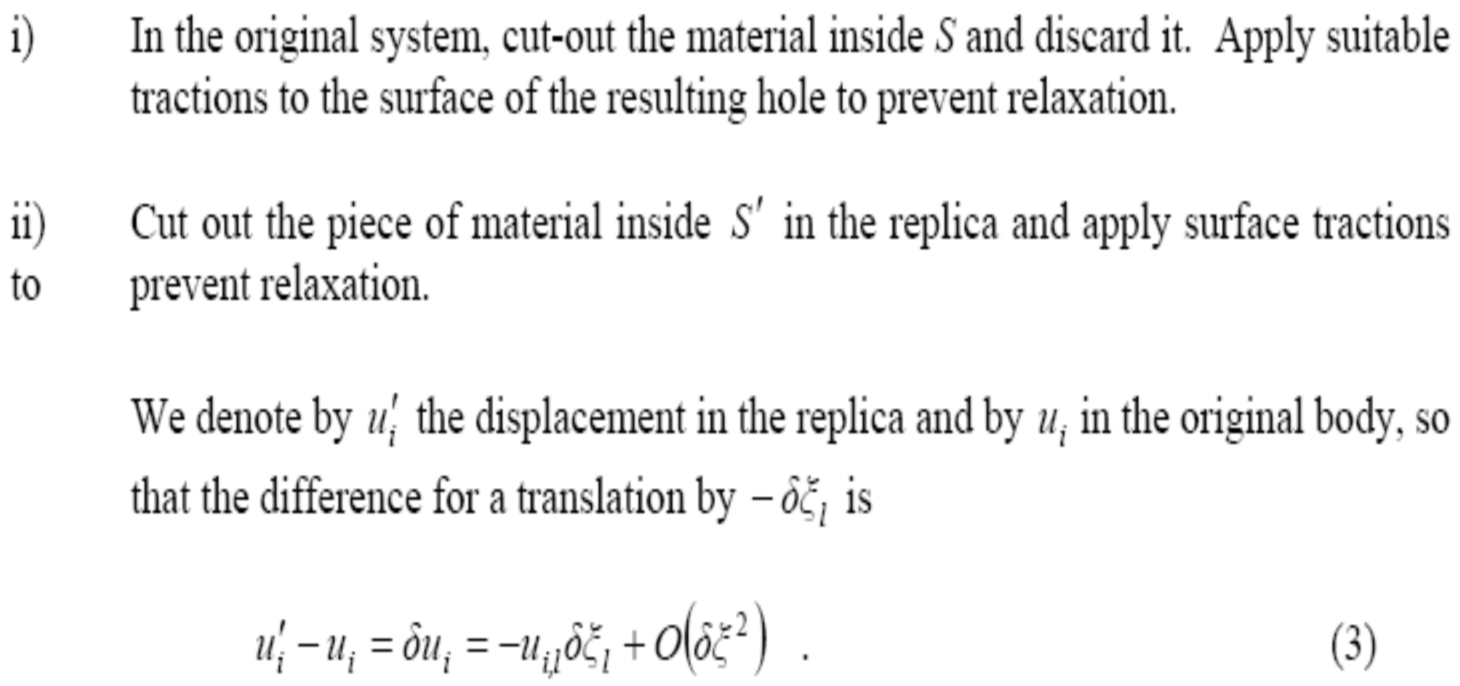
$$F_l(t) = \lim_{z\to 0, x\to l(t^*)} \mu \frac{b}{2\pi} \frac{1}{|\ddot{l}(t^*)|^{1/2}}$$
$$\times \int_{-\infty}^{\infty} \frac{z^2}{\{[x - l(t^*) - \xi]^2 + z^2\}^{5/4}} \ln[x - l(t^*) - \xi]$$
$$\times \frac{\varepsilon}{\varepsilon^2 + \xi^2} d\xi \times \delta(t - t^*),$$

Figure 2: Detachment of the Mach cone from the decelerating dislocation

The red * refers to the current position of the dislocation moving with $x = 2t^{\frac{1}{2}}$ at time t=3. The dislocation motion transits from supersonic to subsonic at time t=1. The blue circles refer to the wavelets let off by the dislocation before t=1. The green circles refer to the wavelets let off after t=1. The ratio of the dislocation velocity at time t=3 versus the shear wave speed is $\dot{l}(t = 3.0)/c_2 = 0.5774$.

Markenscoff and Huang, *APL* , 2009

Eshelby thought experiment



i) In the original system, cut-out the material inside S and discard it. Apply suitable tractions to the surface of the resulting hole to prevent relaxation.

ii) Cut out the piece of material inside S' in the replica and apply surface tractions to prevent relaxation.

We denote by u_i' the displacement in the replica and by u_i in the original body, so that the difference for a translation by $-\delta\xi_l$ is

$$u_i' - u_i = \delta u_i = -u_{i,l}\delta\xi_l + O(\delta\xi^2) \quad . \tag{3}$$

Smearing method

Dynamic J integral for a strip

$$
\begin{aligned}
F_1 &= \lim_{A\to 0}\{ \int_{V\setminus V_A} \frac{\partial}{\partial t}[\rho \hat{\dot{u}}_3 \hat{u}_{3,1}]dV + \int_{S_+\cup S_-} [(\hat{W}-\hat{T})\delta_{j1} - \hat{\sigma}_{3j}\hat{u}_{3,1}]dS_j\} \\
&= \lim_{A\to 0} \int_{S_A+\cup S_{-A}} [(\hat{W}-\hat{T})\delta_{j1} - \hat{\sigma}_{3j}\hat{u}_{3,1}]dS_j .
\end{aligned}
$$

$$
\hat{u}_{3,1} = \int_{-\infty}^{\infty} u_3(\xi,y,t)\frac{1}{\pi}\frac{\partial}{\partial x}[\frac{a}{(x-\xi)^2+a^2}]d\xi .
$$

$$
\begin{aligned}
F_1 = \lim_{A\to 0}\Bigg\{ \int_{-\infty}^{\infty} &[\hat{\sigma}_{32}(x,-A,t)\hat{u}_{3,1}(x,-A,t) \\
&-\hat{\sigma}_{32}(x,A,t)\hat{u}_{3,1}(x,A,t)]\,dx\Bigg\} .
\end{aligned}
$$

Note that this is due only to its own radiated fields.
Applied stress has to be added to consider “an evolution” equation of motion

A CONFIGURATIONAL FORCE ON THE LATTICE DISLOCATION AND THE PEIERLS STRESS

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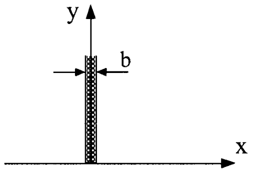
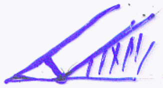
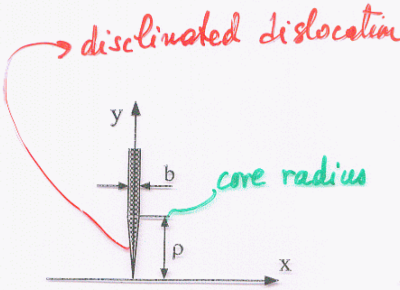
Peierls dislocation in the framework of linear elasticity

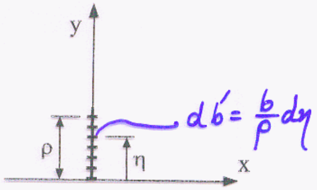


$$\Phi^{\mathrm{V}} = -\frac{\mu b}{4\pi(1-\nu)}\, y\, \ln(x^2+y^2)\,,$$

$$\tau_{xy}^{\mathrm{V}}(x,0) = \frac{\mu}{2\pi(1-\nu)}\,\frac{b}{x}\,.$$



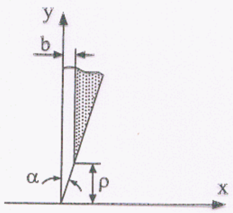




$$\tau_{xy}(x,0) = \frac{\mu b}{2\pi(1-\nu)}\,\frac{x}{\rho}\int_0^\rho \frac{x^2-\eta^2}{(x^2+\eta^2)^2}\,\mathrm{d}\eta\,.$$

$$\tau_{xy}(x,0) = \frac{\mu b}{2\pi(1-\nu)}\,\frac{x}{x^2+\rho^2}\,,$$

Above also follows from



Semi-inverse method:

What slip discontinuity imposed along the x axis would give rise to this $\tau_{xy}(x,0)$?

$\beta(x)$ = **density of infinitesimal dislocations along the slip plane**

$$\frac{\mu}{2\pi(1-\nu)} \int_{-\infty}^{\infty} \frac{\beta(\xi)}{x-\xi}\,\mathrm{d}\xi = \frac{\mu b}{2\pi(1-\nu)} \frac{x}{x^2+\rho^2}$$

$$\text{p.v.} \int_{-\infty}^{\infty} \frac{\beta(\xi)}{x-\xi}\,\mathrm{d}\xi = \frac{bx}{x^2+\rho^2}$$

$$\beta(x) = \frac{b}{\pi}\frac{\rho}{x^2+\rho^2}$$

$\delta(x)$ = **slip discontinuity along the slip plane**

$$\delta(x) = \int_0^x b(\xi)\,\mathrm{d}\xi = \frac{b}{\pi}\int_0^x \frac{\rho}{\xi^2+\rho^2}\,\mathrm{d}\xi$$

$$\underbrace{\delta(x) = \frac{b}{\pi}\tan^{-1}\frac{x}{\rho}}_{\text{recover Peierls-Nabarro}} \quad \sim \quad \rho = \frac{d}{2(1-\nu)} \text{ in Peierls model}$$

disl. width free here

Since by trigonometric identity

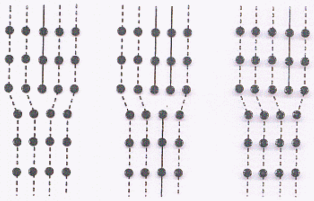
$$\sin\frac{2\pi\delta(x)}{b} = \sin\left(2\tan^{-1}\frac{x}{\rho}\right) \equiv \frac{2\rho x}{\rho^2+x^2}$$

we deduce (rather than assume) the sinusoidal force relation

$$\tau_{xy}(x,0) = \frac{\mu b}{2\pi(1-\nu)}\,\frac{x}{x^2+\rho^2} \qquad \Rightarrow \qquad \tau_{xy} = \frac{\mu b}{4\pi(1-\nu)}\,\frac{1}{\rho}\,\sin\frac{2\pi\delta(x)}{b}$$

Configurational Force on the Lattice Dislocation

Assumption : $\rho = \rho(\Delta)\,, \quad 0 \le \Delta \le b$

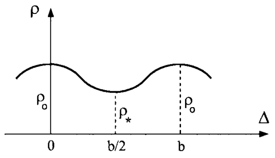


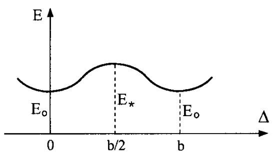
$$\mathcal{F} = -\frac{\partial E}{\partial \Delta} = -\frac{\partial E}{\partial \rho}\,\frac{\mathrm{d}\rho}{\mathrm{d}\Delta}$$

$$E = \frac{\mu b^2}{4\pi(1-\nu)}\,\ln\frac{e^{1/2}R}{2\rho} \quad \Rightarrow \quad \frac{\partial E}{\partial \rho} = -\frac{\mu b^2}{4\pi(1-\nu)}\,\frac{1}{\rho}$$

$$\mathcal{F} = \frac{\mu b^2}{4\pi(1-\nu)}\,\frac{1}{\rho}\,\frac{\mathrm{d}\rho}{\mathrm{d}\Delta}$$

Periodic Variation of the Core Radius





$$\rho(\Delta) = \frac{1}{2}(\rho_o + \rho_*) + \frac{1}{2}(\rho_o - \rho_*) \cos \frac{2\pi\Delta}{b}$$

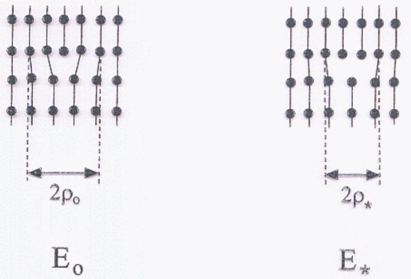
$$\frac{\mathrm{d}\rho}{\mathrm{d}\Delta} = -\frac{\pi}{b}\,(\rho_o - \rho_*) \sin \frac{2\pi\Delta}{b}$$

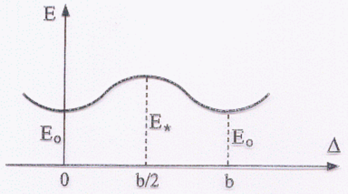
$$\mathcal{F} = \frac{\mu b^2}{4\pi(1-\nu)}\,\frac{1}{\rho}\,\frac{\mathrm{d}\rho}{\mathrm{d}\Delta} \qquad \Rightarrow \qquad \mathcal{F} = -\frac{\mu b}{4(1-\nu)}\,\frac{\rho_o - \rho_*}{\rho} \sin \frac{2\pi\Delta}{b}$$

$$\tau_{\mathrm{PS}} = \frac{\mu}{2(1-\nu)} \sinh(\Gamma)$$

$$\tau_{\mathrm{PS}} = \pi \frac{E_* - E_o}{b^2} \left(1 + \frac{\Gamma^2}{6} + \cdots \right)$$

$$\boxed{\tau_{\mathrm{PS}} \approx \pi \frac{E_* - E_o}{b^2}}$$





An Estimate of the Peierls Stress

$$\frac{\rho_o - \rho_*}{\rho_o} = c \ \exp\left(-k\pi\rho_o/b\right) \longleftarrow$$

difference in the width between stable and unstable more significant if disl. width is narrow (ρ_0 small)

$$\tau_{\mathrm{PS}} = \frac{\mu}{4(1-\nu)} \frac{c \ \exp\left(-k\pi\rho_o/b\right)}{\left[1 - c \ \exp\left(-k\pi\rho_o/b\right)\right]^{1/2}}$$

Recover:

$$c = 8 \ , \ k = 4 \quad \Rightarrow \quad \tau_{\mathrm{PS}} \approx \frac{2\mu}{1-\nu} \exp\left(-4\pi\rho_o/b\right) \quad (\mathrm{P-N} \ \text{formula})$$

1940, 1947

Better fit of experiments:

$$c = 4 \ , \ k = 2 \quad \Rightarrow \quad \tau_{\mathrm{PS}} = \frac{\mu}{1-\nu} \frac{\exp\left(-2\pi\rho_o/b\right)}{\left[1 - 4 \ \exp\left(-k\pi\rho_o/b\right)\right]^{1/2}}$$

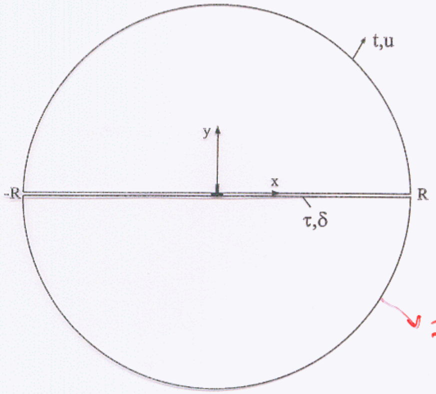
$\downarrow$

$c = 8\left[1+\beta+\beta^2/6\right], \ k = 4a$ Foreman et al (1951)

$c = \left(2.3 + 0.98\,(1-\nu)\right)/32 \ , \ k = 2$ Huntington (1955)

$c = 8 \ , \ k = 2(3-2\nu)$ Dundurs + Lee (1972)

Elastic Strain energy



far field is Volterra

$$E = \frac{1}{2}\int_{-R}^{R} \tau_{xy}(x,0)\delta(x)\,\mathrm{d}x + \frac{1}{2}\int_{0}^{2\pi} \mathbf{t}\cdot\mathbf{u}\,R\mathrm{d}\theta$$

$$E = \frac{\mu b^2}{2\pi^2(1-\nu)}\int_{0}^{R} \frac{x}{x^2+\rho^2}\tan^{-1}\frac{x}{\rho}\,\mathrm{d}x + \frac{\mu b^2}{8\pi(1-\nu)}$$

Lattice Friction Stress

$$\tau_{\mathrm{LF}} = \frac{\mathcal{F}}{b}$$

$$\tau_{\mathrm{LF}} = -\frac{\mu}{4(1-\nu)}\,\frac{\rho_o - \rho_*}{\rho}\sin\frac{2\pi\Delta}{b}$$

$$\tau_{\mathrm{LF}}^{\max} = ?$$

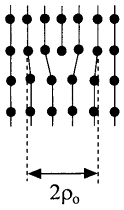
$$\frac{\mathrm{d}\tau_{\mathrm{LF}}}{\mathrm{d}\Delta} = 0 \quad \Rightarrow \quad \cos\frac{2\pi\Delta}{b} = -\frac{\rho_o - \rho_*}{\rho_o + \rho_*}$$

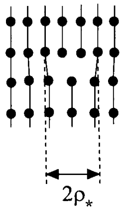
$$\tau_{\mathrm{LF}}^{\max} = \frac{\mu}{4(1-\nu)}\,\frac{\rho_o - \rho_*}{\sqrt{\rho_o\rho_*}}$$

Peierls Stress

$$\tau_{\mathrm{PS}} = \tau_{\mathrm{LF}}^{\max}$$

$$\tau_{\mathrm{PS}} = \frac{\mu}{4(1-\nu)} \frac{\rho_o - \rho_*}{\sqrt{\rho_o \rho_*}}$$





$$R \gg \rho$$

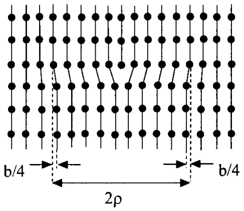
$$E = \frac{\mu b^2}{4\pi(1-\nu)} \ln \frac{R}{2\rho} + \frac{\mu b^2}{8\pi(1-\nu)}$$

$$E = \frac{\mu b^2}{4\pi(1-\nu)} \ln \frac{e^{1/2} R}{2\rho}$$

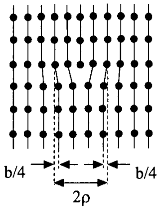
$$\nu = 1/3$$

$$\rho_0 = 2b \quad \Rightarrow \quad \tau_{\mathrm{PS}} = 5.2 \times 10^{-6}\,\mu \quad \text{(Cu)}$$

$$\rho_0 = b/2 \quad \Rightarrow \quad \tau_{\mathrm{PS}} = 7.1 \times 10^{-2}\,\mu \quad \text{(Si)}$$



wide dislocation
(soft metals)



narrow dislocation
(covalent bonding)

Experimental Values

$$\text{Cu} \quad \Rightarrow \quad \tau_{\mathrm{PS}} = 5 \times 10^{-6}\,\mu$$

$$\text{Si} \quad \Rightarrow \quad \tau_{\mathrm{PS}} = 0.1\,\mu$$

Temperature Effect on the Peierls Stress

$$\tau_{\mathrm{PS}} = \frac{\mu}{1-\nu} \frac{\exp\left(-k\pi\rho_o/b\right)}{\left[1-4\,\exp\left(-k\pi\rho_o/b\right)\right]^{1/2}}$$

$$k = k(T) \qquad (T = \text{temperature})$$

($k = 2$: Law Temperature)

$2\rho_o/b$	$(\tau_{\mathrm{PS}}/\mu) \times 10^6$
1.00	71,272.9
1.50	13,723.8
2.00	2,811.7
2.50	582.8
3.00	121.1
3.50	25.16
4.00	5.231
4.50	1.087
5.00	0.2261
5.50	0.0470
6.00	0.0097
6.50	0.0020
7.00	0.0004

($k = 1.75$: Room Temper.)

$2\rho_o/b$	$(\tau_{\mathrm{PS}}/\mu) \times 10^6$
1.00	111,294.5
1.50	25,112.3
2.00	6,194.7
2.50	1,557.5
3.00	393.40
3.50	99.48
4.00	25.17
4.50	6.366
5.00	1.610
5.50	0.4074
6.00	0.1031
6.50	0.0261
7.00	0.0066

The Peierls Stress in terms of an Energy Barrier

$$E = \frac{\mu b^2}{4\pi(1-\nu)} \ln \frac{e^{1/2} R}{2\rho}$$

$$E_* - E_o = D \ln \frac{\rho_o}{\rho_*} \quad \Rightarrow \quad \frac{\rho_o}{\rho_*} = \exp \frac{E_* - E_o}{D}$$

$$D = \frac{\mu b^2}{4\pi(1-\nu)} \quad \longleftarrow \text{ total misfit energy of Peierls disl.}$$

$$\Gamma = \frac{E_* - E_o}{2D} \quad \Rightarrow \quad \frac{\rho_o}{\rho_*} = \exp(2\Gamma)$$

$$\tau_{\mathrm{PS}} = \frac{\mu}{4(1-\nu)} \frac{\rho_o - \rho_*}{\sqrt{\rho_o \rho_*}} \quad \Rightarrow \quad \tau_{\mathrm{PS}} = \frac{\mu}{4(1-\nu)} \left(\sqrt{\frac{\rho_o}{\rho_*}} - \sqrt{\frac{\rho_*}{\rho_o}} \right)$$

$$\tau_{\mathrm{PS}} = \frac{\mu}{2(1-\nu)} \sinh(\Gamma)$$

If $\nu = 1/3$ and $\rho_0 = 2b$, the Peierls stress is $\tau_{\mathrm{PS}} = 5.25 \times 10^{-6}\,\mu$, while for a narrow dislocation with $\rho_o = b/2$ and $\nu = 1/5$, $\tau_{\mathrm{PS}} = 5.4 \times 10^{-2}\,\mu$. The experimental values at low temperature for τ_{PS} in closed-packed Cu is about $5 \times 10^{-6}\,\mu$, while in covalent Si it is about $0.1\,\mu$. If $\rho_o = 1.7b$ and $\nu = 1/3$, $\tau_{\mathrm{PS}} = 3.4 \times 10^{-5}\,\mu$, which is close to an experimentally observed value for hexagonal close-packed (HCP) Zn ($2 \times 10^{-5}\,\mu$ for the basal plane). If $\rho_o = b$ and $\nu = 0.3$, $\tau_{\mathrm{PS}} = 2.67 \times 10^{-3}\,\mu$, which is close to an experimentally observed value for a base-centered cubic (BCC) α-Fe ($5 \times 10^{-3}\,\mu$).

$$\rho_o = \frac{\mu b}{4\pi(1-\nu)\tau_{\max}}\,. \tag{26}$$

t is reasonable to assume that $\tau_{\max}$ is equal to the actual shear strength of the pure crystal under uniform training, either experimentally determined or estimated from atomistic calculations, which is a fraction of the heoretical shear strength $\mu b/2\pi h$ of the pure crystal [33]. Guided by experimental data on the lattice friction tress, we take $\tau_{\max}$ to be one half of the theoretical shear strength, i.e., $\tau_{\max} = \mu b/4\pi h$. For a face-centered ubic (FCC) crystal ($\langle 211\rangle\,\{111\}$ partial, $h/b = \sqrt{2}$), we obtain $\tau_{\max} = 0.056\,\mu$. With $\nu = 1/3$, Eq. (26) ives $\rho_o = 2b$. For a BCC crystal ($\langle 111\rangle\,\{110\}$ glide system, $h/b = \sqrt{2/3}$), we obtain $\tau_{\max} = 0.1\,\mu$ and, with $= 0.3$, Eq. (26) gives $\rho_o = 1.1b$. For an HCP crystal ($\langle 11\bar{2}0\rangle\,\{0001\}$ glide system, $h/b = 1.093$), we obtain $_{\max} = 0.07\,\mu$. With $\nu = 1/3$, Eq. (26) gives $\rho_o = 1.7b$. Finally, for a diamond cubic crystal ($\langle 110\rangle\,\{111\}$ huffle plane, $h/b = 0.4083$), we obtain $\tau_{\max} = 0.2\,\mu$ and, with $\nu = 1/5$, Eq. (26) gives $\rho_o = 0.5b$.

Mixed Screw/Edge Dislocation

$$\delta_s(x) = \frac{b_s}{\pi} \tan^{-1} \frac{x}{\rho_s},$$

$$\tau_s(x) = \frac{\mu}{4\pi} \frac{b_s}{\rho_s} \sin \frac{2\pi\delta_s(x)}{b_s} = \frac{\mu b_s}{2\pi} \frac{x}{\rho_s^2 + x^2},$$

$$E = \frac{\mu b_e^2}{4\pi(1-\nu)} \ln \frac{e^{1/2}R}{2\rho_e} + \frac{\mu b_s^2}{4\pi} \ln \frac{R}{2\rho_s}.$$

$$\rho_s = c\rho_e,$$

$$E = \frac{\mu \bar{b}^2}{4\pi(1-\nu)} \ln \frac{R}{2\rho_e} + \frac{\mu b_e^2}{8\pi(1-\nu)} - \frac{\mu b_s^2}{4\pi} \ln c,$$

$$\bar{b}^2 = b_e^2 + (1-\nu) b_s^2.$$

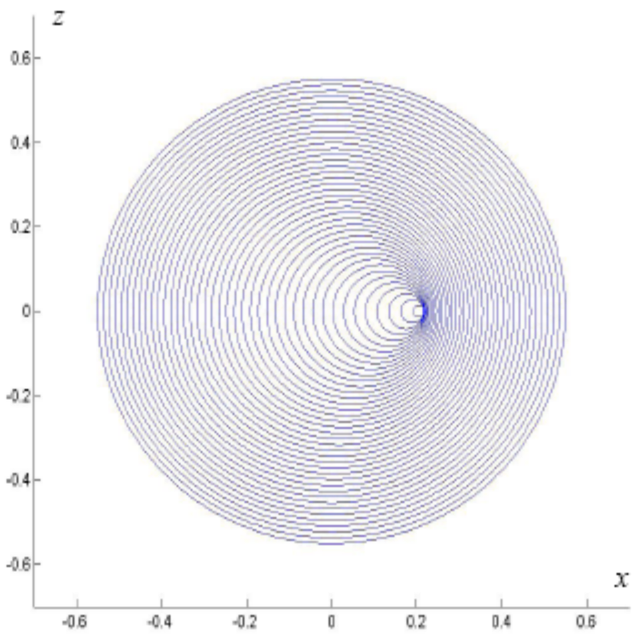


Figure 1: Forming Mach cone for dislocation motion $l(t) = \frac{4}{3}t^3$ at $t = 0.55$; The motion becomes supersonic at $t = 0.5$; the ratio of the dislocation velocity at time $t = 0.55$ versus the shear wave speed is $\dot{l}(t = 0.55)/c_2 = 1.21$; the quantities are dimensionless and the speed c_2 is normalized to 1 for all figures.

$$\rho(\Delta) = \frac{1}{2}(\rho_o + \rho_*) + \frac{1}{2}(\rho_o - \rho_*)\cos\frac{2\pi\Delta}{a}$$

$$\Pi(\Delta) = E(\Delta) - \int_0^{\Delta} b\,\tau_b(\Delta)\,d\Delta$$

$$b = (b_e^2 + b_s^2)^{1/2},$$

$$\tau_b = \tau\cos(\varphi - \psi).$$

$$d\Pi/d\Delta = 0, \qquad b\,\tau_b(\Delta) = dE/d\Delta$$

$$\tau_b(\Delta) = \frac{\mu}{4(1-\nu)}\frac{\bar{b}^2}{ab}\frac{\rho_o - \rho_*}{\rho(\Delta)}\sin\frac{2\pi\Delta}{a}$$

Peierls Stress for Mixed Screw/Edge

$$\tau_b^{\mathrm{PS}} = \frac{\mu}{4(1-\nu)} \frac{\bar{b}^2}{ab} \frac{\rho_o - \rho_*}{\sqrt{\rho_o \rho_*}}.$$

$$E_* - E_o = \bar{D} \ln \frac{\rho_o}{\rho_*}, \quad \bar{D} = \frac{\mu \bar{b}^2}{4\pi(1-\nu)}.$$

$$\tau_b^{\mathrm{PS}} = \frac{\mu}{2(1-\nu)} \frac{\bar{b}^2}{ab} \sinh(\bar{\Gamma}),$$

$$\bar{\Gamma} = \frac{E_* - E_o}{2\bar{D}}.$$

$$\tau_b^{\mathrm{PS}} = \pi \frac{E_* - E_o}{ab} + \text{higher order terms}.$$

Conclusions

- The solution for the Peierls lattice dislocation derived entirely within the framework of linear elasticity.

- The core radius is a free parameter, not constrained by $2\rho = d/(1-\nu)$, as in classical solution.

- The sinusoidal relationship between the shear stress and the slip discontinuity along the glide plane deduced rather than assumed.

- Width of the dislocation changes as the center of the dislocation moves between the two consecutive equilibrium configurations of the dislocation along its glide plane.

- Configurational force on the lattice dislocation is the negative gradient of the elastic strain energy with respect to the dislocation position in the crystal lattice.

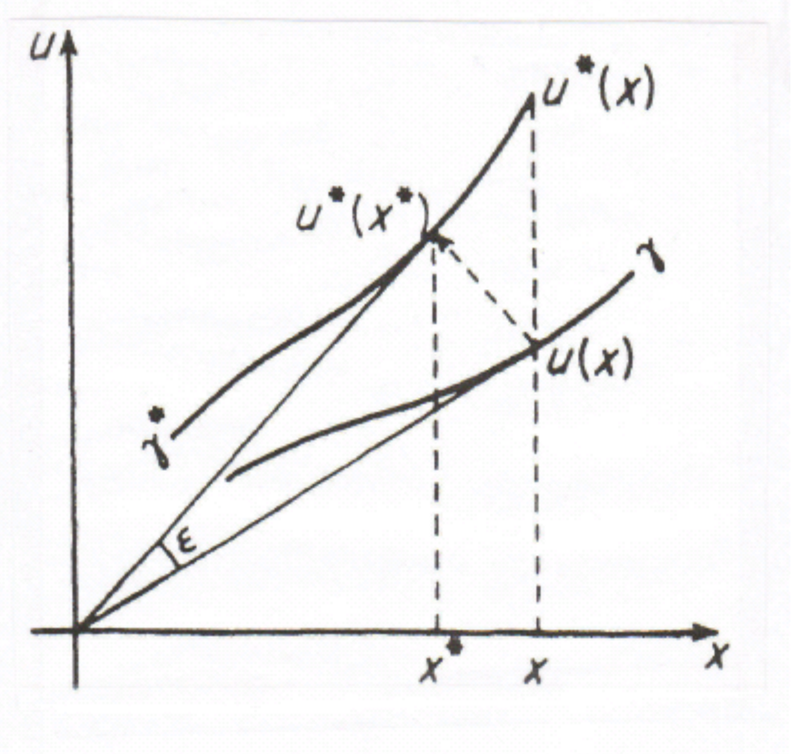
- The simple new expression for the Peierls stress derived in terms on the energy barrier between the unstable and stable equilibrium position of the dislocation.

- Estimates made for the Peierls stress of wide and narrow dislocations based on a proposed expression for the relative change of the dislocation width.

- Good agreement with experimental data to both narrow and wide dislocations (Si, Cu).

- Temperature effects on the Peierls stress discussed.

Variable domain invariance
Noether' s theorem



Noether' s theorem for elastodynamics

$$\Pi(u_i, u_{i,j}, \dot{u}_i) = \int_\Omega (W(x_i, u_i, u_{i,j}) - T(\dot{u}_i))dV \qquad (1)$$

Consider the transformations, $y_\alpha = x_\alpha + \phi_\alpha + O(\varepsilon^2)$ and $v_i = u_i + \psi_i + O(\varepsilon^2)$, where $\alpha = 1$ to 4 and $x_4 = t$ (and therefore $\dot{u}_i \equiv u_{i,4}$). Let $L = W - T$. We obtain,

$$\delta\Pi = \int_\Omega \frac{d}{dx_\alpha}\left(\frac{\partial L}{\partial u_{k,\alpha}}\bar{\psi}_k + L\phi_\alpha\right)dV + \int_\Omega \Psi_i \bar{\psi}_i dV \qquad (2)$$

where $\bar{\psi}_k = \psi_k - u_{k,\alpha}\phi_\alpha$ and,

$$\Psi_i = \frac{\partial L}{\partial u_i} - \frac{d}{dx_\alpha}\frac{\partial L}{\partial u_{i,\alpha}} \qquad (3)$$

Now if we let $\psi_i = 0$ and $\phi_4 = 0$ (i.e. no transformation in the time coordinate), then $\bar{\psi}_k = \psi_k - u_{k,j}\phi_j$ and the relation (2) reduces to,

$$\delta_x\Pi = \int_\Omega B_{\alpha,\alpha} dV - \int_\Omega \Psi_i u_{i,j}\phi_j dV$$

$$B_\alpha = \left(L\delta_{\alpha\beta} - u_{k,\beta}\frac{\partial L}{\partial u_{k,\alpha}}\right)\phi_\beta$$

$$B_4 = u_{k,j}\frac{\partial T}{\partial u_{k,4}}\phi_j$$

$$\delta_x \Pi = \int_{t_1}^{t_2} \int_{\partial\Omega} B_i n_i dA dt + \left(\int_{\Omega} B_4 dV \right)_{t=t_2} - \left(\int_{\Omega} B_4 dV \right)_{t=t_1}$$

substitute $\phi_i = \varepsilon_i$ and use $T = \frac{1}{2}\rho \dot{u}_i^2$.

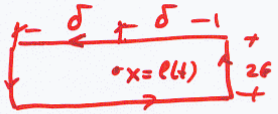
$$= \int_{t_1}^{t_2} \int_{\partial\Omega} \left(L\delta_{ij} - u_{k,j} \frac{\partial W}{\partial u_{k,i}} \right) n_i dA dt + \left(\int_{\Omega} \rho \dot{u}_k u_{k,j} dV \right)_{t=t_2} - \left(\int_{\Omega} \rho \dot{u}_k u_{k,j} dV \right)_{t=t_1}$$

Self-force on an Edge Dislocation Jumping from Rest to Constant Velocity

(a) Circular contour 

(calculation by Mathematica)

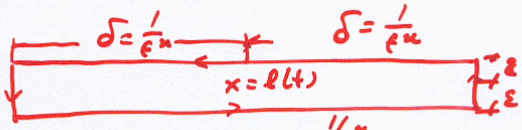
(b) Rectangular contour



$$\dot{\mathcal{E}} = \lim_{\epsilon\to 0} \int_{\ell(t)-\delta}^{\ell(t)+\delta} \left[\sigma_{i3} \frac{\partial u_i}{\partial t}(x,\epsilon,t) - \sigma_{i3} \frac{\partial u_i}{\partial t}(x,-\epsilon,t) \right] dx$$

$n > 1$

(c) Slip-plane



$$\dot{\mathcal{E}} = \lim_{\epsilon\to 0} \int \sigma_{ij} n_j \dot{u}_i \, dS = \lim_{\epsilon\to 0} \int_{-1/\epsilon^n}^{1/\epsilon^n} \sigma_{ij}(x,\epsilon,t) n_j \dot{u}_i (x,\epsilon,t) dx$$

$$= \frac{\Delta u}{d} \int_{-\infty}^{\infty} \sigma_{xz}(x,0,t)\, \delta(x-\ell(t))\, dx = \frac{\Delta u}{d} \lim_{x\to \ell(t)} \sigma_{xz}(\ell(t),0,t)$$

$$\dot{E} = \frac{-\mu(\Delta u_x)^2}{2\pi t} \left\{ \frac{12-8\alpha^2}{\beta^2(1-\alpha^2)^{1/2}} - \frac{(2-\beta^2)(6-7\beta^2)}{\beta^2(1-\beta^2)^{1/2}} - 2\left(1-\frac{\alpha^2}{\beta^2}\right) \right\} > 0$$

$(2-\beta^2)$ $= 0$ at $v_d = \sqrt{2}c_2$

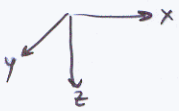
$\alpha = \frac{v_d}{c_1}$, $\beta = \frac{v_d}{c_2}$

Self-force on a dislocation

jumping from rest to a velocity v_d

$d = \frac{1}{v_d}$

(a) Screw dislocation



$b = \frac{1}{c_2}$

Expansion around $x = \ell(t) = \frac{t}{d}$

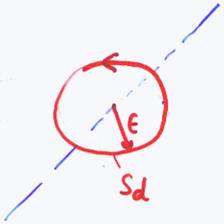
$$\frac{\partial u_y}{\partial z} = \frac{\Delta u}{2\pi}\left\{ \frac{-d^2\cos\theta\sqrt{1-b^2/d^2}}{(d^2-b^2\sin^2\theta)\, \underset{\nwarrow \epsilon}{r}} + \frac{d}{\sqrt{1-\frac{b^2}{d^2}}\, t} - \frac{d}{t} \right\}$$

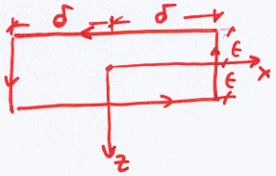
$$\frac{\partial u_y}{\partial t} = \frac{\Delta u}{2\pi}\left\{ \frac{-\sin\theta\sqrt{d^2-b^2}}{(d^2-b^2\sin^2\theta)\, \underset{\nwarrow \epsilon}{r}} + \frac{d\sqrt{d^2-b^2}\sin\theta\,\epsilon}{t^2(d^2-b^2\sin^2\theta)} + \dots \right\}$$

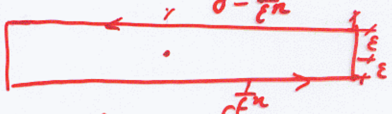
$$\frac{\partial u_y}{\partial x} = \frac{\Delta u}{2\pi}\left\{ \frac{d\sqrt{d^2-b^2}\sin\theta}{(d^2-\sin^2\theta\, b^2)\epsilon} + \frac{d^3\sin\theta\sqrt{d^2-b^2}\,\epsilon}{t^2(-b^2\sin^2\theta+d^2)} + d^2\frac{\sin\theta}{t^2}\epsilon + \dots \right\}$$

$$\dot{\mathcal{E}} = \int_{S_d}\left\{\frac{1}{2}\rho\left(\frac{\partial u}{\partial t}\right)^2 + \frac{1}{2}\mu\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial z}\right)^2\right]\right\}\cos\theta\,\dot{\ell}(t)\,\epsilon\, d\theta + \int_{S_d}\mu\left(\cos\theta\frac{\partial u}{\partial x} + \sin\theta\frac{\partial u}{\partial z}\right)\frac{\partial u}{\partial t}\,\epsilon\, d\theta$$

$n > 1$







$$\lim_{\epsilon\to 0}\int_{-\frac{1}{\epsilon^n}}^{\epsilon^n} \sigma_{yz}(x, z\to 0, t)\cdot\frac{\partial u_y}{\partial t}\, dx =$$

$$\downarrow$$

$$\dot{\ell}(t)\,\delta(x-\ell(t))$$

$$\dot{\mathcal{E}} = \frac{\mu(\Delta u)^2}{2\pi t}\left(\frac{\sqrt{1-b^2/d^2}-1}{\sqrt{1-\frac{b^2}{d^2}}}\right)$$

$$(\;)\lim_{\delta\to 0}\lim_{\epsilon\to 0}\int_{\tan^{-1}-\frac{\epsilon}{\delta}}^{\tan^{-1}\frac{\epsilon}{\delta}} \frac{d\theta}{1-\frac{b^2}{d^2}\sin^2\theta} =$$

$$\dot{\mathcal{E}} = \frac{\Delta u}{2\pi}\,\dot{\ell}(t)\,\underline{\sigma_{yz}}(\ell(t), z\to 0^+, t) + \sigma^{appl}$$

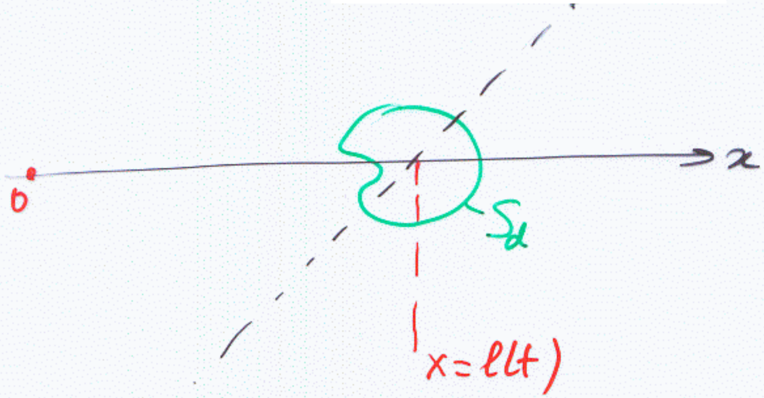
$F = (\sigma\cdot b)\times\xi$ Dynamic Peach-Koehler

Energy-release rate for moving cracks

$$\dot{\mathcal{E}}_{\mathrm{d}} = \int_{S_{\mathrm{d}}} \{\sigma_{ij} n_j v_i + (\tfrac{1}{2}\sigma_{ij} u_{i,j} + \tfrac{1}{2}\rho v_i v_i) v_n\} \,\mathrm{d}S,$$

$$\dot{\mathcal{E}}_0 = \lim_{S_{\mathrm{d}}\to 0} \dot{\mathcal{E}}_{\mathrm{d}}.$$

Atkinson + Eshelby, 1969
Freund, 1972



Define Self-force: $= -\dfrac{\dot{\mathcal{E}}}{v_d}$

Singular asymptotic expansion of integrals

sketch of proof

$$\int_0^\infty \varphi(x)\, F\Big(\overset{y}{\boxed{\frac{\epsilon}{x^2}}}\Big)\,dx$$

$\downarrow$

$\varphi(x)$ has compact support

$$F\Big(x,\overset{y}{\boxed{\frac{\epsilon}{x^2}}}\Big) = \sum_{k=0}^{2m} \frac{x^k}{k!}\,\partial_x^k F\Big(0,\frac{\epsilon}{x^2}\Big)$$

$F(y)$ is smooth as $y \to 0$
(i.e. $x \to \infty$)

$F(y)$ is bounded as $y \to \infty$
(i.e. as $x \to 0$)

$\Big($or even $\displaystyle\int_0^B |F(y)|\,dy < \infty\Big)$

$$\rightarrow F\Big(\frac{1}{x^2}\Big) \le B$$

$$\frac{1}{1+y^2}$$

$$\rightarrow F(y) \sim F^{(0)}(0) + F^{(1)}(0)\frac{\epsilon}{x^2} + \cdots$$

$$R_m\Big(\frac{\epsilon}{x^2}\Big) = F\Big(\frac{\epsilon}{x^2}\Big) - \sum_{k=0}^{m-1} \frac{F^{(k)}(0)}{k!}\Big(\frac{\epsilon}{x^2}\Big)^k$$

As $x \to 0$ $\quad \Big| x^{2(m-1)} R_m\Big(\frac{1}{x^2}\Big)\Big| \le B\, x^{2(m-1)} + \sum_{k=0}^{m-1} x^{2(m-1-k)} \Big|\frac{F^{(k)}(0)}{k!}$

As $x \to \infty$ $\quad \Big| x^{2(m-1)} R_m\Big(\frac{1}{x^2}\Big)\Big| \le \frac{1}{x^2}{}^{2}\Big|\frac{F^{(m)}(0)}{m!}\Big|$

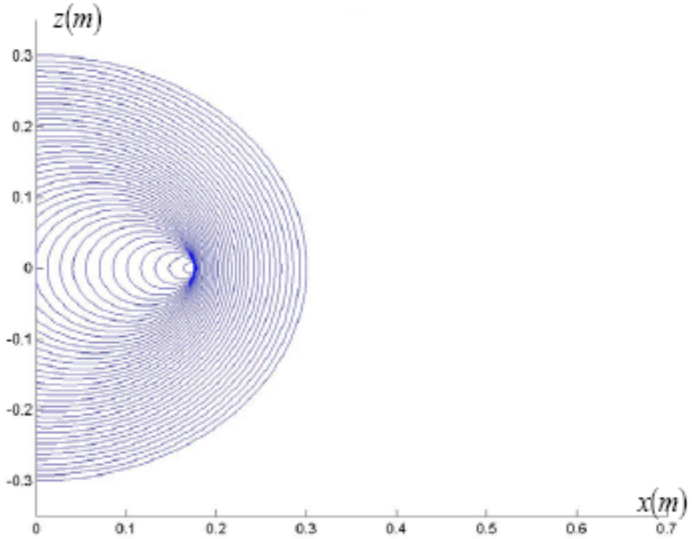


Figure 2 Mach wave front at $t = 0.3s$ for the motion $l(t) = 2t^2$, the motion becomes supersonic at $t = 0.25s$ and the envelope is inside the circle with radius $r = 0.3m$; the speed c is normalized to $1m/s$

$$\partial^n(fg) = \sum_{k=0}^{n} \binom{n}{k} f^{(k)} g^{(n-k)}$$

$$-\frac{1}{(2m-3)!}\int_0^\infty dx\, \ln x\, \partial\Big(\sum_{k=0}^{2m-3}\binom{2m-3}{k}\varphi^{(k)}(x)\,\partial^{2m-3-k}\big(x^{2(m-1)}R_m(\tfrac{\epsilon}{x^2})\big)\Big)$$

$$= -\frac{1}{(2m-3)!}\sum_k \ln x\big(\varphi^{(k)}(x)-\varphi^{(k)}(0)\big)\binom{2m-3}{k}\partial^{2m-3-k}(\;\text{"}\;)\Big|_0^\infty \to 0$$

$x \ln x \to 0$ as $x \to 0$

$$+\frac{1}{(2m-3)!}\int_0^\infty dx \sum_{k=0}^{2m-3}\binom{2m-3}{k}\frac{\varphi^{(k)}(x)-\varphi^{(k)}(0)}{x}\,\partial^{2m-3-k}(\;\text{"}\;)$$

$$-\frac{1}{(2m-3)!}\sum_{k=0}^{2m-3}\binom{2m-3}{k}\varphi^{(k)}(0)\int_0^\infty dx\, \ln x\, \partial^{2m-2-k}\big(x^{2m-2}R_m(\tfrac{\epsilon}{x^2})\big)$$

change of variable $x = x'\epsilon^{1/2}$

$$-\frac{1}{(2m-3)!}\sum_{k=0}^{2m-3}\binom{2m-3}{k}\varphi^{(k)}(0)\,\epsilon^{1/2}\epsilon^{k/2}\int_0^\infty dx'\,(\ln x' + \tfrac{1}{2}\ln\epsilon)\,\partial^{2m-2-k}\big(x'^{2m-2}R_m(\tfrac{1}{x'^2})\big)$$

logarithmic terms in ϵ

+ nonintegral powers in ϵ

Integrate by parts and get integral powers of ϵ

and a true remainder (the integral part)

$$\int_0^\infty dx\, \varphi(x) F\left(\frac{\epsilon}{x^2}\right) = \int \frac{dx}{x^{2m-2}}\, x^{2m-2}\, \varphi(x) \left\{ \sum_{k=0}^{m-1} \frac{F^{(k)}(0)}{k!} \epsilon^k x^{-2k} + R_m\left(\frac{\epsilon}{x^2}\right) \right\}$$

$$= -\frac{1}{(2m-3)!} \int_0^\infty dx \ln x\, \partial_x^{2m-2} \underbrace{\left(\varphi(x) \sum_{k=0}^{m-1} \frac{F^{(k)}(0)}{k!} \epsilon^k x^{2(m-k-1)} \right)}$$

$$- \frac{1}{(2m-3)!} \underbrace{\int_0^\infty dx \ln x\, \partial_x^{2m-2} \left(\varphi\, x^{2(m-1)} R_m\left(\frac{\epsilon}{x^2}\right)\right)}$$

$$\boxed{\frac{1}{x^{2m-2}} = \frac{1}{(2m-3)!}\, \partial_x^{2m-2} \ln x}$$

This term gives integral powers of ϵ in the asymptotic expansion in ϵ

This term gives integral, fractional and logarithmic terms in the asymptotic expansion in ϵ as well as the **true** remainder.

$O(\epsilon^{m-\frac{1}{2}})$, i.e. higher than $\epsilon^{(m-1)}$

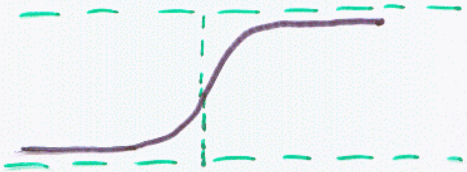
Two options

1) Regularization in the sense of distributions

(Is it unique ?)

2) Smearing out of the core (Eshelby)

Nonuniformly moving ramp-core (Markenscoff + Ni, JMPS 2001)



Are they the same ?

Yes to $O(\ln\varepsilon)$!

not to $O(1)$

Regularization (in a distributional sense)

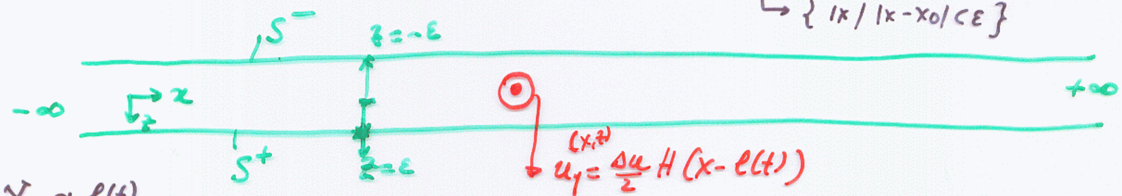
Self-force on an accelerating dislocation

$$\mathcal{F}^{self} \equiv \frac{d}{dt}\int_D \rho \dot{u}_j u_{j,i}\, dV + \int_{\partial D_1} \{ L n_i - u_{j,i}\sigma_{jk} n_k - \rho \dot{u}_j u_{j,i} v_n \} dS$$

$$(F,\phi) = \int f \phi\, dx + \int_B f \Big[\phi - \sum_{|k|<m} D^k\phi(x_0)\frac{(x-x_0)^k}{k!}\Big] dx$$

$$B \hookrightarrow \{ x \,/\, |x-x_0| < \varepsilon \}$$

Choose infinite strip



$X = x - \ell(t)$

$$\int_{-\infty}^{\infty} [\sigma_{yz} u_{y,x}(X,\varepsilon^+) - \sigma_{yz} u_{y,x}(X,\varepsilon^-)] dX =$$

$$= \int_{-\infty}^{\infty} \sigma_{yz}(X,\varepsilon) \{ [u_{y,x}(X,0^+) - u_{y,x}(X,0^-)] + \varepsilon [\quad]' \} dX =$$

$$= \int_{-\infty}^{\infty} \sigma_{yz}(X,\varepsilon) \{ \delta(X) + \varepsilon\delta'(X) + \frac{\varepsilon^2}{2}\delta''(X) + \cdots \} dX =$$

$$= \sigma_{yz}(0,\varepsilon) + \varepsilon\sigma'_{yz}(0,\varepsilon) + \varepsilon^2 \text{--} \quad = \sigma_{yz}(x=\ell(t),\varepsilon) + \varepsilon\sigma'_{yz}(x=\ell(t),\varepsilon) + \cdots$$

$$= \underset{\substack{\downarrow \\ 0}}{A_1} \frac{1}{\varepsilon} + A_2 \ln\varepsilon + A_3 + O(\varepsilon)$$

0 (same as steady-state)

$O(1)$ term in the near-field expansion around a non-uniformly moving dislocation

term: A_3

$$\frac{1}{2}\frac{\boxed{\ddot{\ell}(t)}\,c}{(c^2-v^2(t))^{1/2}}\left[1+\ln\left(\frac{cv}{2(c^2-v^2)}\right)\right]$$

$$+\frac{\boxed{\ddot{\ell}(t)}}{2c^2}\int_0^x \ln s\,\partial_s\left(\qquad\right)ds$$

$$+\frac{\boxed{\ddot{\ell}(t)}\sqrt{c^2-v^2}}{(c^2-v^2)^3}\left[\frac{v(c-v)}{c(c+v)}-\frac{c^2(c+2v)}{v^2(c+v)}\right]$$

$$+\frac{\boxed{\ddot{\ell}(t)}}{(c-v)^3}\left[\frac{c(2c-5v)}{2(c-v)}+\frac{3v^2}{2c}\right]\ln\left(\frac{c+\sqrt{c^2-v^2}}{v}\right)$$

$$-\frac{1}{2\{\ell(t)-\ell(0)\}}\frac{1}{\left(1-\frac{\ell^2(t)}{c^2t^2}\right)^{1/2}}$$

$$+\frac{1}{2c^2}\int_0^{x_0}\ln s\,\partial_s\left[\;—\;\right]ds$$

term A_2: $\frac{\mu(\Delta u)}{4\pi c_2^2}\frac{\boxed{\ddot{\ell}(t)}}{\left(1-\frac{\dot{\ell}^2}{c_2^2}\right)^{3/2}}$

Self-force on a ramp-core dislocation

(a) Rigid-core δ

$$\overset{\text{self}}{\mathcal{F}} = \mu \frac{\Delta u}{4\pi c_2^2} \frac{\ddot{\ell}(t)}{\left(1-\frac{\dot{\ell}^2}{c_2^2}\right)^{3/2}} \int_{-\infty}^{\infty} \ln|x-\ell(t)-\xi| \frac{\delta}{\delta^2+\xi^2}\, d\xi =$$

$$= \qquad '' \qquad \frac{1}{2} \ln\left((x-\ell(t))^2+\delta^2\right) =$$

$x-\ell(t)=\varepsilon$

$\lim\ x \to \ell(t)$

$$= \qquad \mu \frac{\Delta u}{4\pi c_2^2} \frac{\ddot{\ell}(t)}{\left(1-\frac{\dot{\ell}^2}{c_2^2}\right)^{3/2}} \ln\delta$$

(b) Time-Dependent core $\delta(t)$

$$\overset{\text{self}}{\mathcal{F}} = \mu \frac{\Delta u}{4\pi c_2^2} \int_0^t \frac{\ddot{\ell}(t-w)}{\left(1-\frac{\dot{\ell}(t-w)^2}{c_2^2}\right)^{3/2}} \underbrace{\int_{-\infty}^{\infty} \ln|x-\ell(w)-\xi| \frac{\ell'(w)\,\delta(w)}{\delta^2+\xi^2}\, d\xi}_{}$$

$$= \frac{\mu \Delta u}{4\pi c_2^2} \int_0^t \frac{\ddot{\ell}(t-w)}{\left(1-\frac{\dot{\ell}(t-w)^2}{c_2^2}\right)^{3/2}} \ell'(w) \boxed{\ln\delta(w)}\, dw$$

To be determined by matching with discrete model.

Near field parameter $\varepsilon < (2\delta)^{1/3}$

M

Motion of a Frenkel-Kontorova Dislocation

One-dimensional discrete crystal model

Atkinson + Cabrera Phys. Rev 1965

Kresse + Truskinovsky J.M.P.S 2003

$$V=\sum_n \frac{1}{2}E\varepsilon\left(\frac{u_{n+1}-u_n}{\varepsilon}\right)^2+\varepsilon\left[\overset{\text{double-well potential}}{W(\tilde{u}_n)}-\tilde{\sigma}\,u_n\right]$$

$$K=\sum_n \frac{1}{2}\rho\varepsilon\dot{u}_n^2 \qquad u_n(t)=\tilde{u}(\varepsilon n-vt)$$

$$\Omega_0=\varepsilon\sqrt{\frac{C}{E}}$$

"**Radiation damping**" is the loss of energy due to microscopic fluxes at infinity. Tunneling of energy from long to short waves.

Compute $$\frac{d(V+K)}{dt}-\frac{dA}{dt}\equiv\underbrace{G(v)}_{\Omega_0^4\sum_k \frac{1}{k\,|L'(k)|}}\cdot V$$

configurational force

$$L(k)=\Omega_0^4+4\sin^2\frac{k}{2}-v^2k^2$$

Match: Configurational force in outer (continuum) and inner (discrete) models.

Dislocation Dynamics

Open problems

- Given an applied loading what is the ensuing motion of a dislocation (equation of motion of a dislocation)
    - "effective mass" of a generally moving dislocation
    - "Self-force" or "configurational force" on a moving dislocation
- How fast can dislocations move?
    - Can dislocations cross the sound-wave barrier?

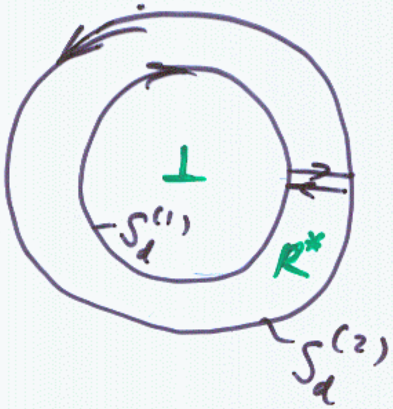
"A supersonic dislocation is a formal possibility"
(Eshelby, 1953)

Self-force for accelerating dislocations

Energy-release rate for moving cracks, see Freund (1972)

$$\dot{\mathcal{E}} = \int_{S_d} \left\{ \sigma_{ij} n_j v_i + \left(\tfrac{1}{2} \sigma_{ij} u_{i,j} + \tfrac{1}{2} \rho v_i v_i \right) v_n \right\} dS$$

$$\downarrow$$



$$\int_{R^*} \left\{ \rho v_i \dot{v}_i + v_n v_{i,n} + \sigma_{ij} \left(v_i + v_n u_{i,n} \right)_{,j} \right\} dA$$

$\longrightarrow 0$

does <u>not</u> vanish as $R^* \to 0$

for accelerating motion of

a dislocation

Self-force and " equation of motion"
for a dislocation suddenly accelerated to constant velocity

Energy-release rate IS path-independent

screw
$$\dot{\mathscr{E}}_0^{\mathrm{s}} = -\frac{\mu b_x^2}{2\pi t}\left(\frac{1-(1-v_{\mathrm{d}}^2/c_2^2)^{\frac{1}{2}}}{(1-v_{\mathrm{d}}^2/c_2^2)^{\frac{1}{2}}}\right),$$

edge
$$\dot{\mathscr{E}}_0^{\mathrm{s}} = \frac{-\mu b_x^2}{2\pi t}\left\{\frac{12-8\alpha^2}{\beta^2(1-\alpha^2)^{\frac{1}{2}}} - \frac{(2-\beta^2)(6-7\beta^2)}{\beta^2(1-\beta^2)^{\frac{1}{2}}} - 2\left(1-\frac{\alpha^2}{\beta^2}\right)\right\}$$

$\beta = v_{\mathrm{d}}/c_2$

$\alpha = v_{\mathrm{d}}/c_1$

Applied shear stress

$$\dot{\mathscr{E}}_0 = \dot{\mathscr{E}}_0^{\mathrm{e}} + \sigma_{yz}^a b_y v_{\mathrm{d}}, \qquad \dot{\mathscr{E}}_0^{\mathrm{s}} = \dot{\mathscr{E}}_0^{\mathrm{s}} + \sigma_{xz}^a b_x v_{\mathrm{d}},$$

$$\sigma_{yz}^a b_y = -\frac{\dot{\mathscr{E}}_0^{\mathrm{s}}}{v_{\mathrm{d}}} \equiv F_{\mathrm{drag}}^{\mathrm{c}}$$

is the driving force required for the elastic fields associated with the disloc
n to have neither an energy source nor an energy sink at the dislocation

Clifton & Markenscoff, *JMPS,* 1981

Singular asymptotic limits of the general motion solution

Limit as $z \to 0$

$$\int_0 \frac{(t-\eta(\xi))\,(x-\xi)^2\,d\xi}{[(x-\xi)^2+z^2]^2\sqrt{(t-\eta(\xi))^2-r^2b^2}} = \frac{1}{z^2}\int_0 \underbrace{\frac{z^2/(x-\xi)^2\quad(t-\eta(\xi))\,d\xi}{\left[1+\frac{z^2}{(x-\xi)^2}\right]^2\sqrt{(t-\eta(\xi))^2-r^2b^2}}}_{f\left(\frac{z}{x-\xi}\right)\,\phi(\xi,z)\,d\xi}$$

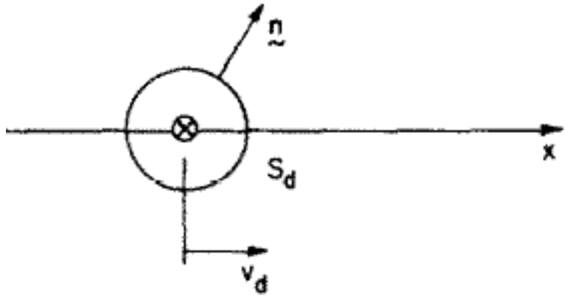
$$\frac{\partial u}{\partial t}(x,0,t) = \frac{\Delta u}{2\pi}\int_{-\infty}^{\infty} \ln|x-\xi|\left(\frac{\partial}{\partial\xi}\right)^2\left[\frac{(t-\eta(\xi))\,\chi(\xi)}{\sqrt{(t-\eta(\xi))^2-b^2(x-\xi)^2}}\right]d\xi$$

$$-\int_0 \frac{(t-\eta(\xi))\,(1-\chi(\xi))\,d\xi}{(\xi-x)^2\sqrt{(t-\eta(\xi))^2-b^2(x-\xi)^2}}$$

Energy flux through a moving dislocation

ESHELBY, 1968; FREUND, 1972

for moving cracks



Energy flux into a moving dislocation.

$$\dot{\mathscr{E}}_{\mathrm{d}} = \int_{S_{\mathrm{d}}} \{\sigma_{ij} n_j v_i + (\tfrac{1}{2}\sigma_{ij} u_{i,j} + \tfrac{1}{2}\rho v_i v_i) v_n\} \, \mathrm{d}S$$

Is path independent in the limit $\dot{\mathscr{E}}_0 = \lim_{S_{\mathrm{d}} \to 0} \dot{\mathscr{E}}_{\mathrm{d}}$

if $\int_{R^*} \{\rho v_i \dot{v}_i + v_n v_{i,n}) + \sigma_{ij}(v_i + v_n u_{i,n})_{,j}\} \, \mathrm{d}a$ vanishes

IN CONSTANT VELOCITY STEADY-STATE DISL. MOTION THE ENERGY FLUX is 0

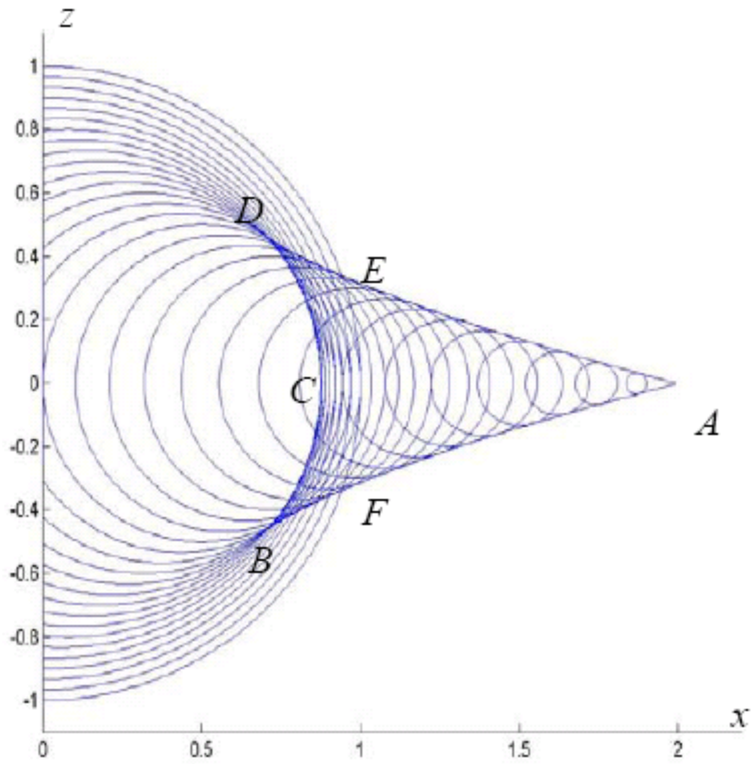


Figure 4 Mach wave front at $t = 1$ for the motion $l(t) = 2t^2$; the motion is supersonic and the envelope grows out of the circle with radius $r = 1$; the speed c_2 is normalized to 1.

Edge dislocation crossing the shear wave speed (transonic)

$$B = \lim_{\xi_0,\xi_1 \to \xi^*} \frac{-\Delta u}{2\pi b^2} \frac{\left(z^2 - (x-\xi^*)^2\right)^2 (t^* - \eta(\xi^*))^4}{[(x-\xi^*)^2 + z^2]^4 \left|\eta''(\xi^*)(t-\eta(\xi^*))\right|^{\frac{1}{2}}} \int_{\xi_0}^{\xi_1} \frac{d\xi}{|(\xi-\xi^*)|}$$

$\left(x-\xi^*\right) = O\left(\xi-\xi^*\right)$.

$\frac{z}{x-\xi^*} = m$, where m is a constant, so that,

as $t \to t^*$, $\left(t-\eta\left(\xi^*\right)\right) \to \left(t^* - \eta\left(\xi^*\right)\right) \to b\sqrt{1+m^2}\left(x-\xi^*\right)$.

$$\lim_{\xi,\xi_0,\xi_1 \to \xi^*} O\left(\frac{\ln\left|(\xi-\xi^*)\right|\Big|_{\xi_0}^{\xi_1}}{\left|\left(\xi-\xi^*\right)\right|^{\frac{1}{2}}} \right)$$