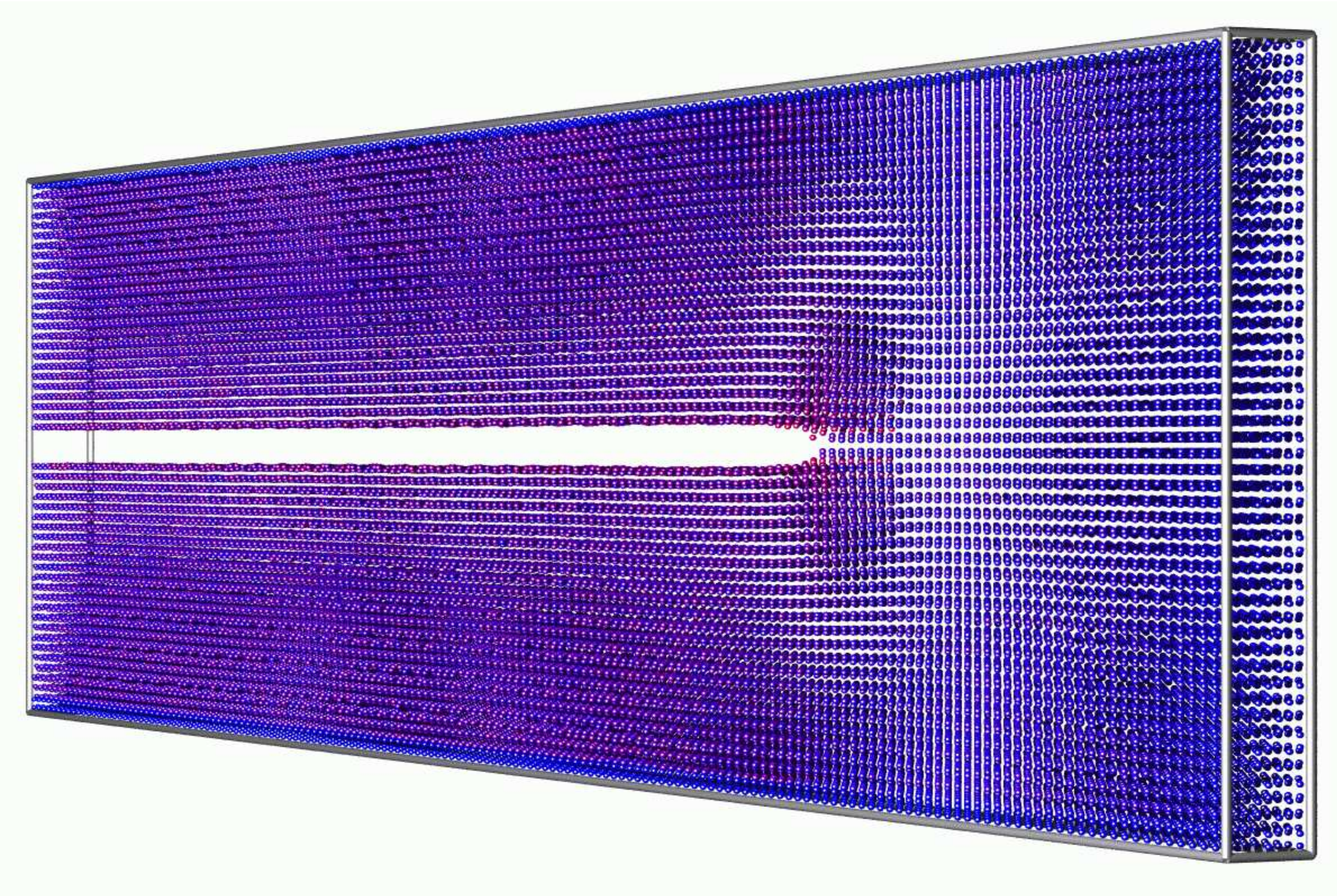
Dislocations and Cracks



Definitions

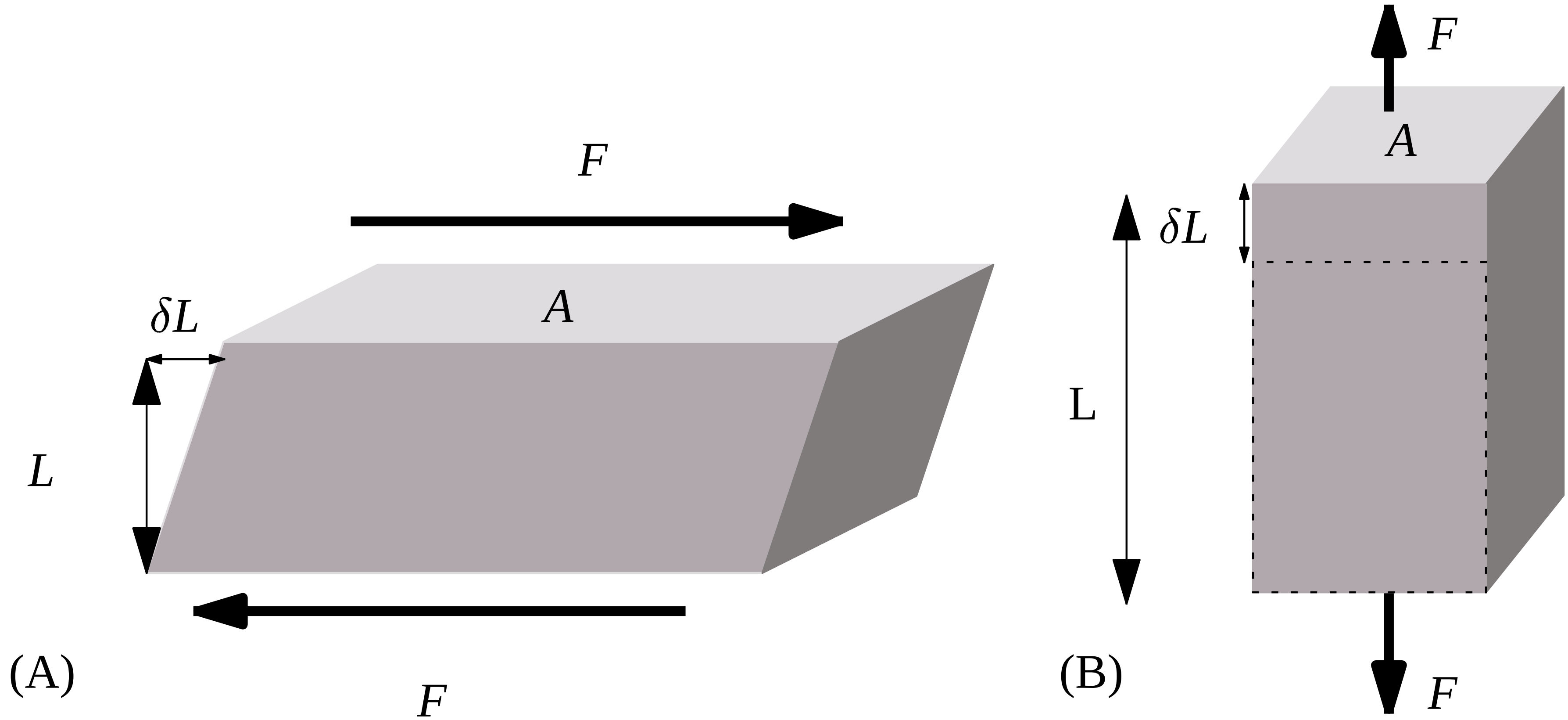
- ☞ Brittle
- ☞ Ductile
- ☞ Dislocation
- ☞ Burgers Vector
- ☞ Glide Plane
- ☞ Frenkel–Kontorova Model
- ☞ Hexatic Phases
- ☞ Orientational Order, Mermin–Wagner Theorem
- ☞ Kosterlitz–Thouless–Berezinkskii Transition
- ☞ Cracks
- ☞ Conformal Mapping
- ☞ Stress Intensity Factor

Definitions

Given surface energy of $\Gamma = 1$ J/m^2, height h at which it pays to split object in two is

$$h = \sqrt{\frac{4\Gamma}{\rho g}} \approx 1.4 \text{ cm.} \quad \text{(L1)}$$

Failure in Shear



$$G\frac{\delta L}{L} = \frac{F}{A}, \tag{L2}$$

Failure in Shear

$$\mathcal{S} = \frac{F}{A} = \begin{cases} \frac{G}{5} & \text{shear} \\ \frac{Y}{5} & \text{tension.} \end{cases} \tag{L3}$$

Material	Shear modulus $G/5$ (10^{11} ergs cm^{-3})	Yield strength (10^{11} ergs cm^{-3})
Iron	1.0–1.6	0.02–1
Copper	1.0	0.005
Titanium	1.0	0.08

Failure in Tension

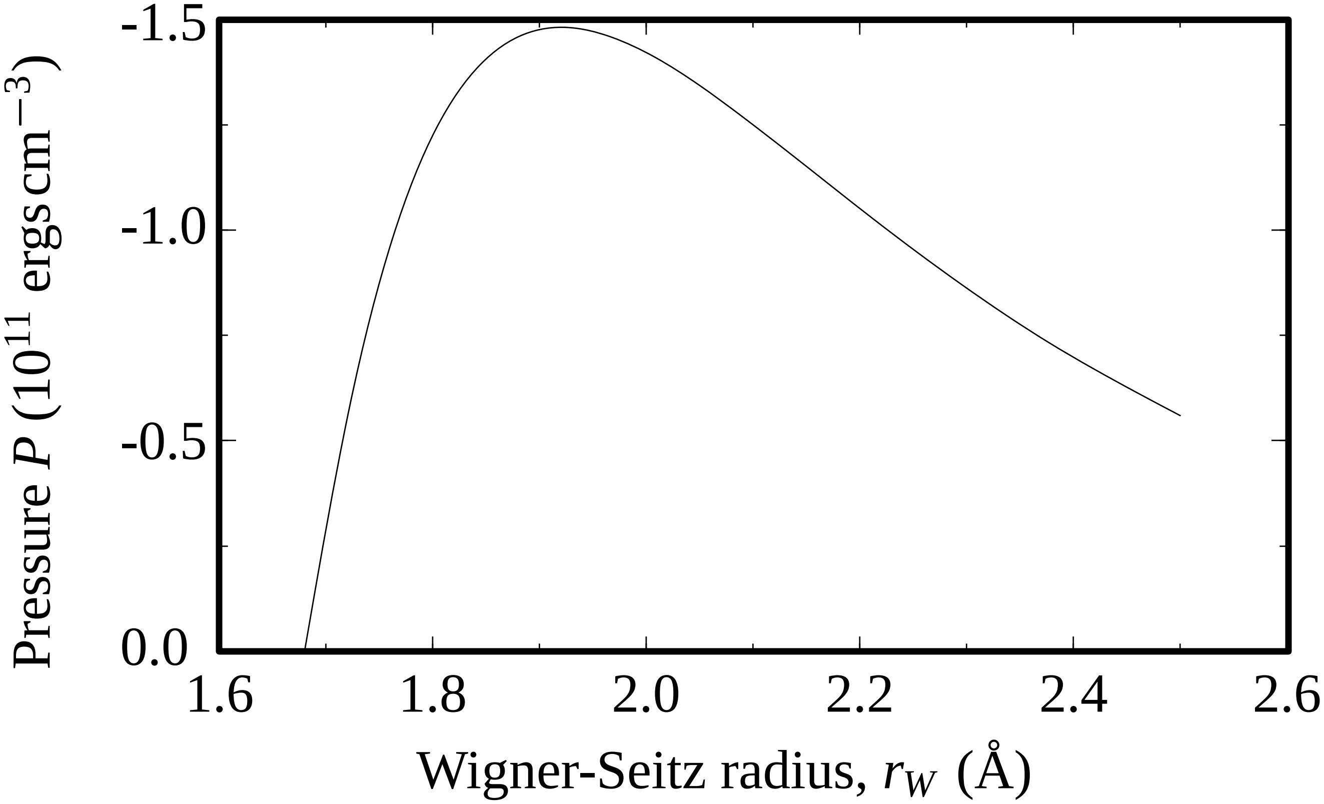
$$\mathcal{S} = \frac{F}{A} = \begin{cases} \frac{G}{5} & \text{shear} \\ \frac{Y}{5} & \text{tension.} \end{cases} \tag{L4}$$

$$Y\frac{\delta L}{L} = \frac{F}{A}. \tag{L5}$$

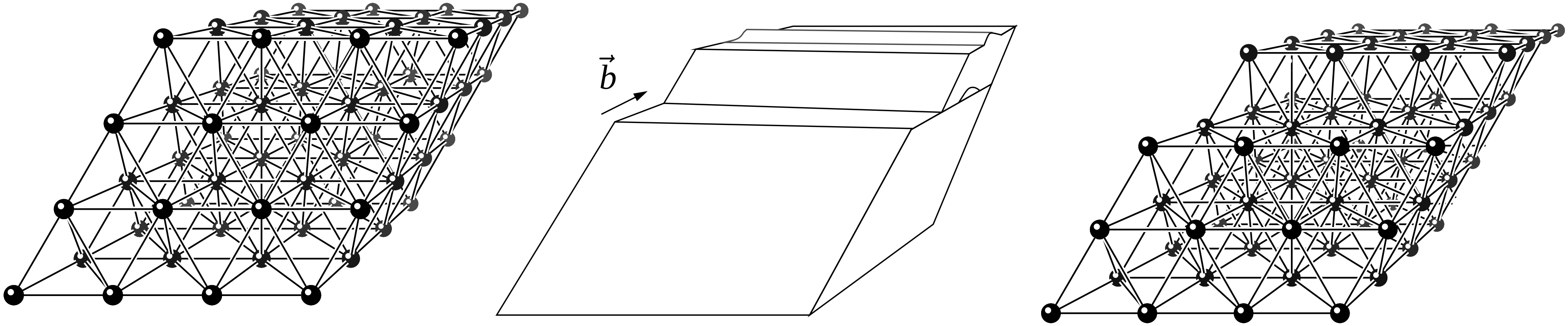
Material	Young's Modulus $Y/5$ (10^{11} ergs cm^{-3})	Theoretical Strength (10^{11} ergs cm^{-3})	Practical Strength (10^{11} ergs cm^{-3})	Ratio
Iron	4.0	4	0.03	0.008
Titanium	2.2	3.1	0.03	0.009
Silicon	3.2	1.5	0.07	0.05
Glass	1.4	4	0.04	0.01

Complete Cohesive Energy Curve

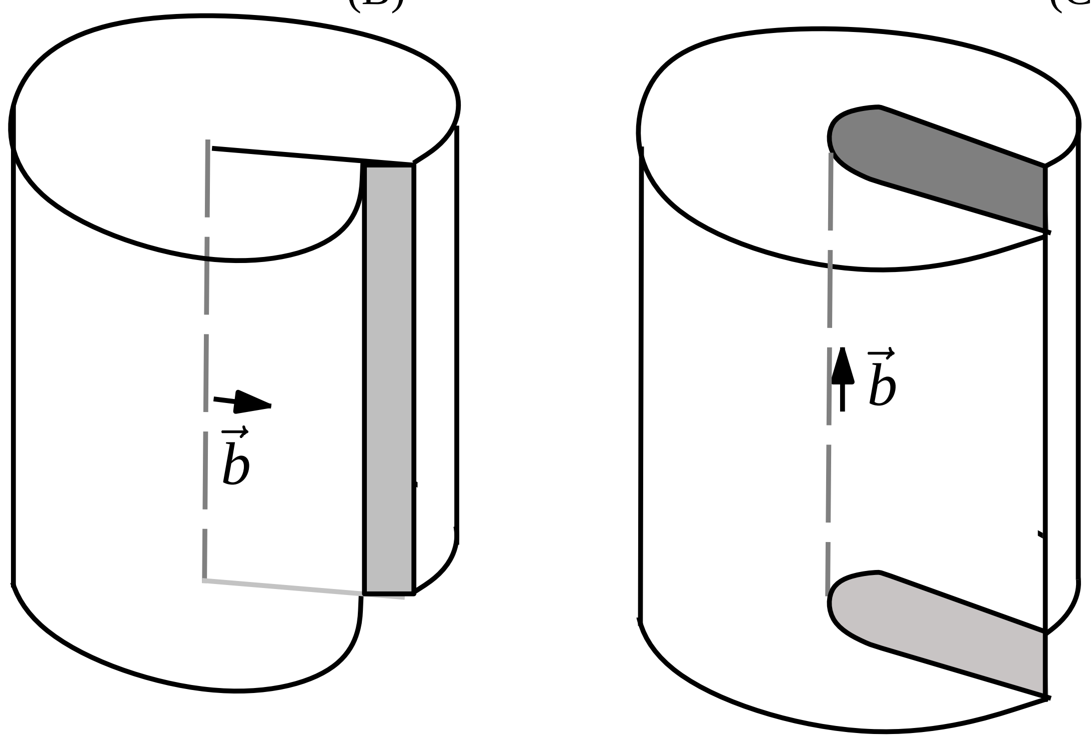
$$-P = \frac{1}{4\pi r_W^2} \frac{\partial \mathcal{E}(r_W)}{\partial r_W}. \tag{L6}$$



Dislocations

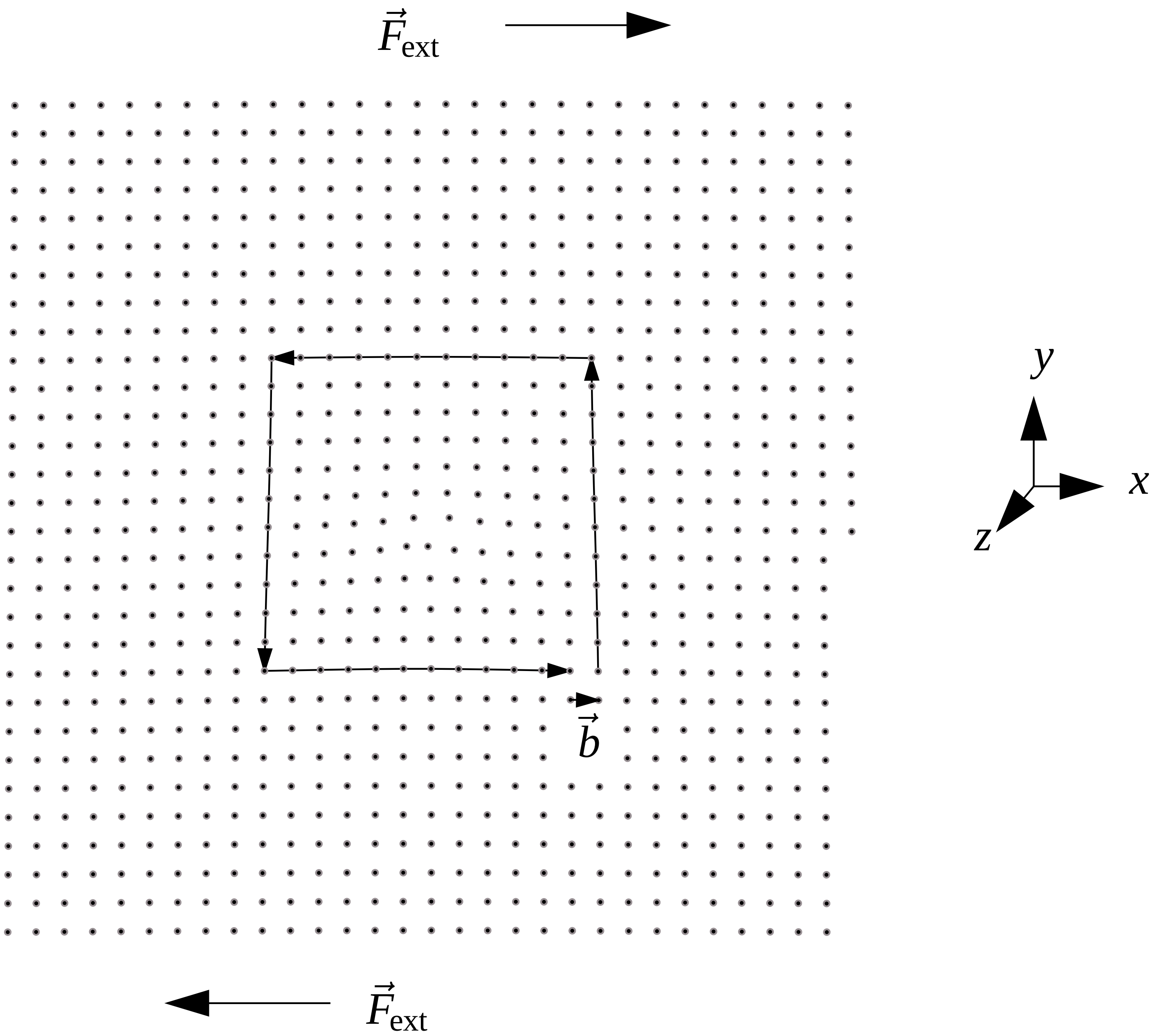


(A) (B) (C)

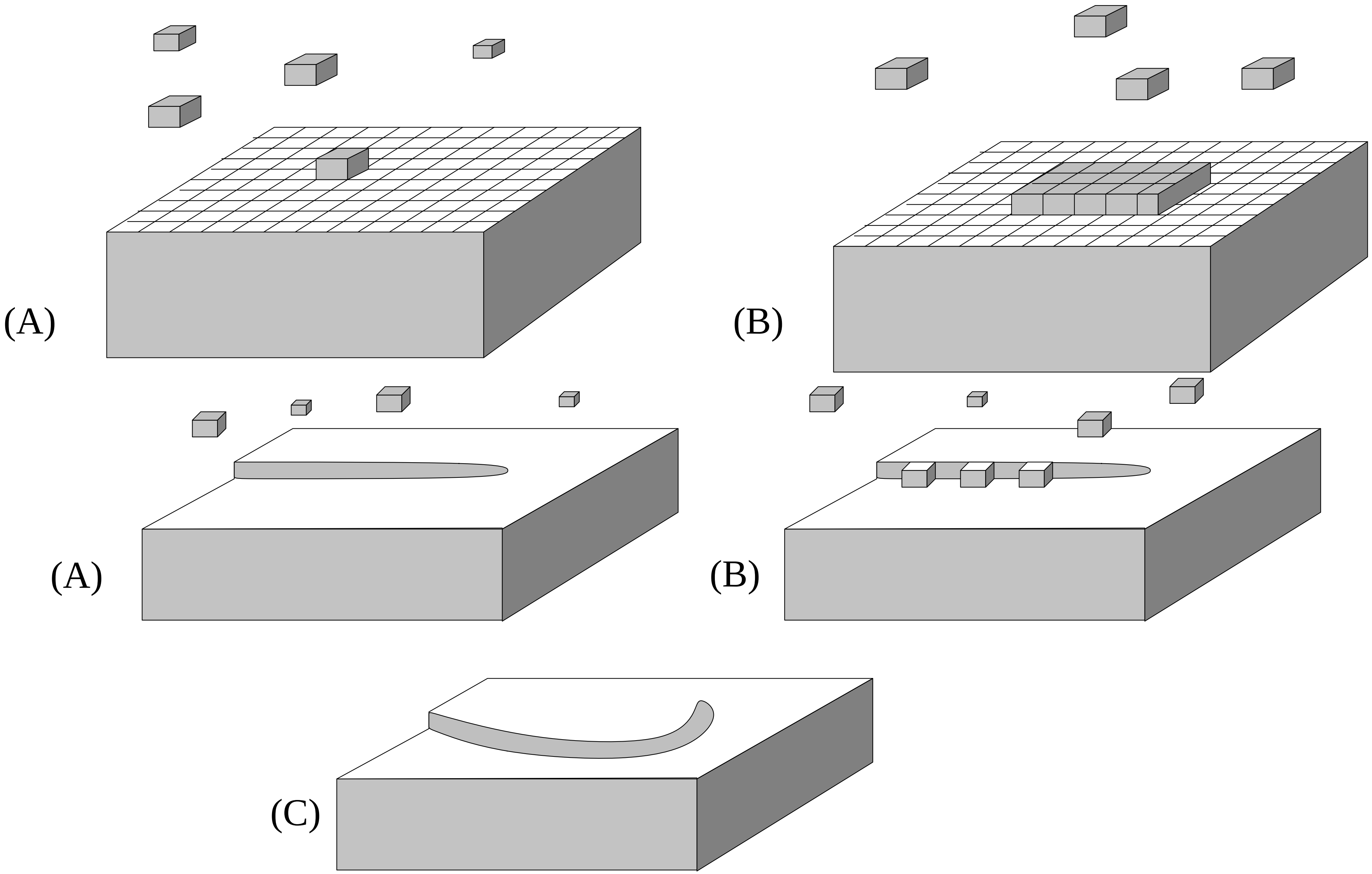


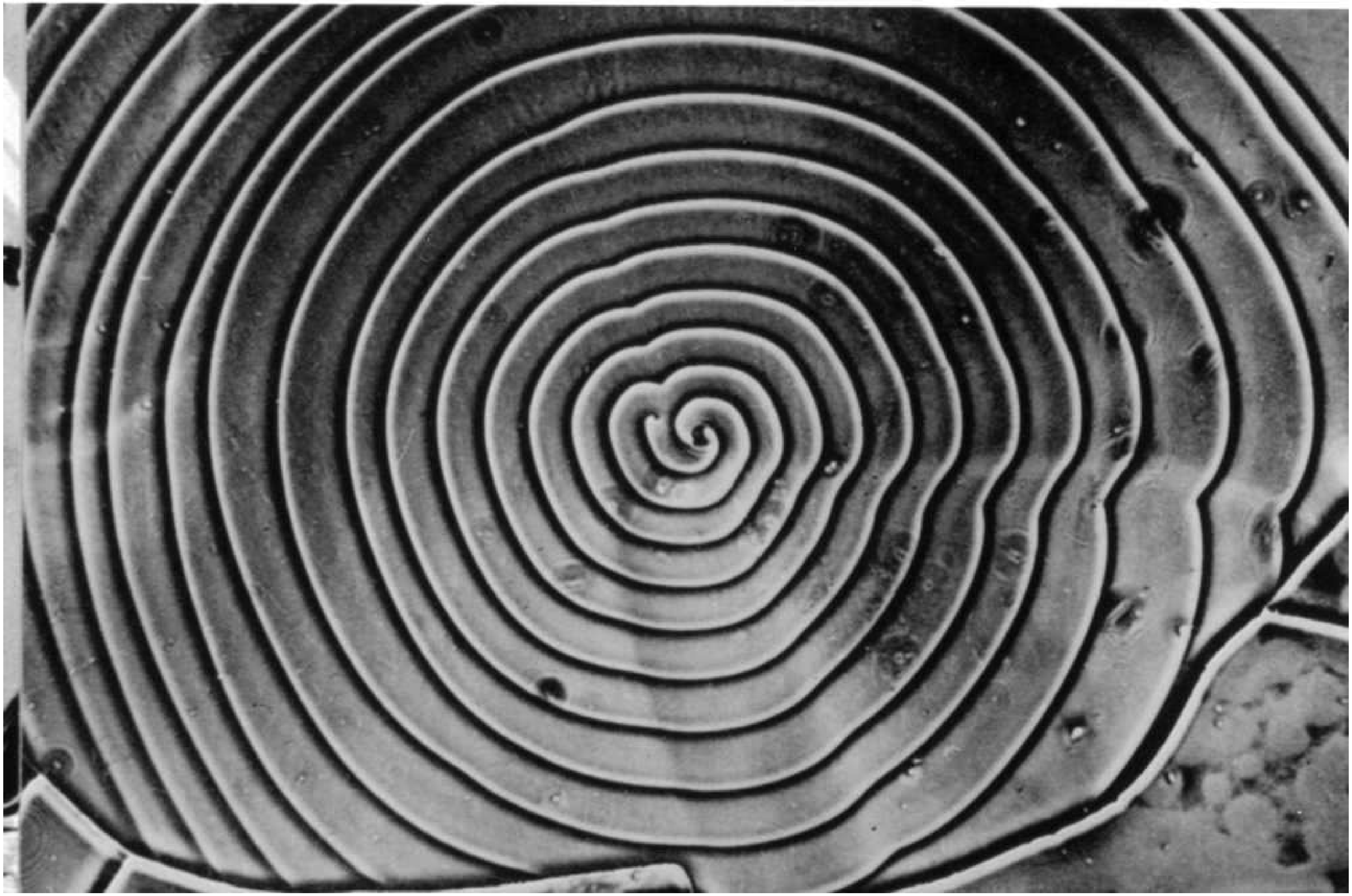
(A) Edge (B) Screw

Burgers Vector

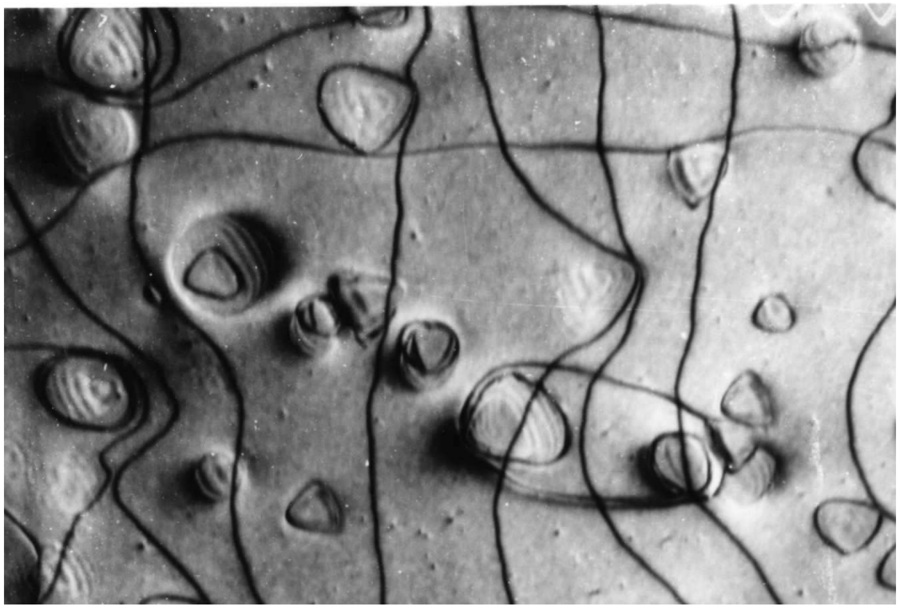
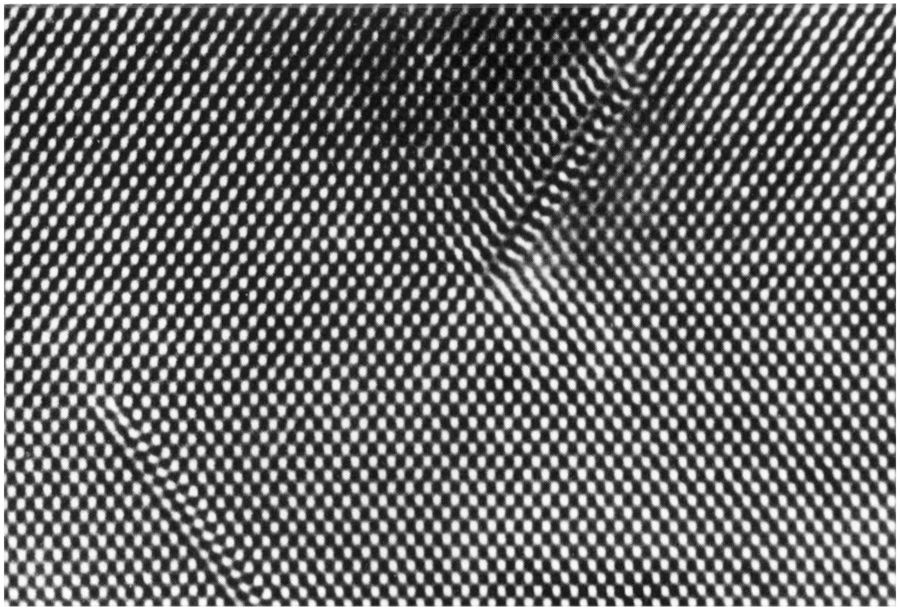


Experimental Observations of Dislocations





[Source: Amelinckx (1964)]

(A)  (B) 

(A) Courtesy of J. Humphreys, Manchester University.)

[(B) Cullis et al. (1985)]

Force to Move a Dislocation

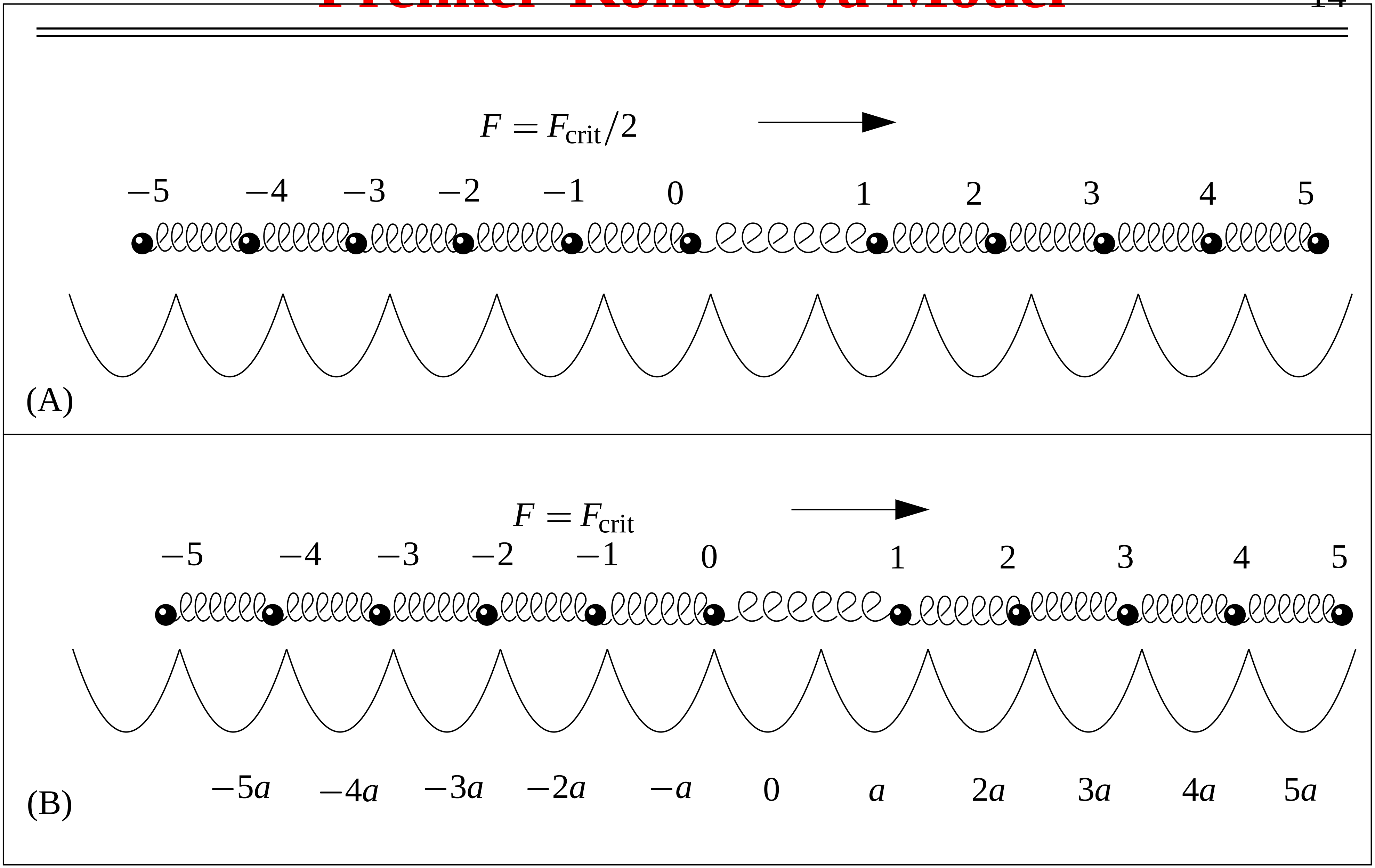
$$f_x = \sigma_{xy} b_x, \tag{L7}$$

$$\sigma_{xy} = \frac{F_{\text{ext}}}{Na^2} \tag{L8}$$

$$\vec{f} = (\sigma \cdot \vec{b}) \times \hat{L}. \tag{L9}$$

Peach–Kohler force

One-Dimensional Dislocations: Frenkel–Kontorova Model



Find force needed to move dislocation in simple one–dimensional model.

One-Dimensional Dislocations: Frenkel–Kontorova Model

$$U(x) = \tfrac{1}{2}\mathcal{K}[x - a\,\mathrm{int}(x/a + \tfrac{1}{2})]^2 - fx, \tag{L10}$$

$$f_n = k[x_{n+1} - x_n - a] + k[x_{n-1} - x_n + a] - \frac{\partial U}{\partial x}. \tag{L11}$$

$$f_n = \begin{cases} k[x_{n+1} - x_n - a] + k[x_{n-1} - x_n + a] + f - \mathcal{K}[x_n - (n-1)a] & \text{for} \quad n \le 0 \\ k[x_{n+1} - x_n - a] + k[x_{n-1} - x_n + a] + f - \mathcal{K}[x_n - na] & \text{for} \quad n > 0. \end{cases} \tag{L12}$$

$$x_n = f/\mathcal{K} + a(n-1) + A_l e^{qn}, \tag{L13}$$

$$k(e^q - 2 + e^{-q}) - \mathcal{K} = 0 \tag{L14}$$

$$x_n = f/\mathcal{K} + an + A_r e^{-qn}. \tag{L15}$$

One-Dimensional Dislocations: Frenkel–Kontorova Model

$$
\begin{aligned}
-a+A_l &= A_r && \text{(L16a)}\\
A_l e^q &= a+A_r e^{-q}, && \text{(L16b)}
\end{aligned}
$$

$$
\begin{aligned}
A_l &= \frac{a}{e^q+1} && \text{(L17a)}\\
A_r &= \frac{-a}{e^{-q}+1}. && \text{(L17b)}
\end{aligned}
$$

$$x_0 = -\frac{a}{2} = \frac{f_c}{\mathcal{K}} - a + A_l \qquad \text{(L18)}$$

$$\Rightarrow f_c = \frac{a\mathcal{K}}{2}\tanh\frac{q}{2}. \qquad \text{(L19)}$$

$$q \approx \sqrt{\frac{\mathcal{K}}{k}} \qquad \text{(L20)}$$

One-Dimensional Dislocations: Frenkel–Kontorova Model

$$f_c \approx \frac{a\mathcal{K}}{4}\sqrt{\frac{\mathcal{K}}{k}}. \tag{L21}$$

Impossibility of Crystalline Order in Two Dimensions

Peierls and Landau showed that two–dimensional crystals are destroyed by thermal fluctuations.

$$U = \int d^2r\,\tfrac{1}{2}C\sum_{\alpha\beta}\frac{\partial u_\alpha}{\partial r_\beta}\frac{\partial u_\alpha}{\partial r_\beta}. \tag{L22}$$

$$u_\alpha(\vec{r}) = \sum_{\vec{k}} e^{i\vec{r}\cdot\vec{k}} u_\alpha(\vec{k}). \tag{L23}$$

$$\vec{u}(\vec{k}) = 0 \text{ for } k > 1/\mathcal{D}. \tag{L24}$$

$$U = \int d^2r\,\tfrac{1}{2}C\sum_{\beta\alpha\vec{k}\vec{k}'} k_\beta k'_\beta e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} u_\alpha(\vec{k})u^*_\alpha(\vec{k}') \tag{L25}$$

$$= \frac{\mathcal{V}C}{2}\sum_{\alpha\vec{k}} k^2|u_\alpha(\vec{k})|^2 \tag{L26}$$

$$\langle u^2 \rangle = \langle \int \frac{d^2r}{\mathcal{V}} \sum_\beta u_\beta(\vec{r}) u_\beta(\vec{r}) \rangle \tag{L27}$$

$$= \sum_{\beta \vec{k}} \langle |u_\beta(\vec{k})|^2 \rangle \tag{L28}$$

$$\vec{u}(\vec{k}) = \vec{u}^*(-\vec{k}) \tag{L29}$$

$$\langle |u_\beta(\vec{k})|^2 \rangle$$

$$= \frac{\int \prod_{\alpha \vec{k}'} du_\alpha(\vec{k}') |u_\beta(\vec{k})|^2 e^{-\beta \frac{\mathcal{V}C}{2} \sum_{\alpha \vec{k}'} k'^2 |u_\alpha(\vec{k}')|^2}}{\int \prod_{\alpha \vec{k}'} du_\alpha(\vec{k}') e^{-\beta \frac{\mathcal{V}C}{2} \sum_{\alpha \vec{k}'} k'^2 |u_\alpha(\vec{k}')|^2}} \tag{L30}$$

$$= \frac{\int du_\beta(\vec{k}) |u_\beta(\vec{k})|^2 e^{-\beta \mathcal{V}Ck^2 |u_\beta(\vec{k})|^2}}{\int du_\beta(\vec{k}) e^{-\beta \mathcal{V}Ck^2 |u_\beta(\vec{k})|^2}} \tag{L31}$$

$$= \frac{\int du^r du^i [(u^r)^2 + (u^i)^2] e^{-\beta \mathcal{V}Ck^2 [(u^r)^2 + (u^i)^2]}}{\int du^r du^i e^{-\beta \mathcal{V}Ck^2 [(u^r)^2 + (u^i)^2]}} \tag{L32}$$

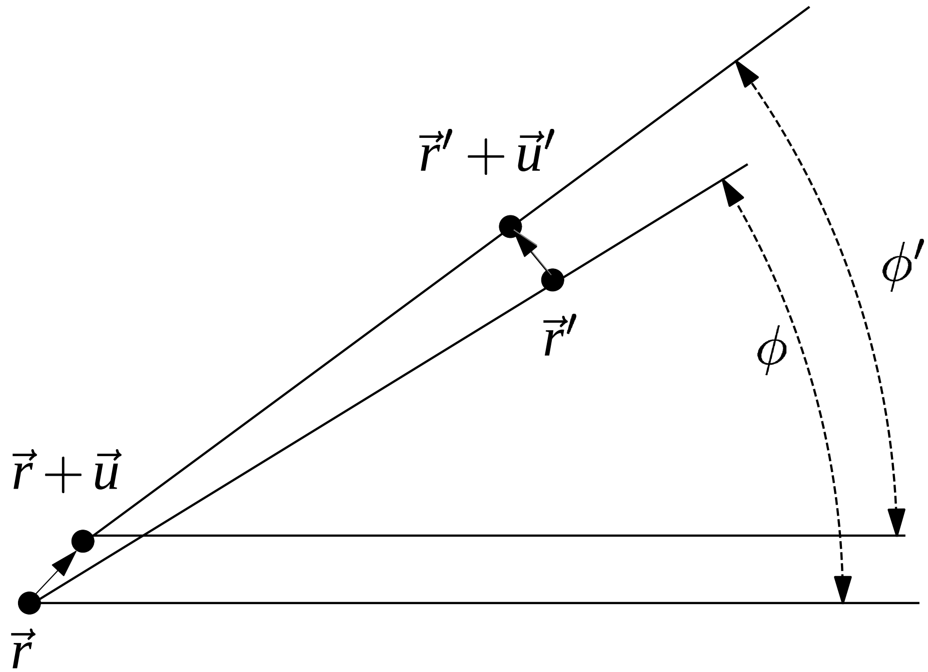
$$= \frac{k_B T}{\mathcal{V} C k^2}. \tag{L33}$$

$$\langle u^2 \rangle = \sum_{\alpha \vec{k}} \frac{k_B T}{\mathcal{V} C k^2} \tag{L34}$$

$$= 2 \int \frac{d^2 k}{(2\pi)^2} \frac{k_B T}{C k^2} \tag{L35}$$

$$= 2 \int_0^{1/\mathcal{D}} \frac{dk}{2\pi k} \frac{k_B T}{C} \to \infty. \tag{L36}$$

Orientational Order



$$(dx, dy) = \vec{r}' - \vec{r}. \tag{L37}$$

$$\phi = \tan^{-1}(dy/dx). \tag{L38}$$

$$\vec{r} + \vec{u}(\vec{r}) \quad \text{and} \quad \vec{r}' + \vec{u}(\vec{r}'). \tag{L39}$$

Orientational Order

$$\phi' = \tan^{-1}\left(\frac{dy+\partial u_y/\partial x\,dx+\partial u_y/\partial y\,dy}{dx+\partial u_x/\partial x\,dx+\partial u_x/\partial y\,dy}\right) \tag{L40}$$

$$\approx \phi+\frac{dx\,dy}{dx^2+dy^2}\left[\left(\frac{\partial u_y}{\partial y}-\frac{\partial u_x}{\partial x}\right)+\frac{dx}{dy}\frac{\partial u_y}{\partial x}-\frac{dy}{dx}\frac{\partial u_x}{\partial y}\right] \tag{L41}$$

$$\Rightarrow \phi'-\phi = \cos\phi\sin\phi\left(\frac{\partial u_y}{\partial y}-\frac{\partial u_x}{\partial x}\right)+\cos^2\phi\frac{\partial u_y}{\partial x}-\sin^2\phi\frac{\partial u_x}{\partial y}. \tag{L42}$$

$$\delta\phi(\vec r) = \frac{1}{2}\left(\frac{\partial u_y}{\partial x}-\frac{\partial u_x}{\partial y}\right). \tag{L43}$$

$$\delta\phi(\vec r) = \frac{1}{2}\sum_{\vec k}(ik_x u_y(\vec k)-ik_y u_x(\vec k))e^{i\vec k\cdot\vec r}. \tag{L44}$$

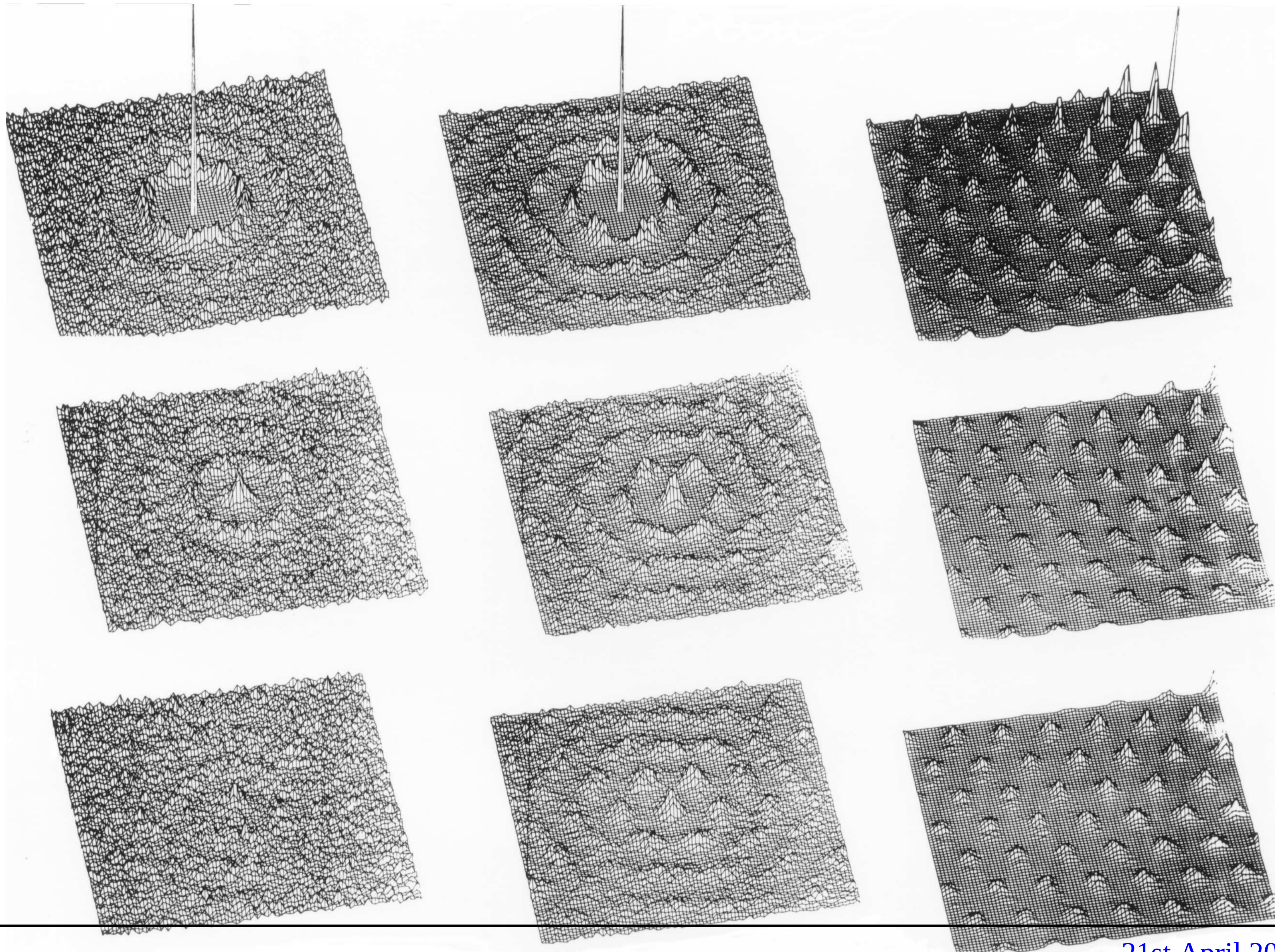
$$\int\frac{d^2r}{\mathcal{V}}\langle\delta\phi(\vec r)\delta\phi(\vec r)\rangle \tag{L45}$$

$$= \tfrac{1}{4}\sum_{\vec k}k_x^2\langle|u_x(\vec k)|^2\rangle+k_y^2\langle|u_y(\vec k)|^2\rangle-k_xk_y\langle(u_x(\vec k)u_y^*(\vec k)+u_y(\vec k)u_x^*(\vec k))\rangle \tag{L46}$$

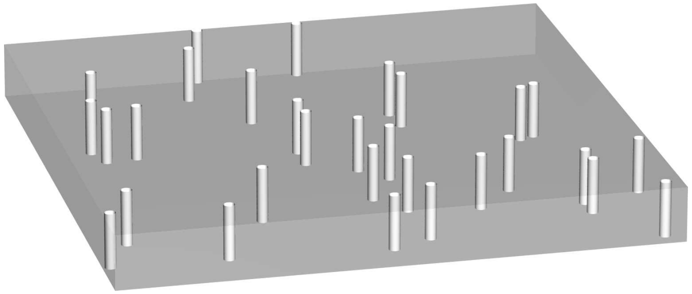
$$= \quad \tfrac{1}{4}\sum_{\vec{k}} \frac{k_BT}{C\mathcal{V}k^2}(k_x^2+k_y^2) \tag{L47}$$

$$= \quad \frac{k_BT}{4C}\int_0^{2\pi} d\theta \int_0^{1/\mathfrak{D}} \frac{dk\,k}{(2\pi)^2} = \frac{k_BT}{16\pi\mathfrak{D}^2 C}. \tag{L48}$$

Kosterlitz–Thouless–Berezinskii Transition



[Murray and Grier (1996)]



$$u_x = 0, \quad u_y = 0, \quad u(x,y) = u_z(x,y). \tag{L49}$$

$$U = \frac{a\mu}{2} \int d^2r \, (\nabla u)^2 \tag{L50}$$

$$\nabla^2 u = 0. \tag{L51}$$

$$u(x,y) = \frac{a}{2\pi} \mathrm{Im} \ln[x + iy]. \tag{L52}$$

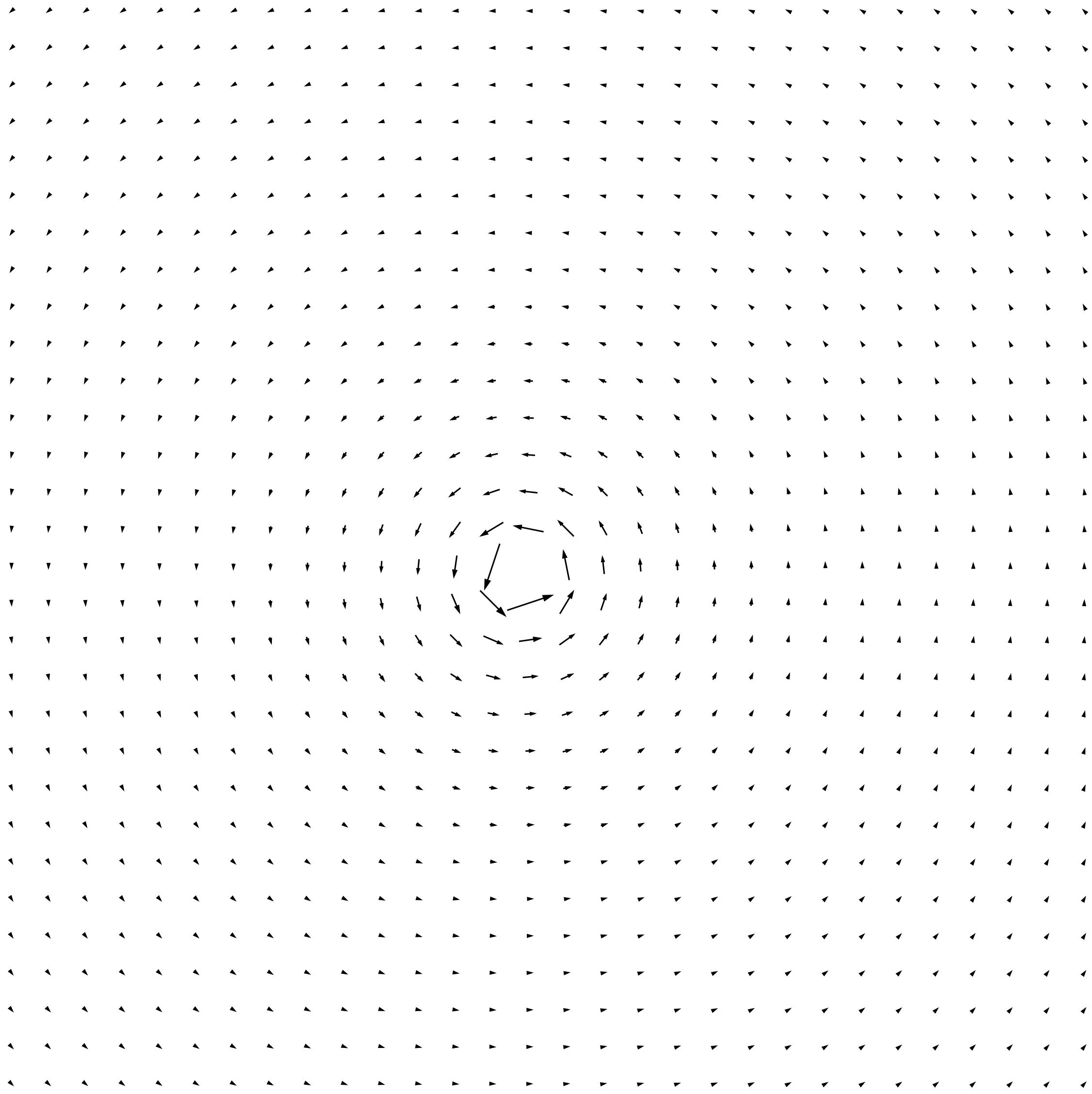
$$U = \frac{a\mu}{2} \left(\frac{a}{2\pi}\right)^2 \int d^2r \left[\frac{-y}{x^2+y^2}\right]^2 + \left[\frac{x}{x^2+y^2}\right]^2 \tag{L53}$$

$$= \quad \frac{a\mu}{2}\left(\frac{a}{2\pi}\right)^2 \int_a^R dr\, 2\pi r \frac{1}{r^2} \tag{L54}$$

$$\to \quad \frac{1}{4\pi}(a^3\mu)\ln\left(\frac{R}{a}\right) + w. \tag{L55}$$

$$u(x,y) = \frac{a}{2\pi}\mathrm{Im}\left\{\ln[x+iy] - \ln[x - x_0 + iy]\right\}. \tag{L56}$$

$$2q^2 \ln\left(\frac{x_0}{a}\right) + 2w \quad \text{with } q^2 = \frac{a^3\mu}{4\pi}. \tag{L57}$$



$$S = 2k_B \ln(L/a), \quad \text{(L58)}$$

$$\mathcal{E} = q^2 \ln(L/a). \tag{L59}$$

$$k_B T_c = \frac{q^2}{2}. \tag{L60}$$

$$\mathcal{H} = \frac{1}{2}\sum_{i \neq j} U(|\vec{r}_i - \vec{r}_j|) + 2w \quad \text{with} \quad U(r) = 2q^2 \ln(r/a) \tag{L61}$$

$$\langle r^2 \rangle = \frac{\int_a^\infty dr\, 2\pi r\, r^2 e^{-\beta U(r)}}{\int_a^\infty dr\, 2\pi r e^{-\beta U(r)}} \tag{L62}$$

$$= a^2 \left[\frac{\beta q^2 - 1}{\beta q^2 - 2}\right]. \tag{L63}$$

$$Z_{\text{gr}} = 1 + \sum_{\vec{r}_1 \vec{r}_2} e^{-\beta U(|\vec{r}_1 - \vec{r}_2|) - 2\beta w} + \ldots. \tag{L64}$$

$$n(r)dr = \frac{dr}{R^2}\langle\delta_{r,|\vec r_1-\vec r_2|}\rangle = \frac{dr}{R^2}\sum_{\vec r_1\vec r_2} e^{-\beta U(|\vec r_1-\vec r_2|)-2\beta w}\delta_{r,|\vec r_1-\vec r_2|}+\dots \tag{L65}$$

$$\approx \frac{1}{a^2}\frac{2\pi r^2 dr}{a^2}e^{-\beta U(r)-2\beta w}. \tag{L66}$$

$$\vec p = \alpha\vec E = rq\langle(\cos\theta,\sin\theta)\rangle \tag{L67}$$

$$= \int\frac{d\theta}{2\pi}e^{-\beta U(r)-2\beta w+\beta Eqr\cos\theta}rq(\cos\theta,\sin\theta) \tag{L68}$$

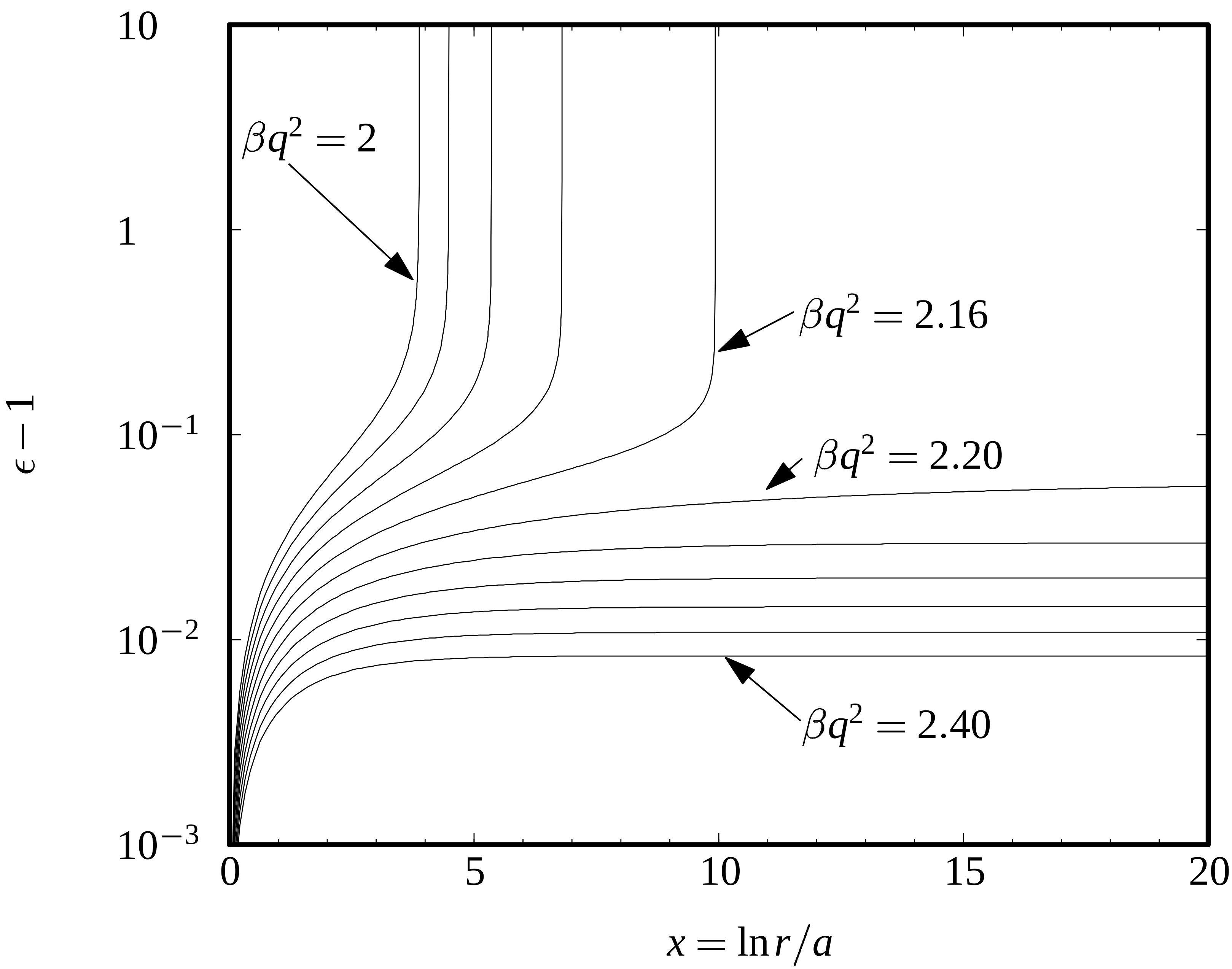
$$= \frac{1}{2}\beta q^2 r^2\vec E. \tag{L69}$$

$$d\chi(r) = n(r)\,dr\,\alpha(r) = \frac{1}{2}\beta q^2\left(\frac{r}{a}\right)^2\frac{2\pi r\,dr}{a^2}e^{-\beta U/\epsilon(r)-2\beta w}. \tag{L70}$$

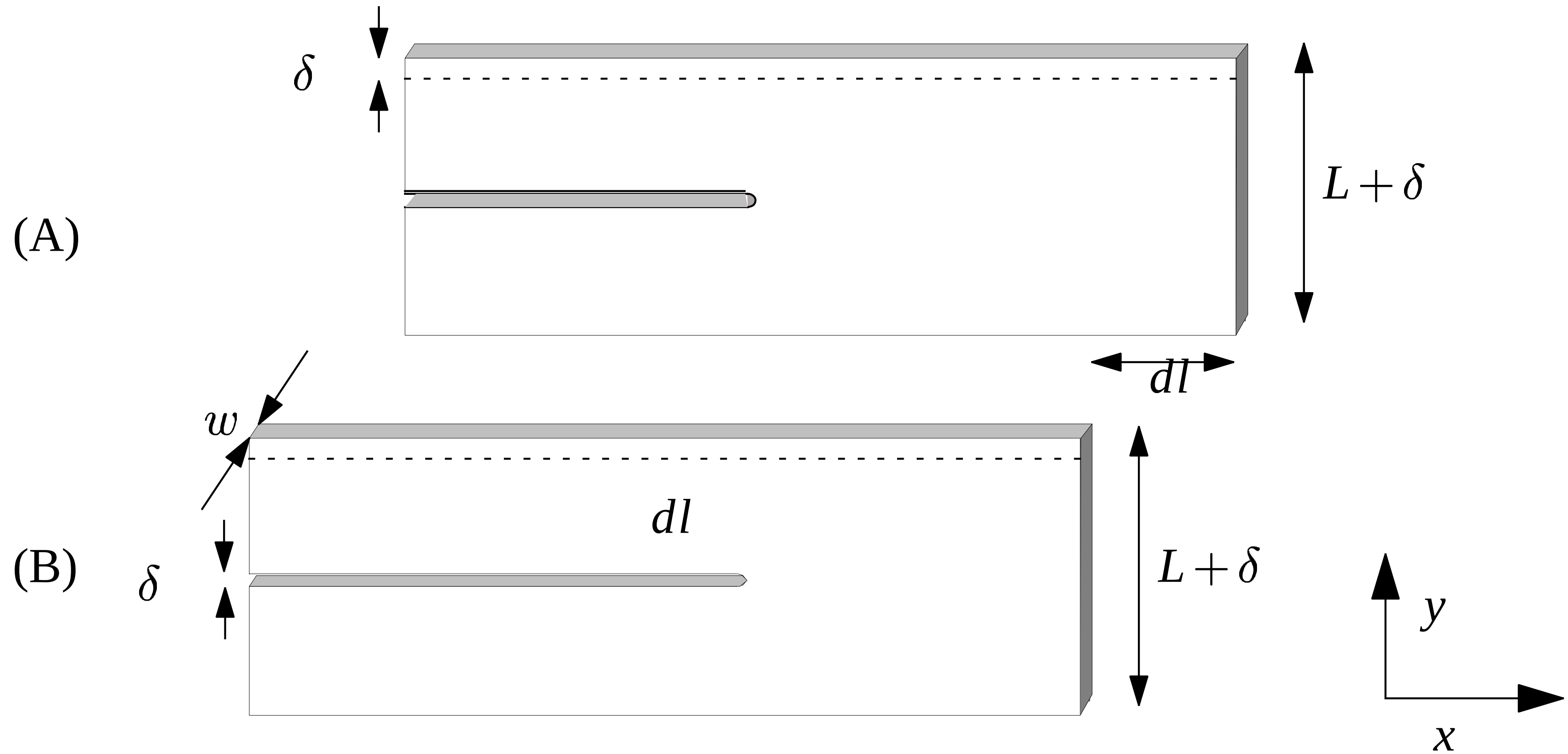
$$\epsilon(r) = 1+4\pi\int^r d\chi = 1+4\pi\int_a^r dr'\,n(r')\alpha(r') \tag{L71}$$

$$\Rightarrow \frac{d\epsilon(r)}{dr} = 4\pi^2\beta q^2 \frac{r^3}{a^4} e^{-\beta U(r)/\epsilon(r) - 2\beta w} \tag{L72}$$

$$\Rightarrow \frac{d\epsilon(x)}{dx} = 4\pi^2\beta q^2 x^{3-2\beta q^2/\epsilon(x)} e^{-2\beta w}. \tag{L73}$$


10
1
10^{-1}
10^{-2}
10^{-3}
0
5
10
15
20
$\epsilon - 1$
$x = \ln r/a$
$\beta q^2 = 2$
$\beta q^2 = 2.16$
$\beta q^2 = 2.20$
$\beta q^2 = 2.40$

Fracture of a Strip



$$U = \frac{1}{2}\delta^2 w \frac{Y}{L}, \qquad \text{(L74)}$$

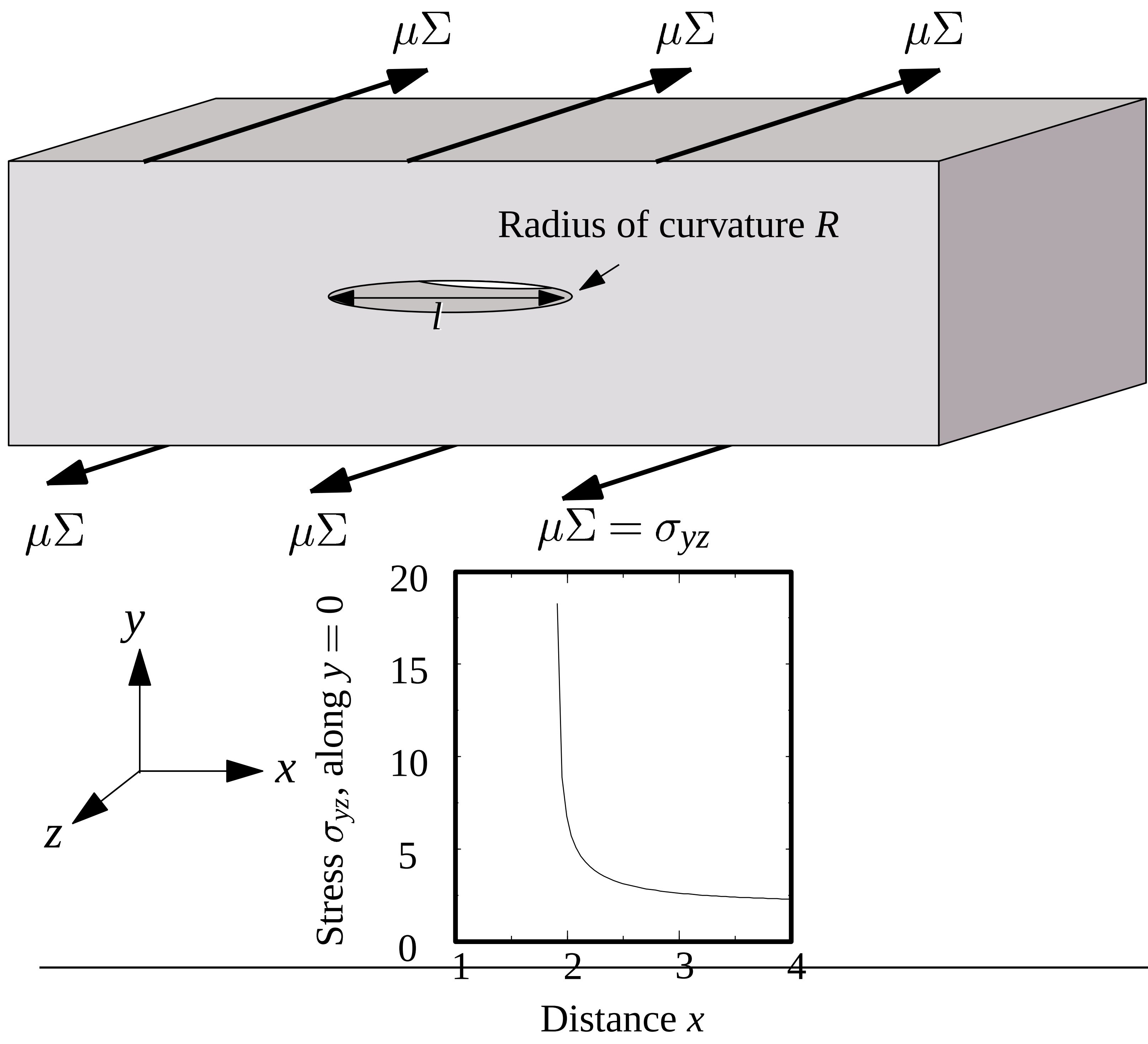
$$dU = dl\,\frac{1}{2}\delta^2 w \frac{Y}{L}. \qquad \text{(L75)}$$

Fracture of a Strip

$$\Gamma w\, dl = dl \frac{1}{2} \delta^2 w \frac{Y}{L} \tag{L76}$$

$$\Rightarrow \quad \delta = \sqrt{\frac{2\Gamma L}{Y}} \quad \text{and} \quad \sigma_{yy} = Y \frac{\delta}{L} = \sqrt{\frac{2\Gamma Y}{L}}. \tag{L77}$$

Fracture of a Strip



Fracture of a Strip

$$\frac{\text{Maximum stress}}{\text{applied stress}} \propto \sqrt{\frac{l}{R}}, \qquad \text{(L78)}$$

$$\nabla^2 u = 0. \tag{L79}$$

$$u = \frac{\phi(\zeta) + \overline{\phi(\zeta)}}{2}, \tag{L80}$$

$$\sigma_{yz} = \mu \frac{\partial u}{\partial y} = \frac{\mu}{2}[i\phi'(x+iy) - i\overline{\phi'(x+iy)}] \tag{L81}$$

$$\Rightarrow \quad \phi'(\zeta) \to -i\Sigma \text{ for } \zeta \to \infty. \tag{L82}$$

$$(x(t), y(t)) \tag{L83}$$

$$\vec{T} = \left(\frac{\partial x}{\partial t}, \frac{\partial y}{\partial t}\right) \quad \text{and} \quad \vec{N} = \left(-\frac{\partial y}{\partial t}, \frac{\partial x}{\partial t}\right) \tag{L84}$$

$$(\sigma_{xz}, \sigma_{yz}) \cdot \vec{N} = 0 \tag{L85}$$

$$\Rightarrow \quad \mu\left(\frac{\partial u}{\partial x},\frac{\partial u}{\partial y}\right)\cdot\left(-\frac{\partial y}{\partial t},\frac{\partial x}{\partial t}\right)=0\Rightarrow\frac{\partial u}{\partial y}\frac{\partial x}{\partial t}-\frac{\partial u}{\partial x}\frac{\partial y}{\partial t}=0 \tag{L86}$$

$$\Rightarrow \quad \left(-\frac{\partial\phi}{\partial ix}+\frac{\partial\overline{\phi}}{\partial ix}\right)\frac{\partial x}{\partial t}=\left(\frac{\partial\phi}{\partial iy}-\frac{\partial\overline{\phi}}{\partial iy}\right)\frac{\partial y}{\partial t} \tag{L87}$$

$$\Rightarrow \quad \frac{\partial\phi}{\partial t}=\frac{\partial\overline{\phi}}{\partial t} \tag{L88}$$

$$\Rightarrow \quad \phi(\zeta)=\overline{\phi(\zeta)} \tag{L89}$$

$$\zeta=\omega+\frac{p}{\omega}, \tag{L90}$$

$$\omega=e^{i\theta}, \tag{L91}$$

$$\phi(\omega)=\overline{\phi(\omega)}=\bar{\phi}(\frac{1}{\omega}), \tag{L92}$$

$$\omega=\frac{\zeta+\sqrt{\zeta^2-4p}}{2}. \tag{L93}$$

$$\phi(\omega) \to -i\Sigma\omega \quad \text{for } \omega \to \infty. \tag{L94}$$

$$\bar{\phi}(1/\omega) \to -i\Sigma\omega \quad \text{for } \omega \to \infty, \tag{L95}$$

$$\bar{\phi}(\omega) \quad \to \quad \frac{-i\Sigma}{\omega} \quad \text{for } \omega \to 0 \tag{L96}$$

$$\phi(\omega) \quad \to \quad \frac{i\Sigma}{\omega} \quad \text{for } \omega \to 0. \tag{L97}$$

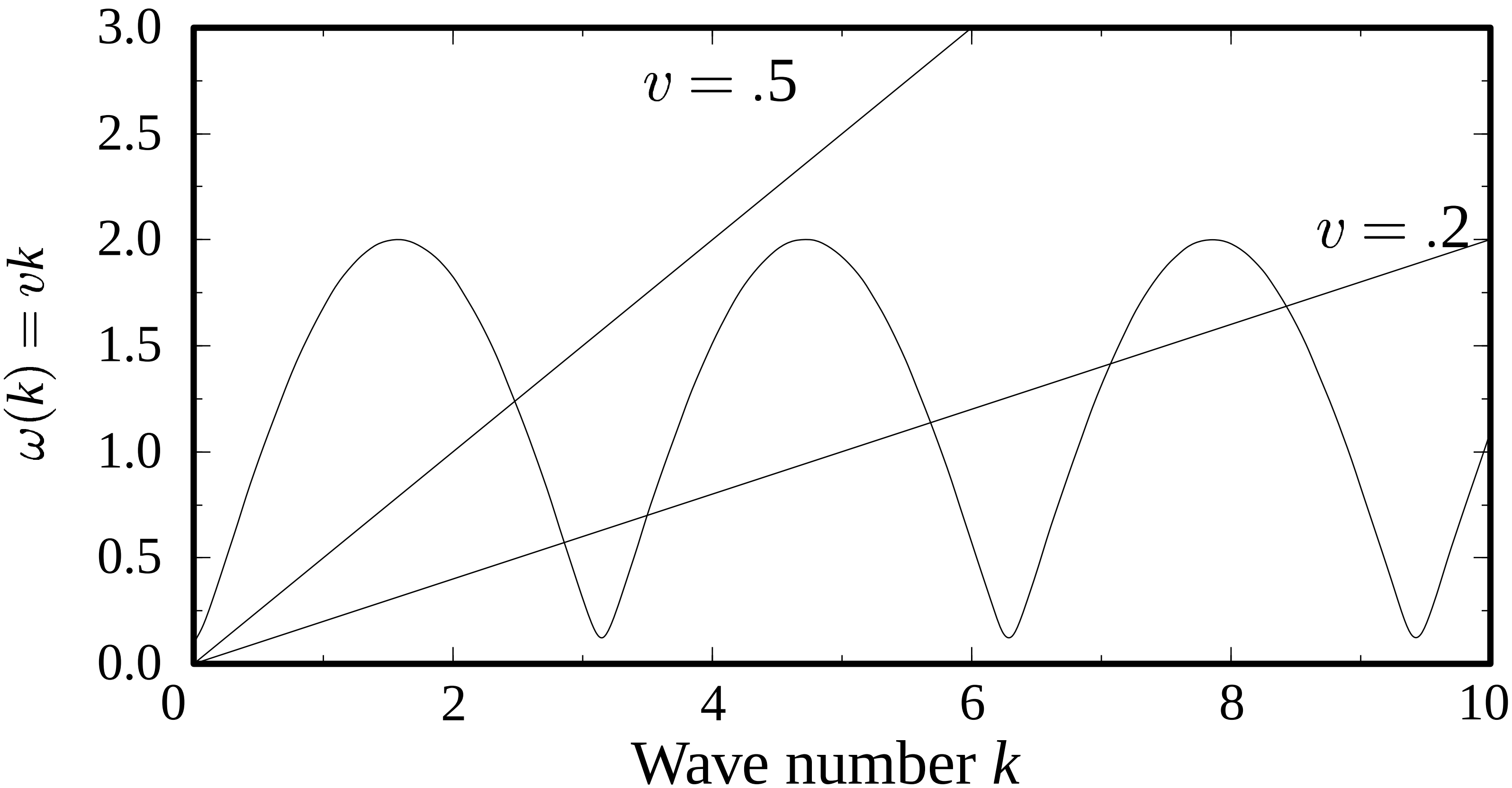
$$\phi(\omega) \quad = \quad -i\Sigma\omega + i\frac{\Sigma}{\omega} \tag{L98}$$

$$\Rightarrow \phi(\zeta) \quad = \quad -i\Sigma\frac{\zeta}{2}(1+\sqrt{1-4p/\zeta^2}) + i\Sigma\frac{\zeta}{2p}(1-\sqrt{1-4p/\zeta^2}). \tag{L99}$$

Stress Intensity Factor

$$\sigma_{yz} = \mu \frac{\partial u}{\partial y} = \frac{\mu \Sigma x}{\sqrt{x-2}\sqrt{x+2}} \rightarrow \frac{\mu \Sigma}{\sqrt{x-2}} \quad \text{as } x \rightarrow 2. \tag{L100}$$

$$K = \lim_{r \rightarrow 0} \sqrt{2\pi r}\,\sigma_{yz}. \tag{L101}$$



$$\vec{r} \rightarrow \vec{r} + \vec{R} \qquad \text{(L102a)}$$

$$t \rightarrow t + a/v. \qquad \text{(L102b)}$$

$$e^{i\vec{k}\cdot(\vec{r}+\vec{R})-i\omega(t+a/v)} = e^{i\vec{k}\cdot\vec{r}-i\omega t} \tag{L103}$$

$$\Rightarrow \quad e^{i\vec{k}\cdot\vec{R}-i\omega a/v} = 1 \tag{L104}$$

$$\Rightarrow \quad (\vec{k}+\vec{K})\cdot\vec{v} = \omega(\vec{k}) \tag{L105}$$

$$\Rightarrow \quad \vec{k}\cdot\vec{v} = \omega(\vec{k}). \tag{L106}$$