A new criterion for crack formation in disordered materials*

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* P.F. Arndt and T.N., Phys. Rev. B63, 134204 (2001)

Theory of Disorder Dominated Effects

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Research Topics

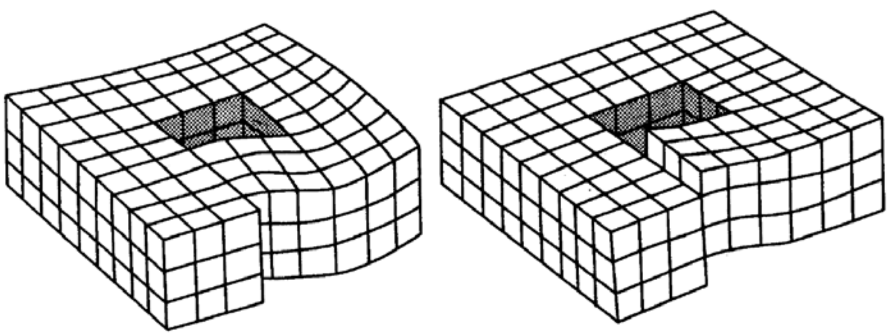
Disordered quantum wires
Charge density waves
Vortex physics
Random magnets
Friction
Crack formation *
Localization of Bosons
Helium 3 in Aerogels

Outline:

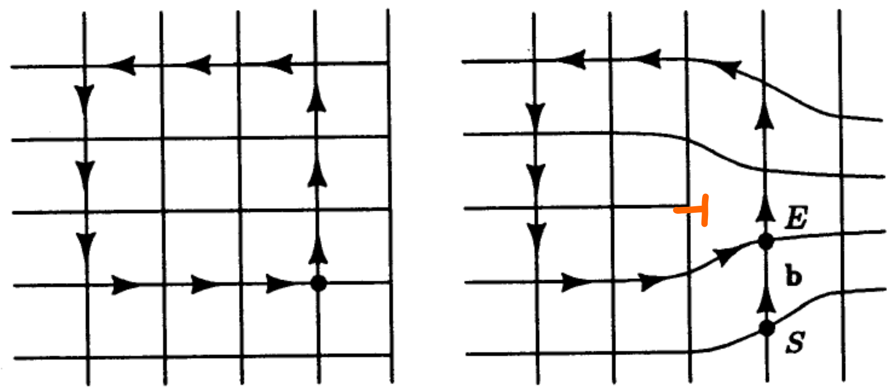
- Elasticity theory
- Griffith criterion
- The new criterion: orders of magnitude estimates
- The 2-dimensional case
- Epilogue

Elasticity theory – a primer:

- elastic displacement $\mathbf{u}(\mathbf{r}) = \mathbf{r}' - \mathbf{r}$ $u_{ik} = (\partial_k u_i + \partial_i u_k)/2$
- force $K_i(\mathbf{r}) = \partial_k \sigma_{ik}$
- free energy density $F = \lambda\, u_{ii}^2/2 + \mu\, u_{ik}^2$ $\sigma_{ik} = \partial F/\partial u_{ik}$
  - simple strain $\sigma_{zz} = p \rightarrow u_{zz} = p/Y$ $Y = \mu(3\lambda + 2\mu)/(\lambda + \mu)$
- dislocation $\oint \partial_k u_i \, dx_k = b_i$

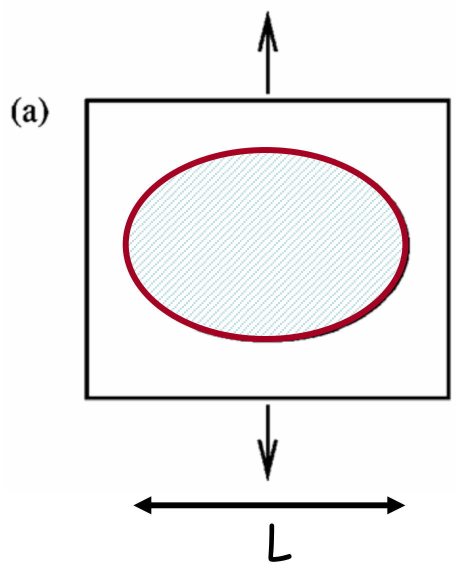


edge skrew



(a) (b)

Griffith criterion for critical cracks (1920)



pull (or shear) a solid

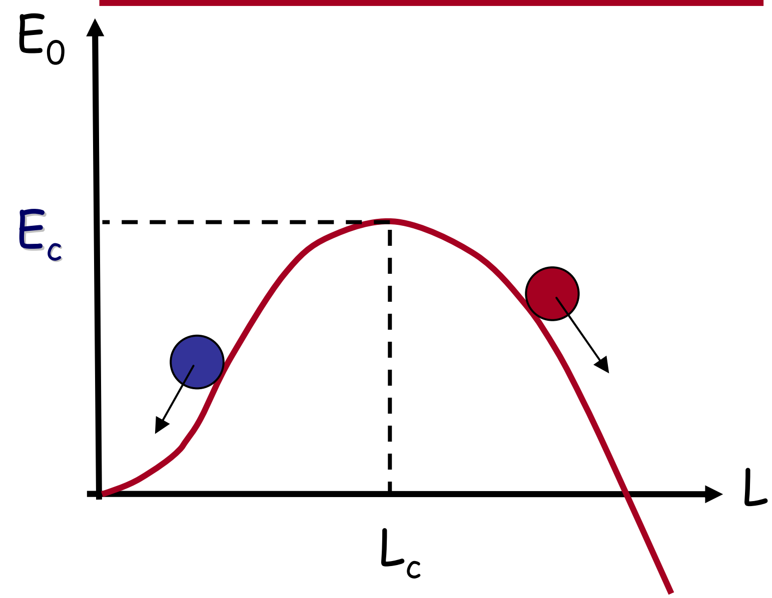
create a crack of extension L

→ energy increases by

→

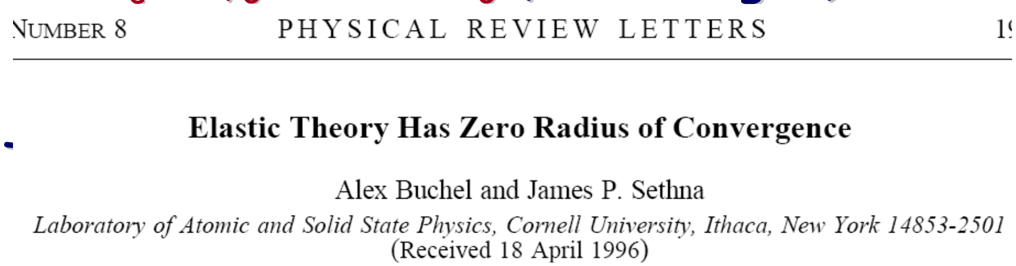
bond strength

$$E_0(L) = \gamma_0 L^{d-1} - \sigma^2 L^d / Y$$



- $L > L_c \sim \gamma_0 Y/\sigma^2 \gg a_0$ (bond length)

-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Elastic Theory Has Zero Radius of Convergence

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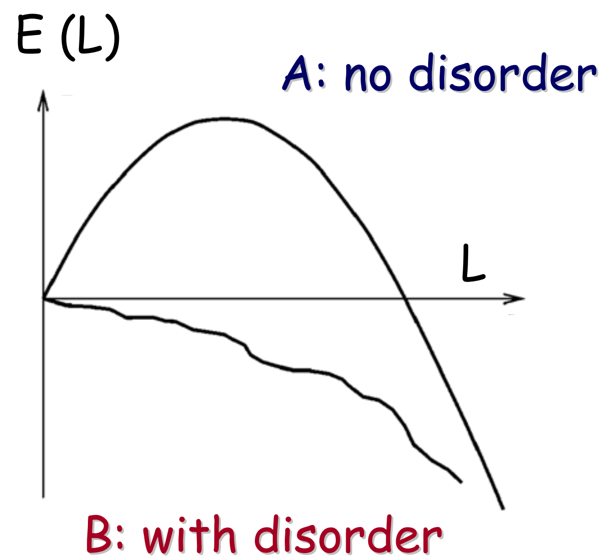
(on times scale of the age of the universe: $\tau \sim \tau_0 e^{E_c/T}$)

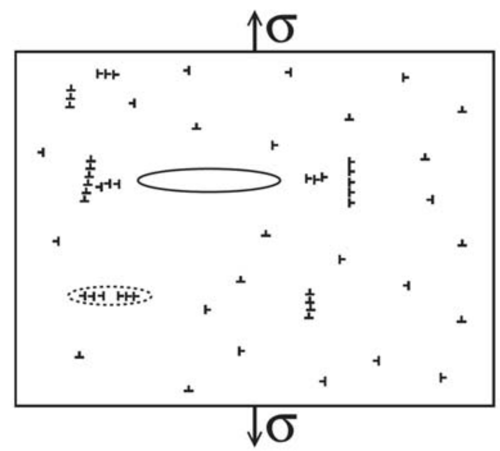
- $E_c \sim T_m (L_c/a_0)^{d-1}$ $T_m \sim \gamma_0 a_0^{d-1}$ melting temperature

Here: new criterion in the presence of disorder

Types of disorder:

- random bond strength between atoms
- randomly distributed frozen impurities and dislocations





goal: condition for the occurence of B

(i) E(L) < 0

(ii) dE/dL < 0

Qualitative discussion in d - dimension

Disorder $\rightarrow$ reduced bond energy and increased stress

may decrease nucleation energy

(i) Fluctuations in atomic bond strength:

$$\gamma_0 \rightarrow \gamma_0 + \delta\gamma(\mathbf{x}), \quad \langle\delta\gamma(\mathbf{x})\rangle = 0, \quad \langle\delta\gamma(\mathbf{x})\,\delta\gamma(\mathbf{x}')\rangle = \delta\gamma^2\,\delta(\mathbf{x}-\mathbf{x}')a_0^{d-1}$$

$\rightarrow$ E(L) gaussian distributed with mean $E_0(L)$ and variance $\delta\gamma^2\,(La_0)^{d-1}$

Probability that energy barrier is negative

$$W_{E<0} \sim \min_{\{L\}} \int_{-\infty}^{0} dE\, e^{-(E-E_0)^2/\delta\gamma^2(La_0)^{d-1}} \sim e^{-E_c^2/\delta\gamma^2(L_c a_0)^{d-1}} \sim e^{-E_c/T_{eff}}$$

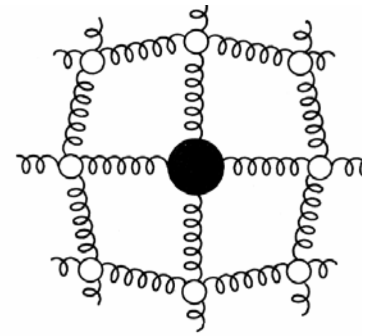
$T_{eff} = T_m(\delta\gamma/\gamma_0)^2$

(ii) Randomly distributed impurities (d'=0):

single impurity: additional stress $\delta\sigma \sim Y\Omega/L^d$

$\Omega \sim \delta R\, R^{d-1}$ change in local volume due to impurity, $\langle\delta R\rangle=0$

consider $c_i L^d$ impurities in volume $L^d \to \Delta\sigma_i \sim Y\Omega(c_i/L^d)^{1/2}$



(iii) Randomly distributed dislocations (d'=d-2)

single dislocation line creates stress $\delta\sigma \sim Yb/L$ $\langle b\rangle=0$

consider $c_{fd}L^2$ dislocation of random orientation $\to$ $\Delta\sigma_{fd} \sim Ybc_{fd}^{1/2}$

$$E_0 \to E_0 - 2L^d\sigma_e(\Delta\sigma_i + \Delta\sigma_{fd})/Y + O(\Delta\sigma^2)$$

Total variance of crack energy:

$$\Delta E^2 = \delta\gamma^2(La_0)^{d-1} + \sigma^2 c_i \Omega^2 L^d + \sigma^2 c_{fd} b^2 L^{2d}$$

Total variance of crack energy:

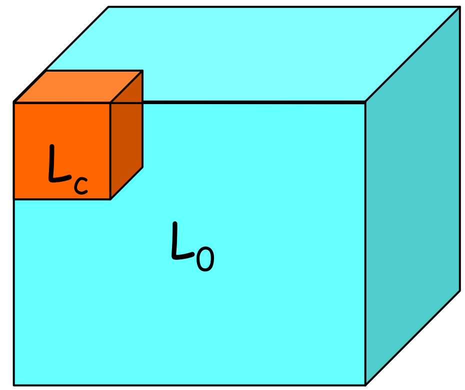
$$\Delta E^2(L) = \delta\gamma^2 (L a_0)^{d-1} + \sigma^2 c_i \Omega^2 L^d + \sigma^2 c_{fd} b^2 L^{2d}$$

Probability that energy of crack of length L is negative

$$W_{E<0} \sim \int_{-\infty}^{0} dE\, e^{-(E-E_0)^2/\Delta E^2(L)} \sim e^{-[E_0(L)/\Delta E(L)]^2}$$

Probability for crack formation dominated by

$$\mathrm{Min}_L\, W_{E<0}(L) \sim e^{-E_c/T_{eff}}$$



- $T_{eff,s} \sim T_m(\delta\gamma/\gamma_0)^2$
- $T_{eff,i} \sim \Omega\, c_i Y$ $\qquad T_{eff} \gg T$
- $T_{eff,fd} \sim a_0^2 L_c^{d-2} Y b c_{fd}$

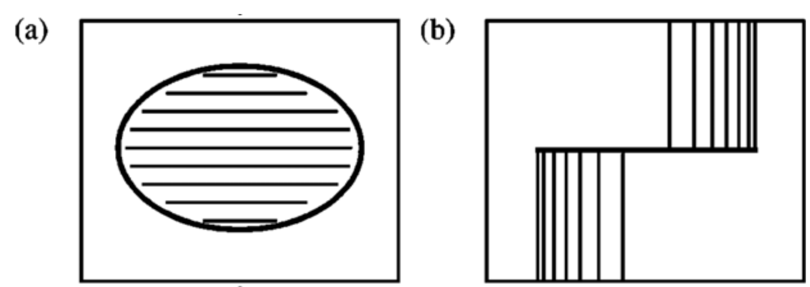
Critical system size :

$$(L_0/L_c)^d\, e^{-E_c/T_{eff}} \sim 1$$

- So far only necessary condition
- Sufficient condition : force on crack tip always positiv

Crack in a thin plate of thickness h: no disorder

- Lame coefficients $$\overline{\lambda} = 2\lambda h/(\lambda + 2\mu), \quad \overline{\mu} = \mu h$$
- crack position -a < x a, y=0 (L→ 2a!)
- non-zero stress mode I: $\overline{\sigma}_{yy}^{(e)}$ mode II: $\overline{\sigma}_{xy}^{(e)} = \overline{\sigma}_{yx}^{(e)}$
- crack filled by virtual lattice planes→ no free crack surface



- → crack dislocations with Burgers vector **b**$^{(c)}$ (x,0)

- Energy of the crack dislocation in the stress field

$$E^{(\mathrm{e})} = -\epsilon_{xl}\overline{\sigma}^{(\mathrm{e})}_{lm}\sum_{\alpha} x_{\alpha} b^{(\mathrm{c})}_{\alpha,m} = -\overline{\sigma}^{(\mathrm{e})}_{ym}\int_{-a}^{a} dx\, x\, b^{(\mathrm{c})}_{m}(x).$$

sum over dislocations

- Stress field generated by dislocations

$$\overline{\sigma}_{ij} = \epsilon_{ik}\epsilon_{jl}\partial_k\partial_l\chi(\mathbf{r})$$

$$(\nabla^2)^2\chi(\mathbf{r}) = \overline{Y}\epsilon_{ji}\partial_j b_i(\mathbf{r})$$

$$\overline{Y} = 4\overline{\mu}(\overline{\lambda}+\overline{\mu})/(2\overline{\mu}+\overline{\lambda})$$

- Solution for Airy stress function

$$\chi(\mathbf{r}) = \overline{Y}\int d^2\mathbf{r}'\, g(\mathbf{r}-\mathbf{r}')\epsilon_{ij}\partial'_i b_j(\mathbf{r}')$$

$$g(\mathbf{r}) = \mathbf{r}^2(\ln|\mathbf{r}| + C)/(8\pi)$$

- crack energy $$E^{(c)}=\frac{1}{2}\int d^2\mathbf{r}\overline{\sigma}_{ij}u_{ij}$$

$$=-\frac{\overline{Y}}{2}\int d^2\mathbf{r}\int d^2\mathbf{r}'\,\epsilon_{ij}\epsilon_{kl}b_j(\mathbf{r})b_l(\mathbf{r}')\partial_i\partial_k g(\mathbf{r}-\mathbf{r}')$$

- elastic deformation $$u_{ik}=\frac{1}{2\overline{\mu}}\overline{\sigma}_{ik}-\frac{\overline{\lambda}}{4\overline{\mu}(\overline{\lambda}+\overline{\mu})}\delta_{ik}\overline{\sigma}_{ll}$$

$$E^{(c)}=-\frac{\overline{Y}}{8\pi}\int_{-a}^{a}dx\int_{-a}^{a}dx'\,b^{(c)}(x)b^{(c)}(x')\ln\left|\frac{x-x'}{a_0}\right|$$

- total energy $E = E^{(c)} + E^{(e)} + 2\int_{-a}^{a}\gamma(x)$

- minimization $$b_0^{(c)}(x,a)=\frac{4\overline{\sigma}^{(e)}}{\overline{Y}}\frac{x}{(a^2-x^2)^{1/2}},$$

$\Rightarrow$ elliptic crack of height $2\overline{\sigma}^{(e)}a/\overline{Y}$.

Crack in a thin plate of thickness h: disorder

- random bond strength

$$E^{(s)} = 2\int_{-a}^{a} dx\,\overline{\gamma}(x) = 4\,\overline{\gamma}_0 a + E_1^{(s)}(a)$$

$\langle ... \rangle$ disorder average

$$\langle [E_1^{(s)}(a) - E_1^{(s)}(a')]^2 \rangle = \Delta_{(s)} |a - a'|$$

- random impurities and dislocation E(d)= $\int d^2\mathbf{r}\,\overline{\sigma}_{ij}^{(d)} u_{ij}^{(c)}$

stress field from disorder

strain field from crack

$$E^{(d)} = -\frac{\overline{Y}}{4\pi}\int_{-a}^{a} dx\, b^{(c)}(x)\, V(x)$$

$$V(x) = V^{(fd)}(x) + V^{(i)}(x).$$

$$V^{(fd)}(x) = 4\pi \int d^2\mathbf{r}'\,\epsilon_{ij}[\partial_k \partial_i g(\mathbf{r} - \mathbf{r}')]_{y=0} b_j^{(fd)}(\mathbf{r}')$$

$$V^{(i)}(x) = \Omega \int d^2\mathbf{r}'\, c(\mathbf{r}') \left(\partial_k \ln\left|\frac{\mathbf{r} - \mathbf{r}'}{a_0}\right| \right)_{y=0}$$

$\mathbf{b}_j(\mathbf{r})$, c($\mathbf{r}$) random

Crack shape in the presence of disorder

- $E=E^{(e)}+E^{(c)}+E^{(s)}+E^{(d)}$ depends on $b^{(c)}(x)$
- saddle point equation

$$\frac{4\pi}{\overline{Y}}\overline{\sigma}^{(e)}+\int_{-a}^{a}dx'\,b^{(c)}(x')\,\frac{1}{x-x'}+V'(x)=0$$

- solution

$$b^{(c)}(x)=\int_{-a}^{a}dx'\,f(x,x';a)\left(\frac{4\pi}{\overline{Y}}\overline{\sigma}^{(e)}+V'(x')\right)$$

$$f(x,x';a)=-\frac{1}{\pi^2}\left(\frac{a^2-x'^2}{a^2-x^2}\right)^{1/2}\frac{1}{x'-x}$$

- total energy as a function of crack length 2a

$$E(a)=\frac{\overline{Y}}{8\pi}\int_{-a}^{a}dx\int_{-a}^{a}dx'\,b^{(c)}(x)b^{(c)}(x')\,\ln\left|\frac{x-x'}{a_0}\right|+2\int_{-a}^{a}dx\,\overline{\gamma}(x)$$

- Total energy $E(a) = E_0(a) + E_1^s + E_1^{(i)}(a) + E_1^{(fd)}(a)$
- non-random part

$$E_0(a) = 4\overline{\gamma_0}a - \frac{\pi a^2 \overline{\sigma_{(e)}^2}}{\overline{Y}} = 4\overline{\gamma_0}a\left(1 - \frac{a}{2a_c}\right)$$

maximum at $a=a_c$, $E_0(a_c) = 2\gamma_0 a_c$

- random part

$$\langle[E_1^{(i)}(a) - E_1^{(i)}(a')]^2\rangle = \Delta_{(i)}|a^2 - a'^2|$$

$$\Delta_{(i)} = (\pi/2)\overline{c_{(i)}}(\Omega\overline{\sigma_{(e)}})^2 = \overline{c_{(i)}}\Omega^2\overline{\gamma_0}\,\overline{Y}/a_c$$

$$\langle[E_1^{(fd)}(a) - E_1^{(fd)}(a')]^2\rangle = \Delta_{(fd)}(a^2 - a'^2)^2$$

$$\Delta_{(fd)} = (3/\pi)c_{(fd)}(b_{(fd)}\overline{\sigma^{(e)}})^2 = 6c_{(fd)}b_{(fd)}^2\overline{\gamma_0}\,\overline{Y}/(\pi^2 a_c)$$

- $\Rightarrow$ complete characterization of the crack

Probability $W_{E<0}(a)$ that crack has negative energy?

$$W_{E<0}(a) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{-\phi(a)} dx e^{-x^2/2}$$

$$\phi(a) = \frac{4\overline{\gamma_0} a[1 - a/(2a_c)]}{(\Delta_{(s)} a + \Delta_{(i)} a^2 + \Delta_{(fd)} a^4)^{1/2}}$$

Minimization with respect to a:

$$E_0(a) = 4\overline{\gamma_0} a - \frac{\pi a^2 \overline{\sigma^2_{(e)}}}{\overline{Y}} = 4\overline{\gamma_0} a \left(1 - \frac{a}{2a_c}\right)$$

$\Delta_{(s)}>0$: $a=2a_c$
$\Delta_{(i)}>0$: $a \approx a_0$
$\Delta_{(fd)}>0$: $a \approx a_0$

Probability $W_{f>0}$ (a) that force f(a) on crack tip is always positive?

$$f(a) = -\frac{\partial E(a)}{\partial a} = f_0(a) + f_1(a)$$

$$f_0(a) = 4\bar{\gamma}_0\left(1 - \frac{a}{a_c}\right),$$

$$f_1(a) = f_1^{(s)}(a) + f_1^{(i)}(a) + f_1^{(fd)}(a)$$

$$\langle f_1^{(s)}(a) f_1^{(s)}(a')\rangle = \Delta_{(s)} \delta_{a_0}(a - a'),$$

$$\langle f_1^{(i)}(a) f_1^{(i)}(a')\rangle = 2a\Delta_{(i)} \delta_{a_0}(a - a'),$$

$$\langle f_1^{(fd)}(a) f_1^{(fd)}(a')\rangle = 4aa'\Delta_{(fd)}.$$

$$W_{f>0}(a) = \int_{-\infty}^{-f_0(a)/\langle f_1^2(a)\rangle^{1/2}} \mathrm{d}x \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$$

$$\ln \tilde{W}_{f>0} = \sum_a \ln W_{f>0}(a) \approx -\int_0^{a_c} \frac{\mathrm{d}a}{2a_0}\left(\frac{f_0^2(a)}{\langle f_1^2(a)\rangle} + \ln \frac{\langle f_1^2(a)\rangle}{2\pi f_0^2(a)}\right).$$

		Glass	SiC
Y	$[10^9$ Pa$]$	70	400
γ_0	[J m^{-2}]	1.0	4.0
Random surface energy			
Weak disorder: $\delta\gamma/\gamma_0 = 0.1$, $a_0 = 5\times10^{-10}$ m			
$T_{\rm eff}^{(s)}(d=2)$	[K]	1087	4348
$A^{(s)}$	[Pa^2 m^{-1}]	5.9×10^{30}	1.36×10^{32}
Strong disorder: $\delta\gamma/\gamma_0 = 0.3$, $a_0 = 10^{-6}$ m			
$T_{\rm eff}^{(s)}(d=2)$	[K]	3.9×10^{10}	1.57×10^{11}
$A^{(s)}$	[Pa^2 m^{-1}]	1.65×10^{23}	3.77×10^{24}
Random impurities			
Weak disorder: $\Omega = 2.5\times10^{-19}$ m^2, $c = 8\times10^{24}$ m^{-3}			
$T_{\rm eff}^{(i)}(d=2)$	[K]	158.5	905.8
$A^{(i)}$	[Pa^2 m^{-1}]	4.07×10^{31}	6.5×10^{32}
Strong disorder: $\Omega = 10^{-15}$ m^2, $c = 10^{17}$ m^{-3}			
$T_{\rm eff}^{(i)}(d=2)$	[K]	1.26×10^{5}	7.24×10^{5}
$A^{(i)}$	[Pa^2 m^{-1}]	5.09×10^{28}	4.15×10^{29}
Random frozen dislocations			
Weak disorder: $b_{(fd)} = 5\times10^{-10}$ m, $c_{(fd)} = 10^{14}$ m^{-2}, $h = 10^{-3}$ m			
$T_{\rm eff}^{(fd)}$(plate)	[K]		1.83×10^{19}
$a_0 = 5\times10^{-9}$ m			
$A^{(fd)}$	[Pa^2 m^{-1}]		1.71×10^{30}
Strong disorder: $b_{(fd)} = 5\times10^{-10}$ m, $c_{(fd)} = 10^{16}$ m^{-2}, $h = 10^{-3}$ m			
$T_{\rm eff}^{(fd)}$(plate)	[K]		1.83×10^{21}
$a_0 = 5\times10^{-10}$ m			
$A^{(fd)}$	[Pa^2 m^{-1}]		1.71×10^{31}

Conclusions

- We considered crack formation by frozen disorder:
  random atomic bonds, impurities, frozen dislocation

- Disorder can reduce or eliminate energy barrier for the formation of supercritical crack

- We calculated the probability to find supercritical crack in d=2
  large but finite volume

- Briefly discussed: extension to higher dimension

Epilogue:

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Slow Crack Propagation in Heterogeneous Materials

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Statistics and thermally activated dynamics of crack nucleation and propagation in a two-dimensional heterogeneous material containing *quenched randomly distributed* defects are studied theoretically. Using the generalized Griffith criterion we derive the equation of motion for the crack tip position accounting for dissipation, thermal noise, and the random forces arising from the defects. We find that aggregations of defects generating long-range interaction forces (e.g., clouds of dislocations) lead to anomalously slow creep of the crack tip or even to its complete arrest. We demonstrate that heterogeneous materials with frozen defects contain a large number of arrested microcracks and that their fracture toughness is enhanced to the experimentally accessible time scales.