The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

1959-17

Workshop on Supersolid 2008

18 - 22 August 2008

Dislocations and Supersolidity in solid He-4

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CUNY, USA

Dislocations and Supersolidity in ^{4}He

Anatoly Kuklov (CUNY,CSI)

supersolid 2008, ICTP, Trieste

First principles QMC

Massimo Boninsegni (Univ of Alberta)
Lode Pollet (ETH)
Nikolay Prokof'ev (UMASS)
Gunes Soyler (UMASS)
Boris Svistunov (UMASS)
Matthias Troyer (ETH)

Dislocation roughening

Darya Aleinikava (CUNY,CSI)
Eugene Dedits (CUNY,CSI)
David Schmeltzer (CUNY,CCNY)

Thanks to: NSF and CUNY grants

Outline

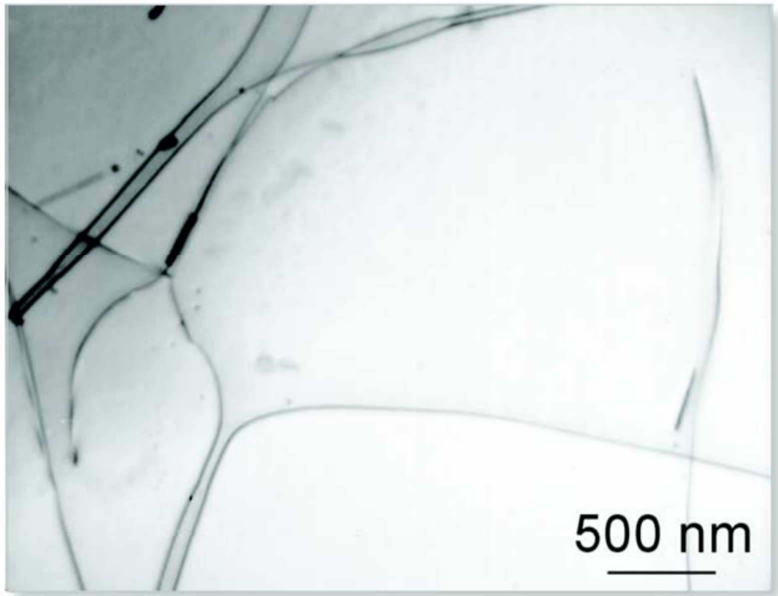
- Motivation: search for superfluid network of defects
- History: Studies of dislocations in He4

- Types of dislocations and their superfluid properties
- Core splitting and self-pinning
- Mechanical strain and vacancy gap
- Approximate phase diagram

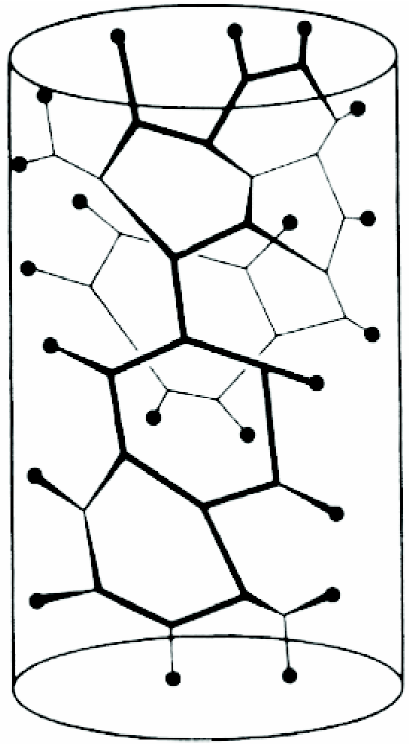
- Quantum roughening
- Long-range forces between kinks
- Kosterlitz-Thouless, RG and MC arguments against quantum roughening
- J. Day & J. Beamish experiment

- Summary

Superfluid network of dislocation (?)

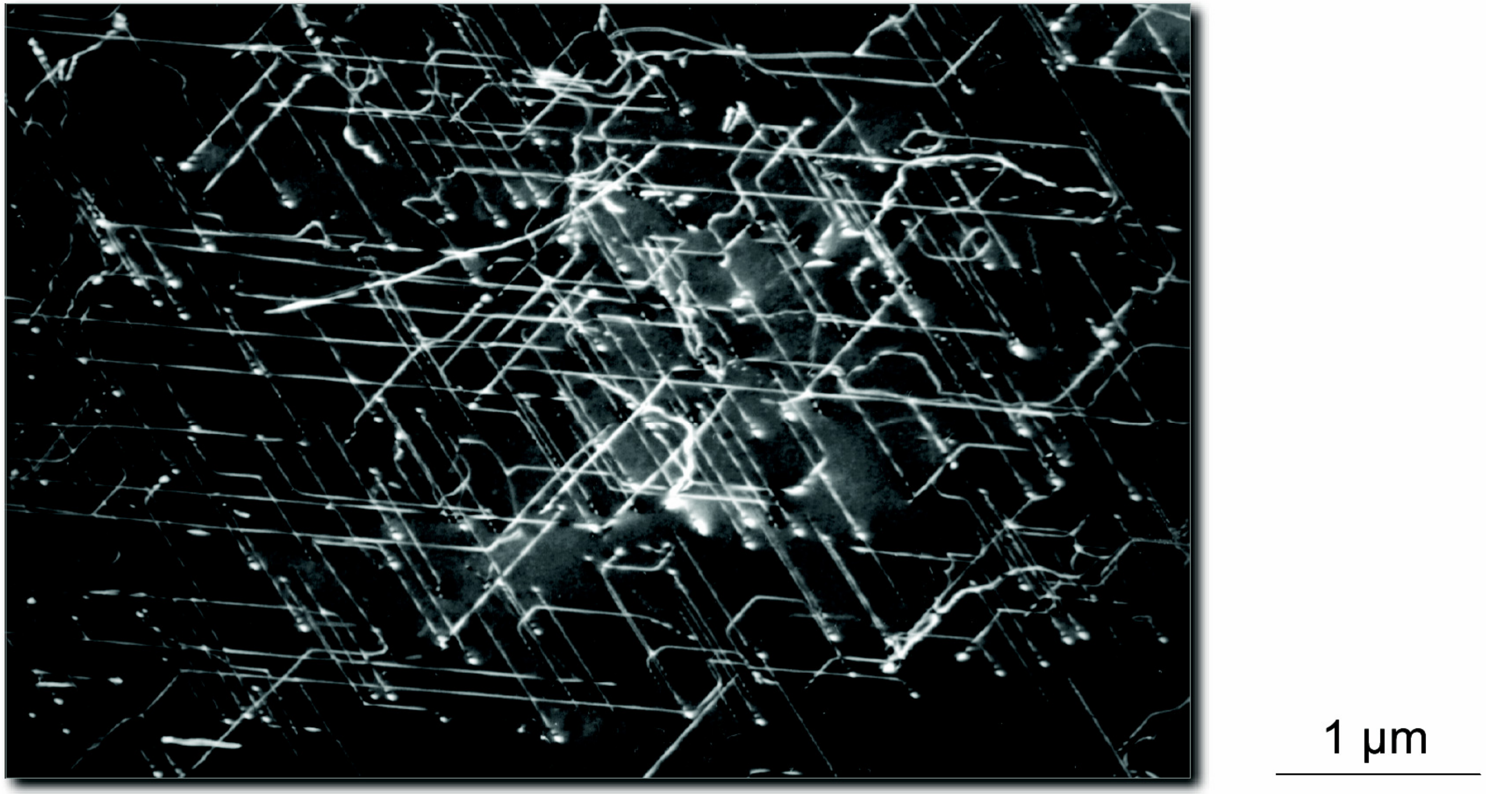


Transmission electron microscopy of plastically deformed GaAs (diffraction contrast image)



Arrangement of dislocations in a well annealed crystal

in metals: dislocation densities $\sim 10^{6}$-10^{14} cm^{-2}

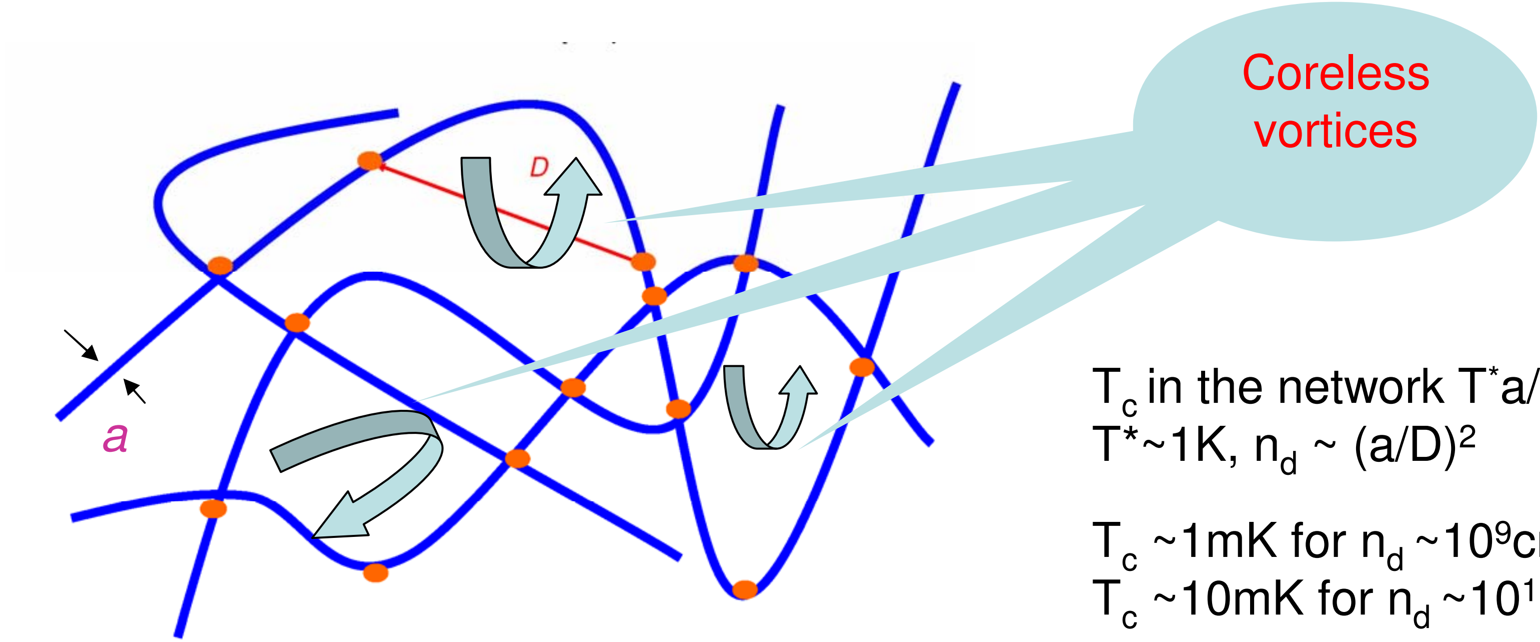


TEM image of dislocations in silicon plastically deformed in a single-slip

Shevchenko state of quasi-1D SF random netwok

S.I. Shevchenko, Sov. J. Low Temp. Phys. 14, 553 (1988).

"Incompressible vortex fluid" by P.W. Anderson, cond-mat/0705.1174



T_c in the network $T^*a/D \sim 1/D$
$T^* \sim 1K$, $n_d \sim (a/D)^2$

$T_c \sim 1mK$ for $n_d \sim 10^9 cm^{-2}$
$T_c \sim 10mK$ for $n_d \sim 10^{11}\ cm^{-2}$

$T_c < T < T^*$, wide range of quasi-superfluid frequency dispersive response

$\omega < \tau$ normal state at $T>T_c$

$\omega > \tau$ superfluid response at $T>T_c$

time of phase slip in a single loop:

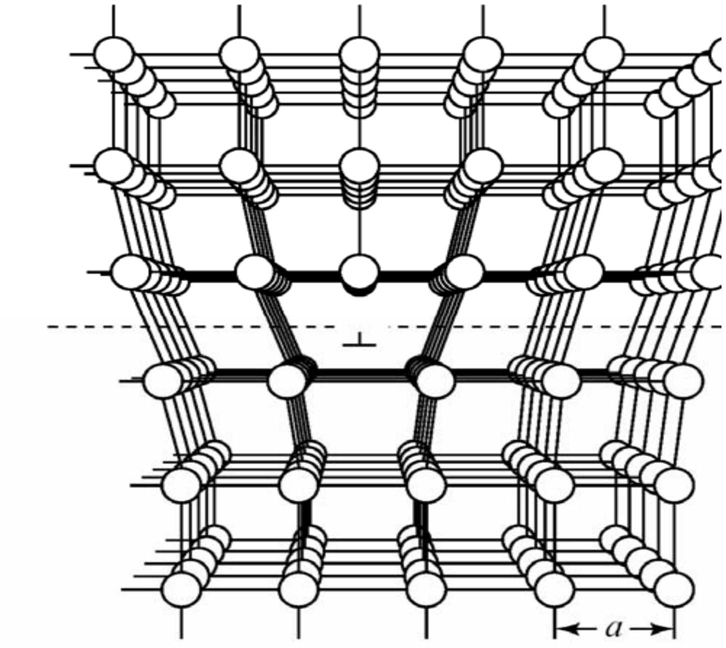
$$\tau \sim \left(\frac{T^*}{T}\right)^{\frac{2}{K_{SF}}-1} \frac{1}{T^*} \sim 10^{-2} - 10^{-1} s$$

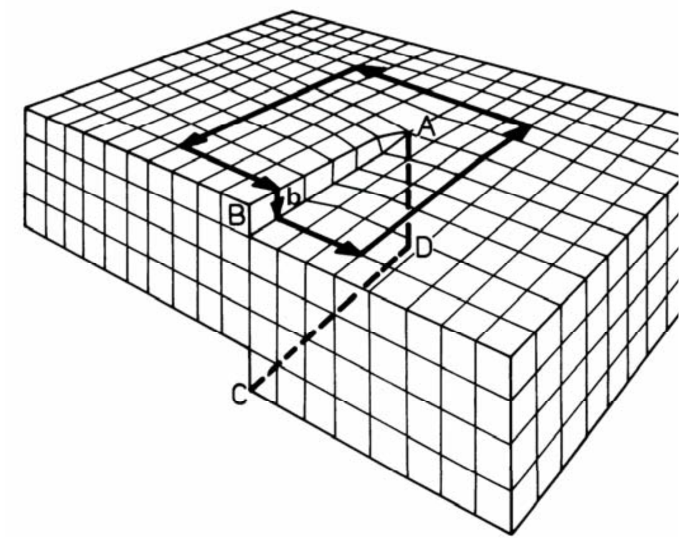
K_{SF} -Luttinger parameter; T^* ~ 1K; K =0.205(20); T_c~0.1K

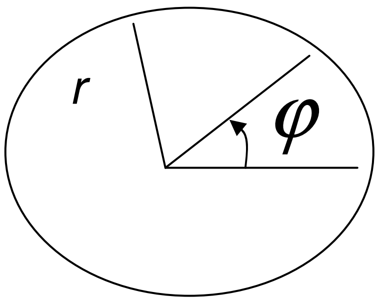
V.A. Kashurnikov, et al, PRB, **53**, 13091 (1996); Yu. Kagan, et al, PRA,**61**, 045601 (2000).

Not much is known about dynamics in the network!

Edge and screw dislocations







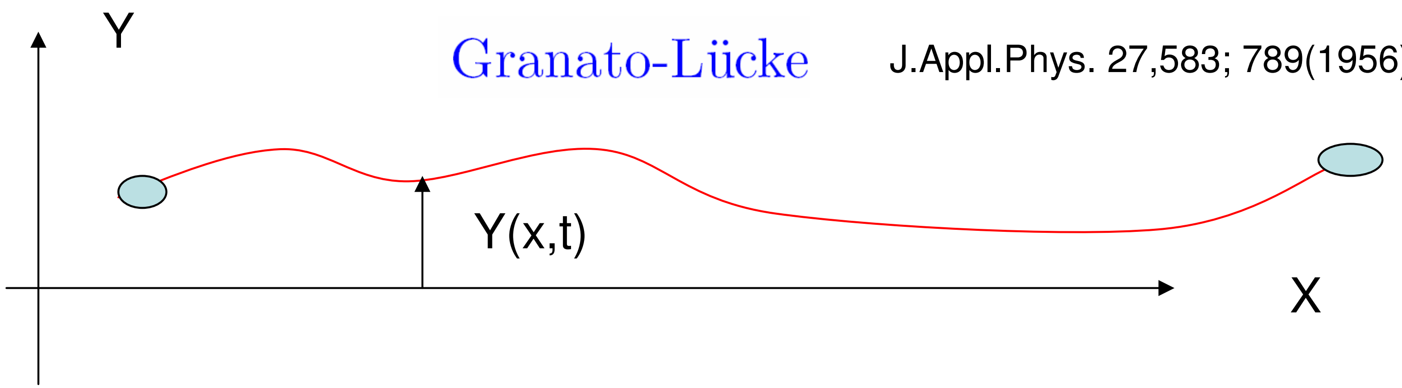
deformation vector $u \sim \frac{b\varphi}{2\pi}$

strain and stress $\partial u \sim \sigma \sim b / r$

b - Burgers vector

Dislocation as almost free classical string

Granato-Lücke J.Appl.Phys. 27,583; 789(1956)



Peierls barrier (still classical)

Peierls, Frenkel-Kontorova, in the book
A. M. Kosevich, "*The Crystal Lattice: Phonons, Solitons, Dislocations, Superlattices",* Wiley, 2005

Measurements of sound absorption and internal friction in solid He4

R.Wanner, I.Iwasa, S.Wales, Solid State Commun., **18**,853(1976)
Y.Hiki, F. Tsuruoka, Phys.Lett. **56A**, 484; **62A**, 50(1977);
V.L.Tsymbalenko, JETP **47**,787(1978); **49**, 859(1979)
I.Iwasa,K.Araki, H.Suzuki, J.Phys.Soc.Jpn **46**, 1119(1979)
J.Beamish, J.P.Frank, PRL **47**,1736(1981)
....

Quantum effects

Semiclassical tunneling of kinks: B.V. Petukhov and V.L. Pokrovsky, JETP 36, 336 (1973)

Kinks as quantum quasiparticles: A.Andreev, Soviet Uspekhi, 19, 137(1976)

Semiclassical description of dislocation dynamics in sound absorption:
A. Y.Hiki, F. Tsuruoka, PRB **27**, 696(1983)
I.Iwasa, N.Saito, H.Suzuki, J.Phys.Soc. Japan **52**, 952(1983)
A.V.Markelov, JETP **61**,118(1985)

Models of quantum kinks+ superfluid properties:
P.G. de Gennes ,*C.R.* Physique 7, 561(2006)
G.Biroli,J.P. Bouchaud, cond-mat 0710.3087
see review S. Balibar and F. Caupin**,** J. Phys.: Condens. Matter **20,** 173201 (2008)

Role of deformations in inducing core SF :

V. M. Nabutovskii and V. Ya. Shapiro, JETP 48, 480 (1978)
S. I. Shevchenko, Sov. J. Low Temp. Phys. **13**, 61; 553 (1987)
A. T. Dorsey,P.M. Goldbart, J. Toner PRL **96,** 055301 (2006)
J. Toner, PRL **100,** 035302(2008)

Main focus of the talk

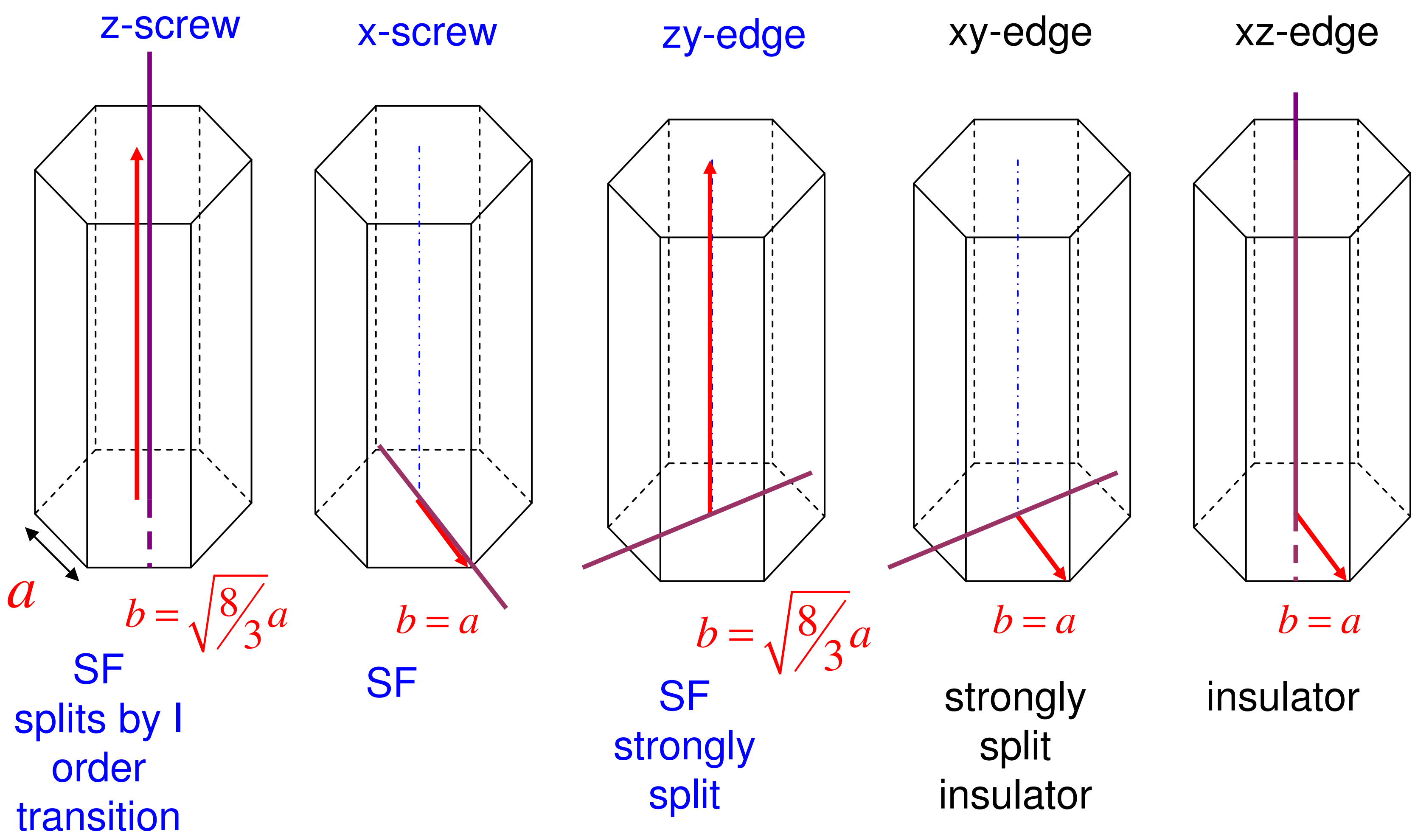
Deformations, structure and core superfluidity

M. Boninsegni, et al., PRL **99**, 035301 (2007)
L. Pollet, et al, cond-mat 08053713

Mechanically gapped dislocations and J. Day & J. Beamish experiment

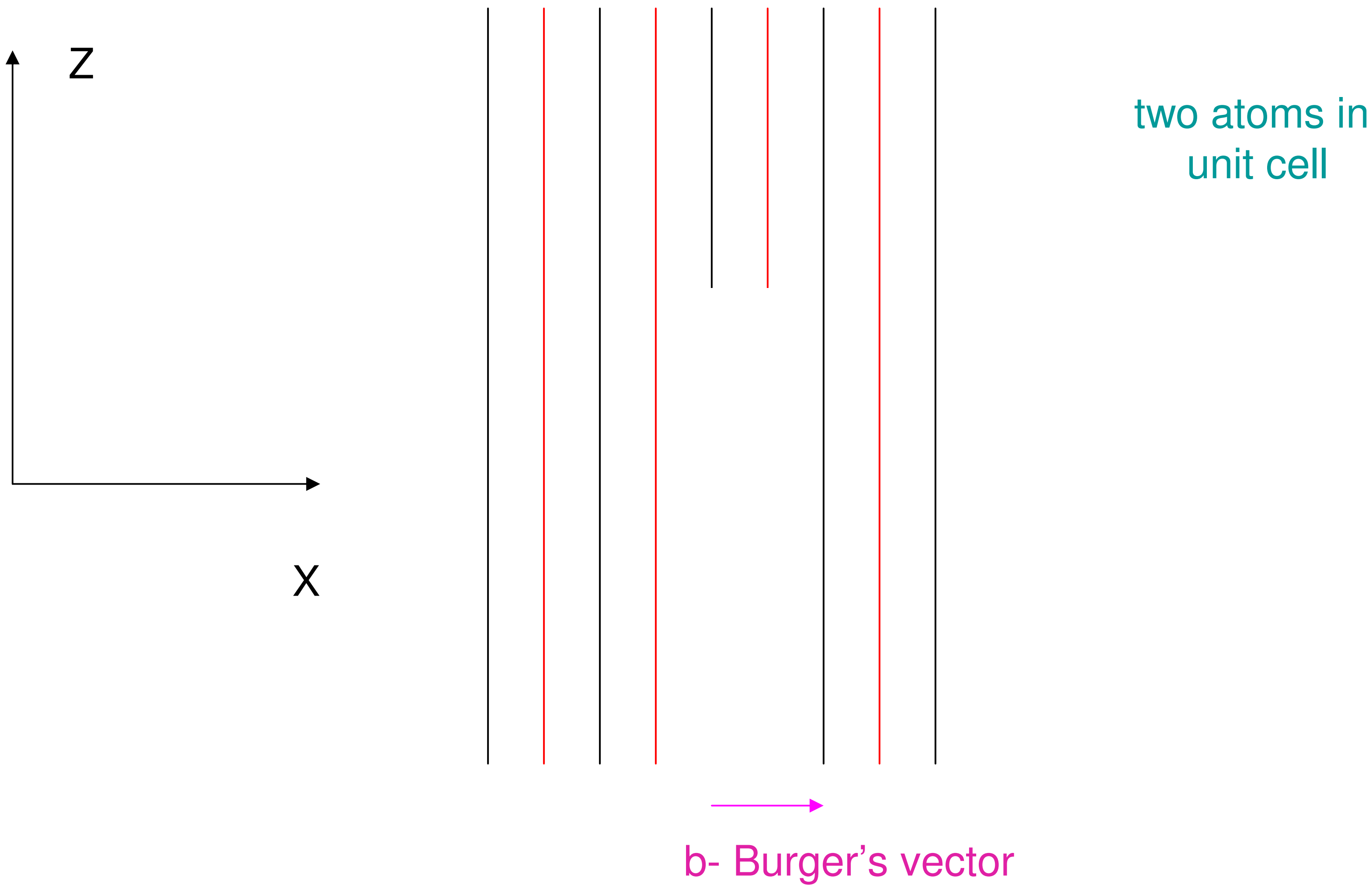
Nature **450**, 853 (2007)

Stable dislocations in *hcp* He4

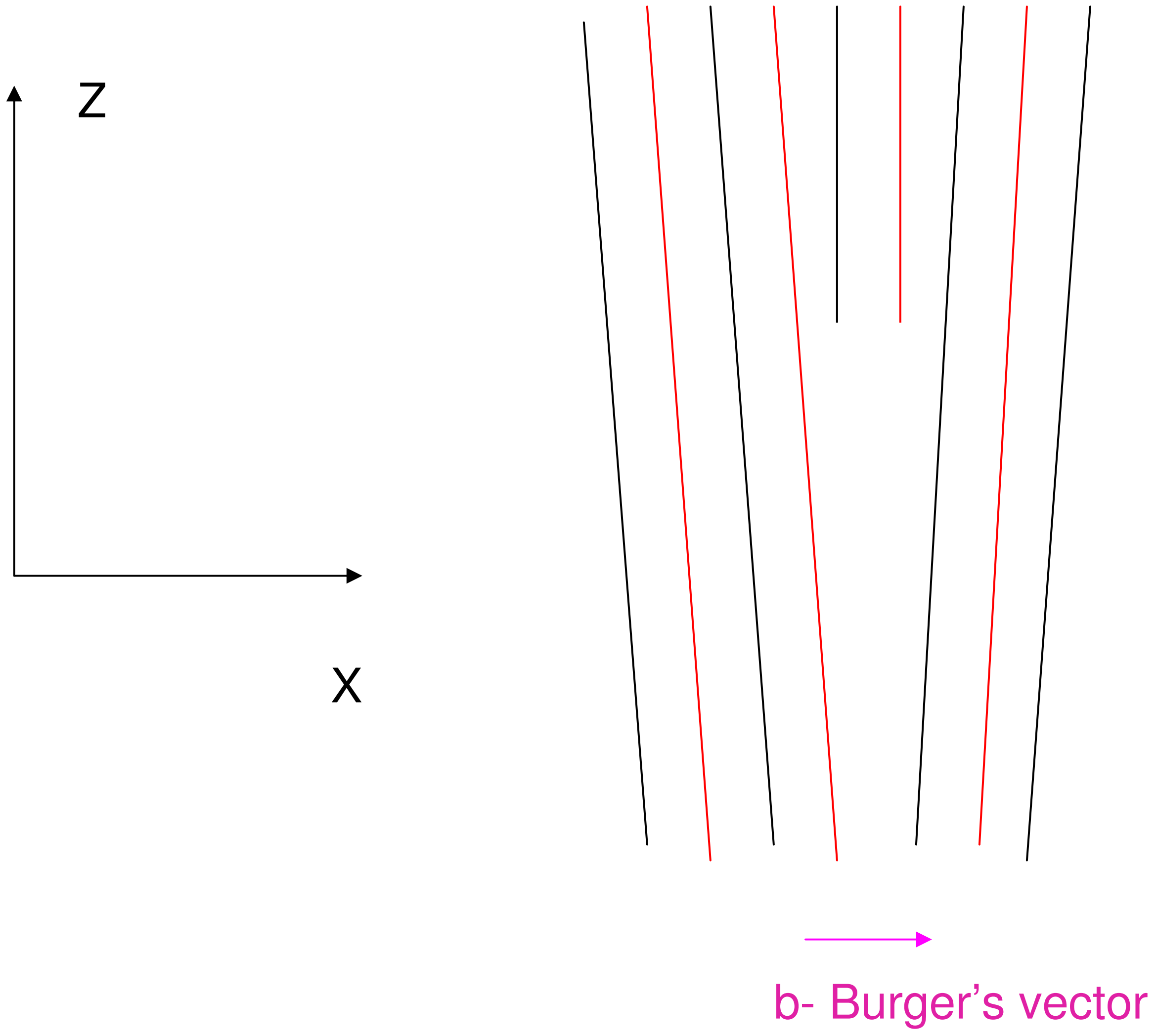


Core splitting (partial dislocations) in He4

Full edge dislocation

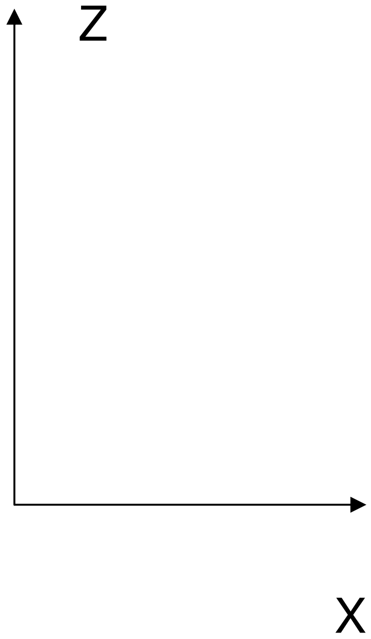


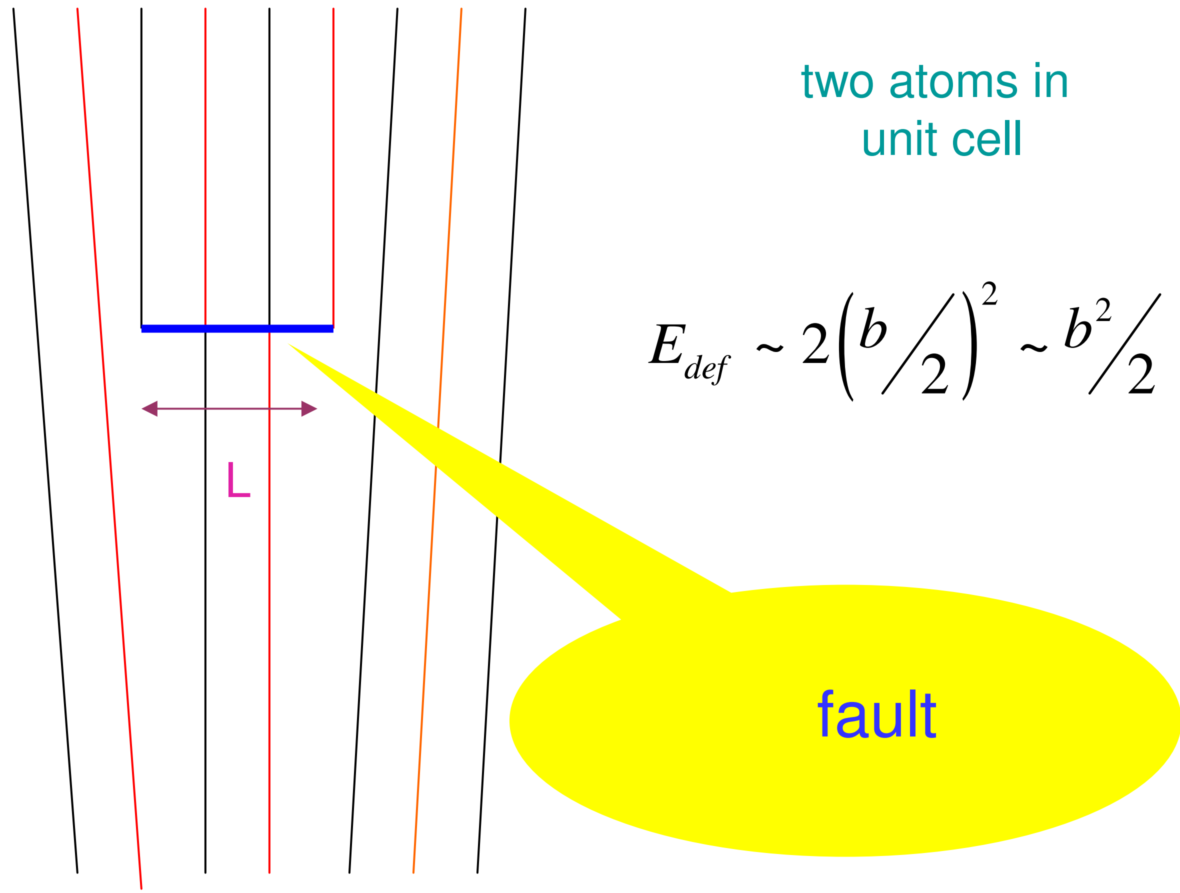
Full edge dislocation



$$E_{def} \sim b^2$$

Partial (split) edge dislocation

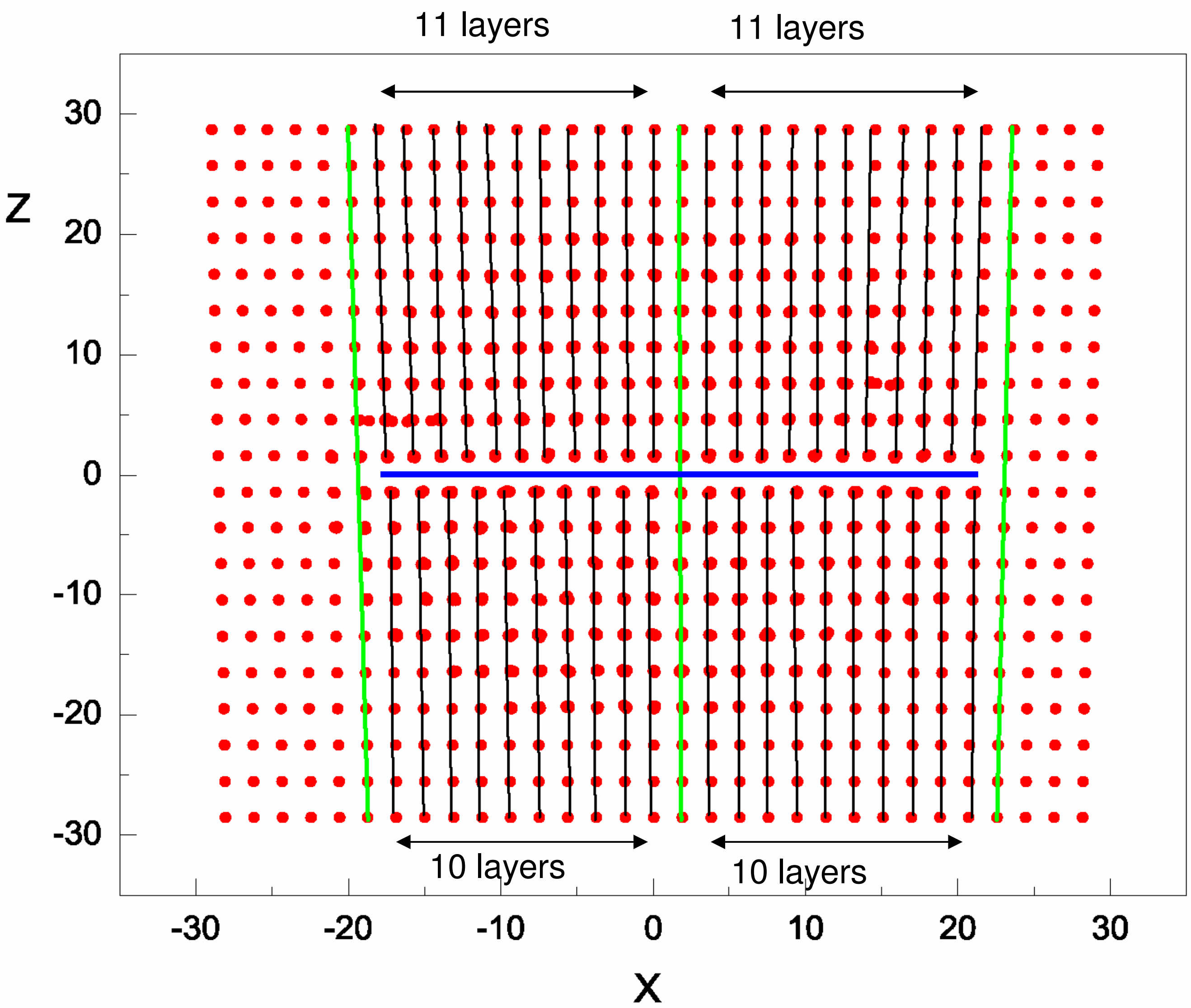




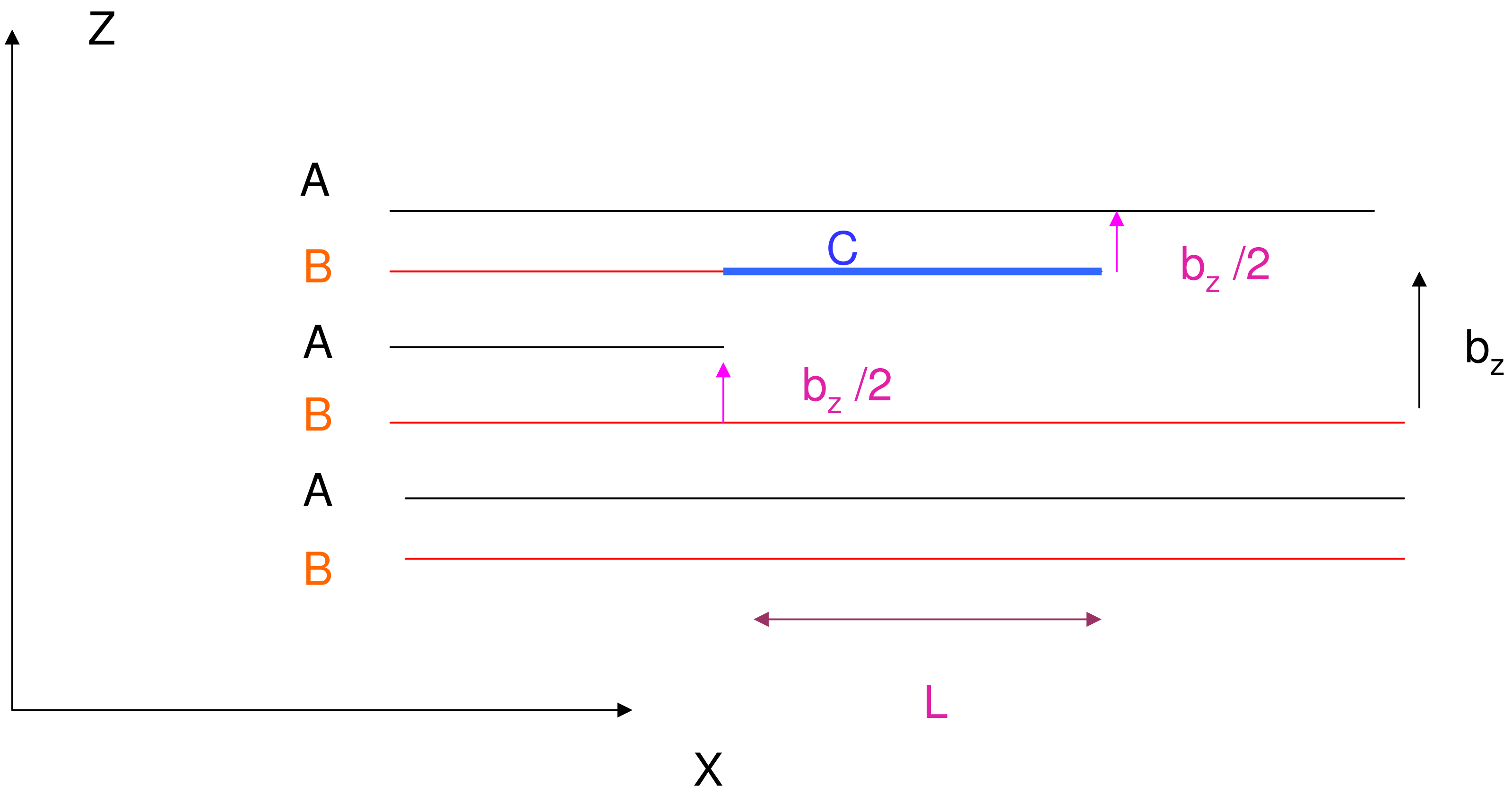
two atoms in
unit cell

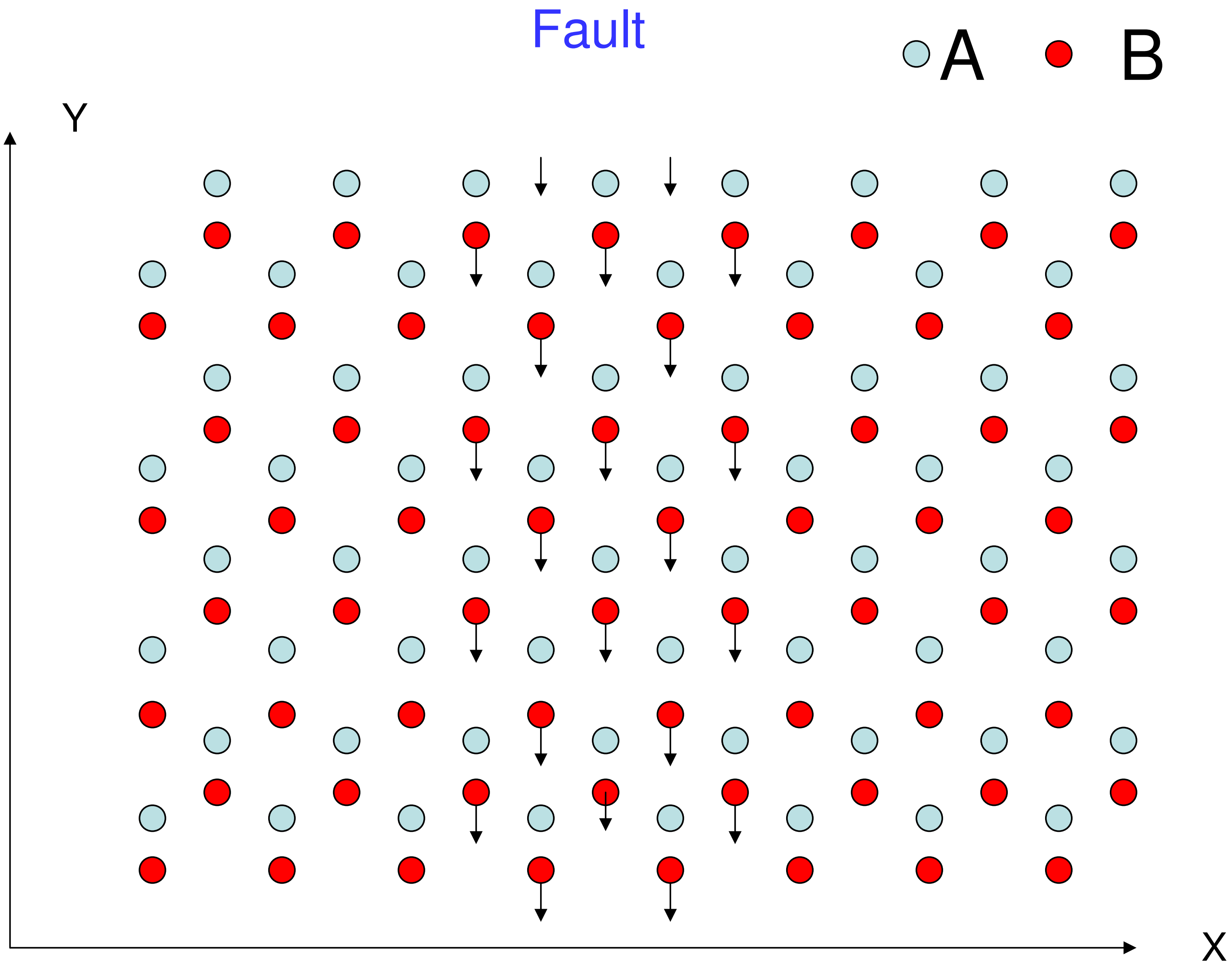
$$E_{def} \sim 2\left(b/2\right)^2 \sim b^2/2$$

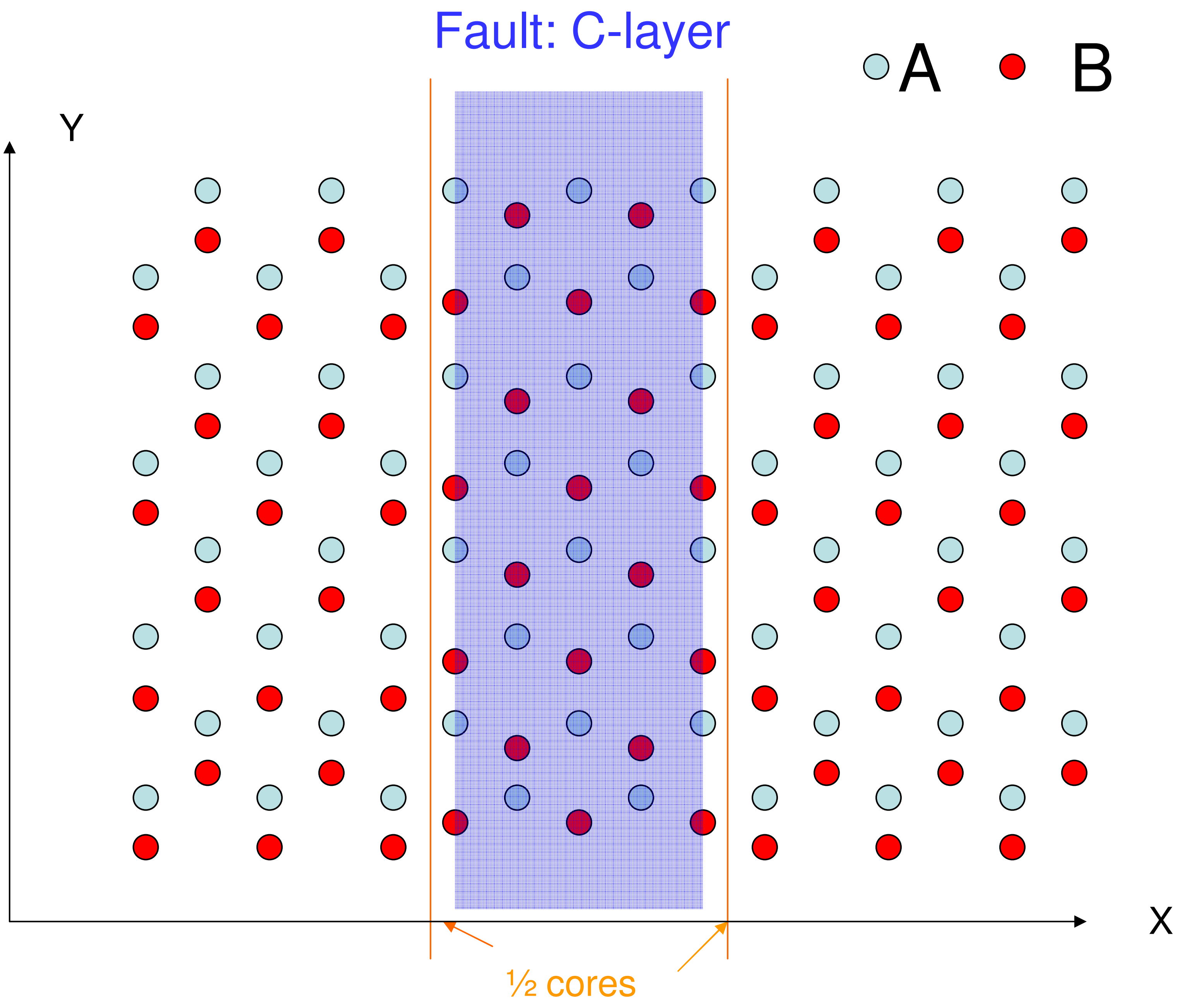
PIMC simulations (columnar view): split xy-edge dislocation



Split ZY-edge dislocation

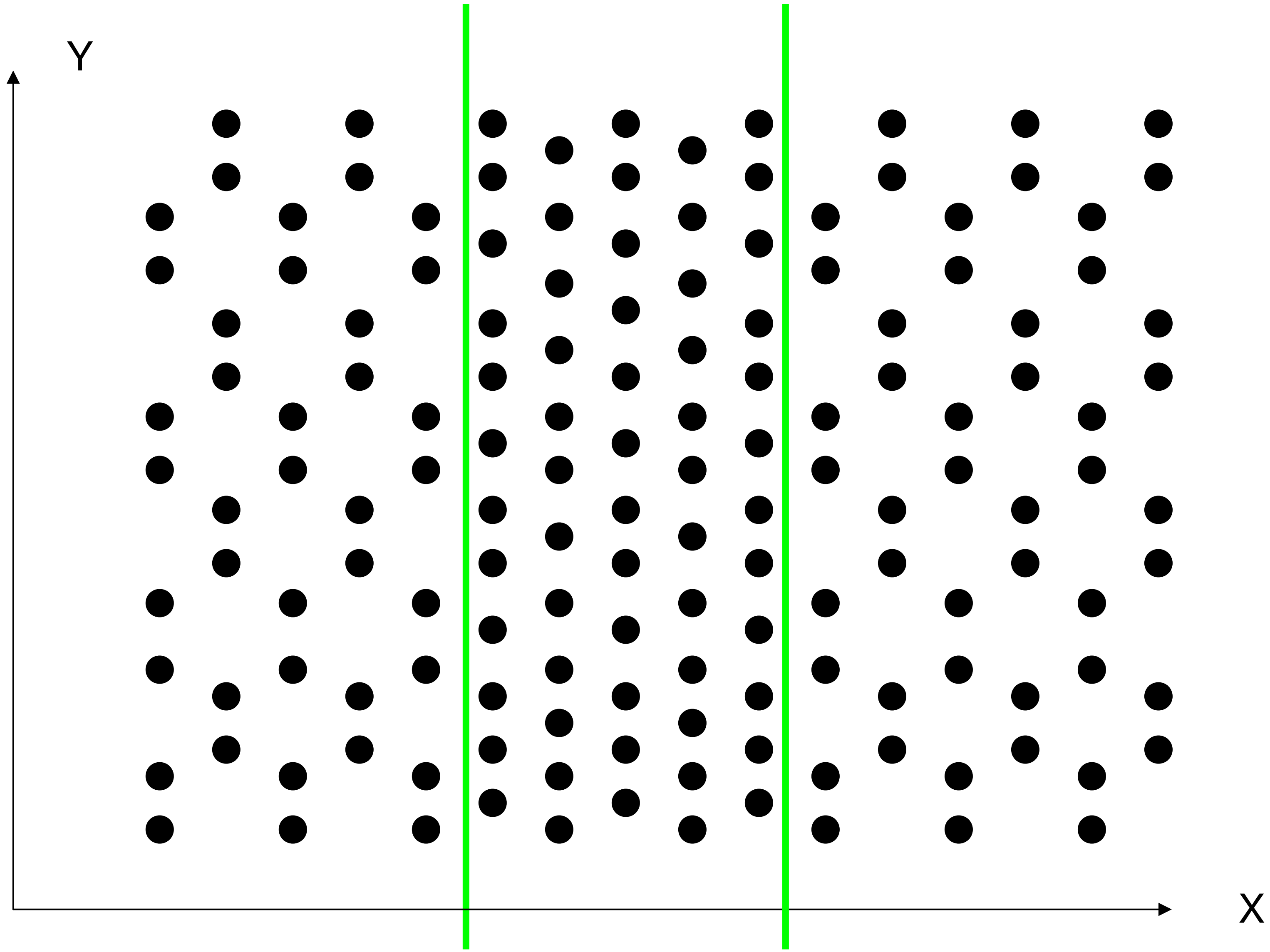



Fault
A
B
Y
X

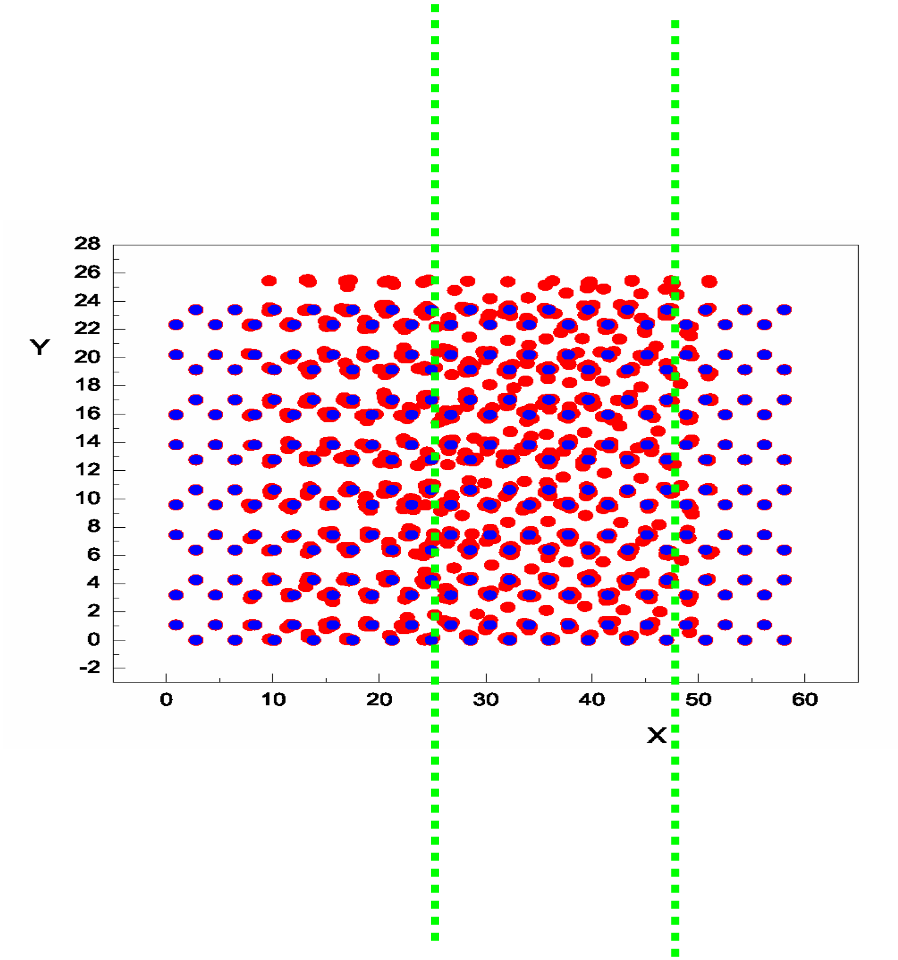


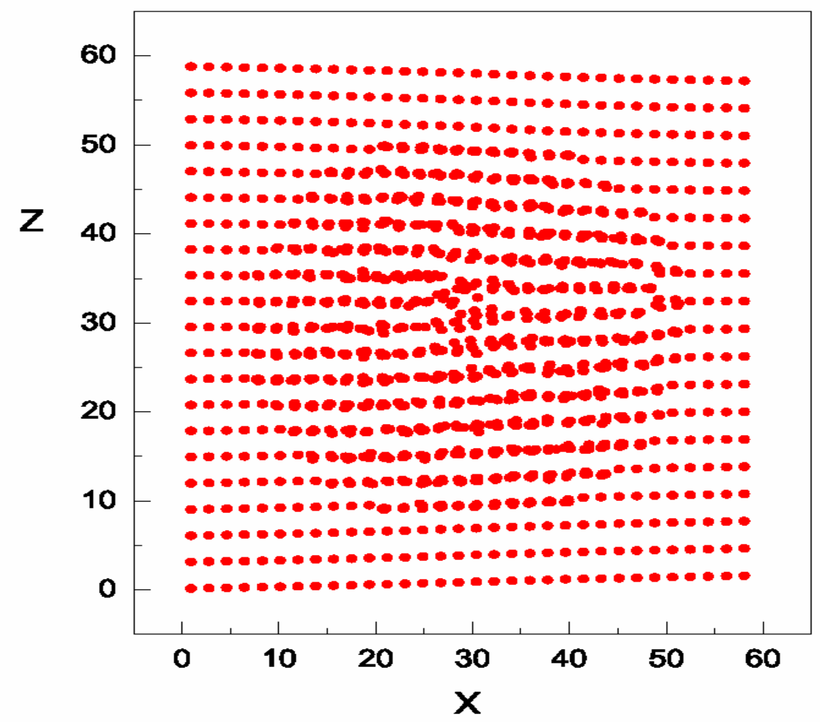
Fault: C-layer
A
B
Y
X
½ cores

Columnar view of fault + split core: many layers

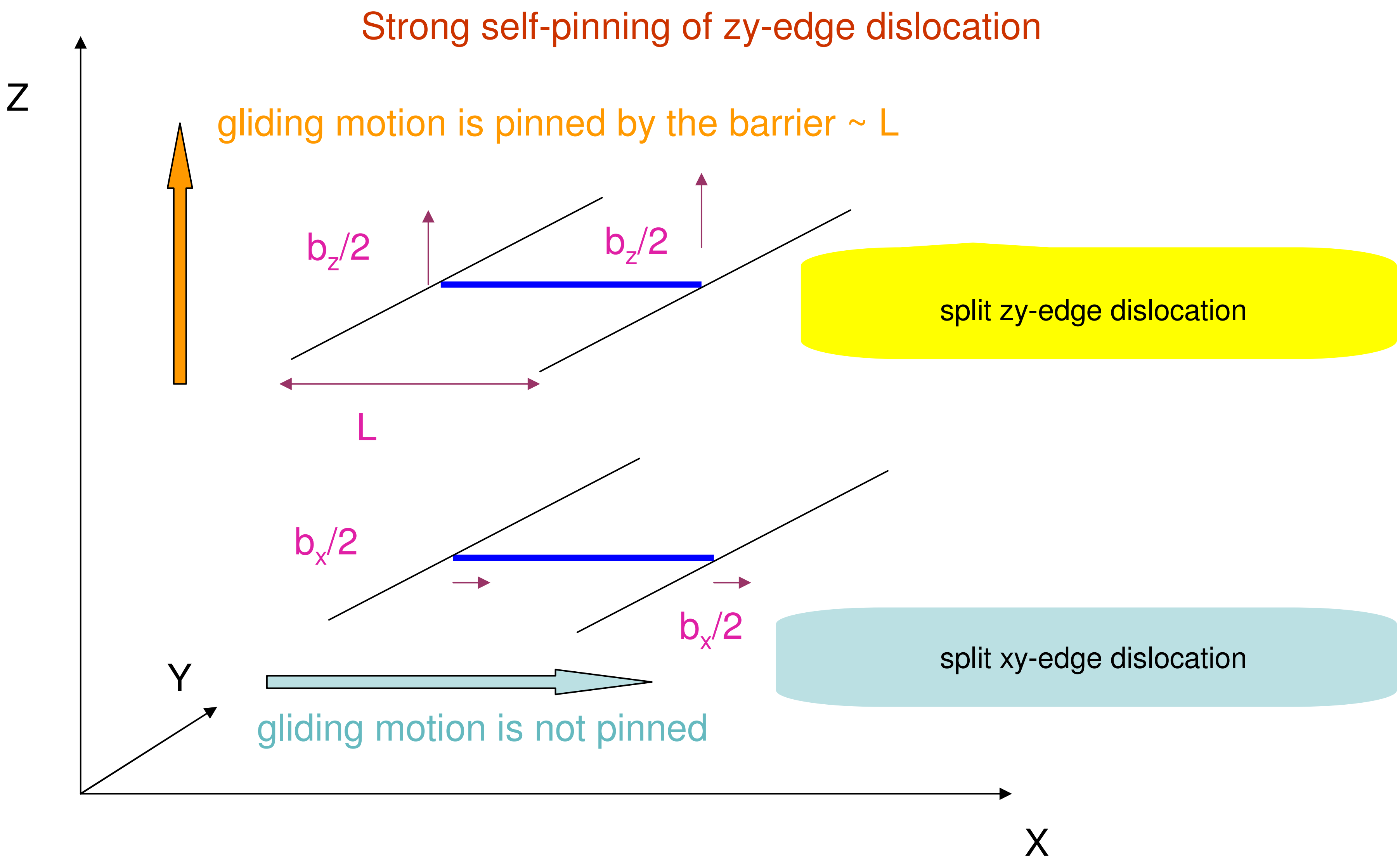


PIMC simulations (columnar view): zy-edge (SF) dislocation





½ cores


Strong self-pinning of zy-edge dislocation
Z
gliding motion is pinned by the barrier ~ L
$b_z/2$
$b_z/2$
split zy-edge dislocation
L
$b_x/2$
$b_x/2$
split xy-edge dislocation
Y
gliding motion is not pinned
X

Fault size

$$E_{full} = \frac{b^2\mu}{4\pi}\ln R$$

$$E_{split} - E_{full} = -\frac{b^2\mu}{8\pi}\ln L + \sigma L$$

$$L = \frac{b^2\mu}{8\pi\sigma}, \quad \sigma - \text{fault surface tension}$$

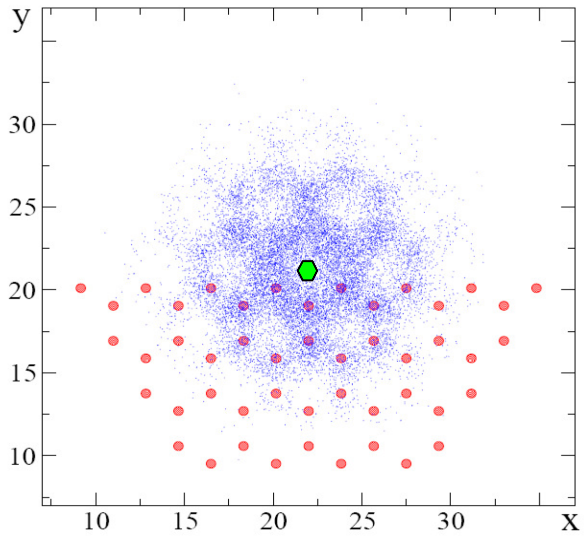
MC simulations: $\sigma < 0.1K\,/\,particle$

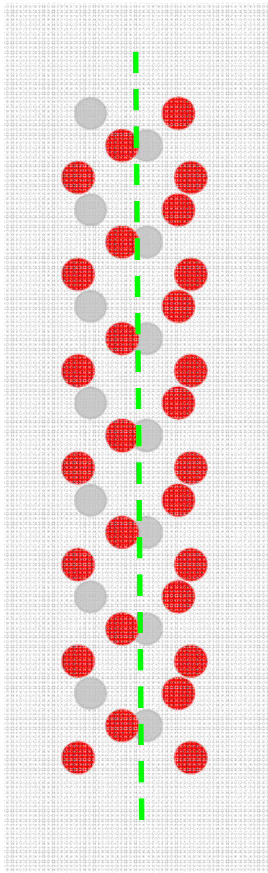
$$b = 3.7\,\text{Å}, \qquad \mu \approx 100 - 200\text{bar}$$

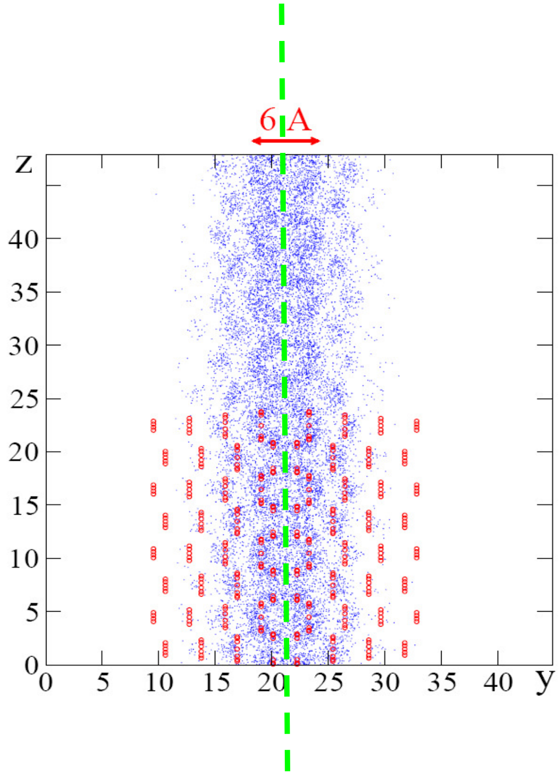
$$L > 75 - 150\,\text{Å}$$

condensate map

Z-Screw

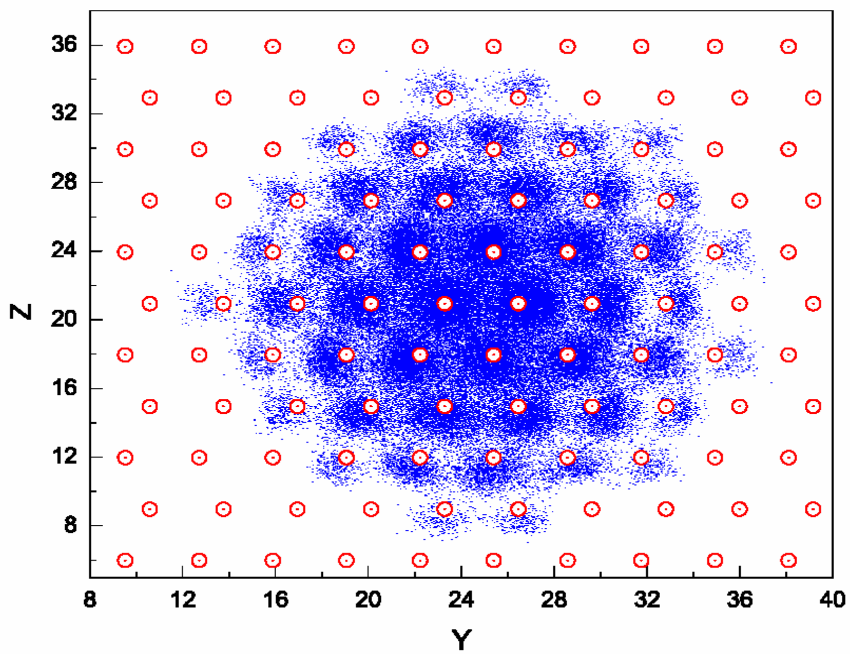


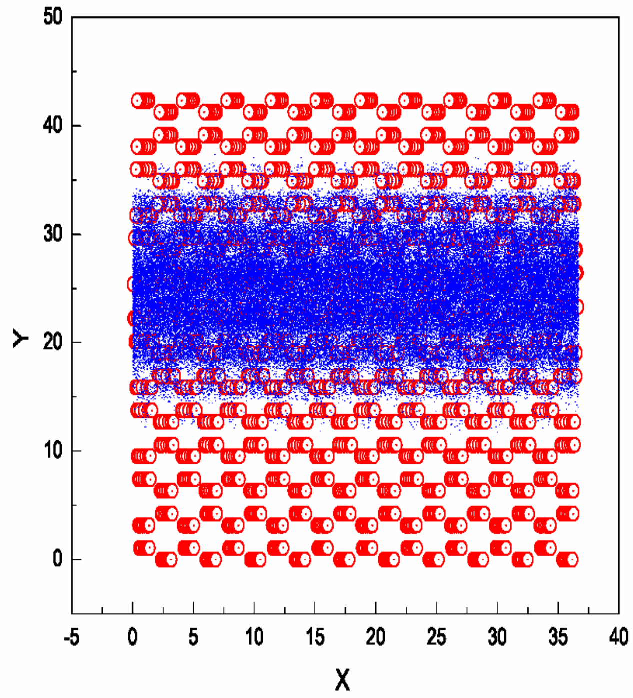




M. Boninsegni, et al., PRL **99**, 035301 (2007) condensate map

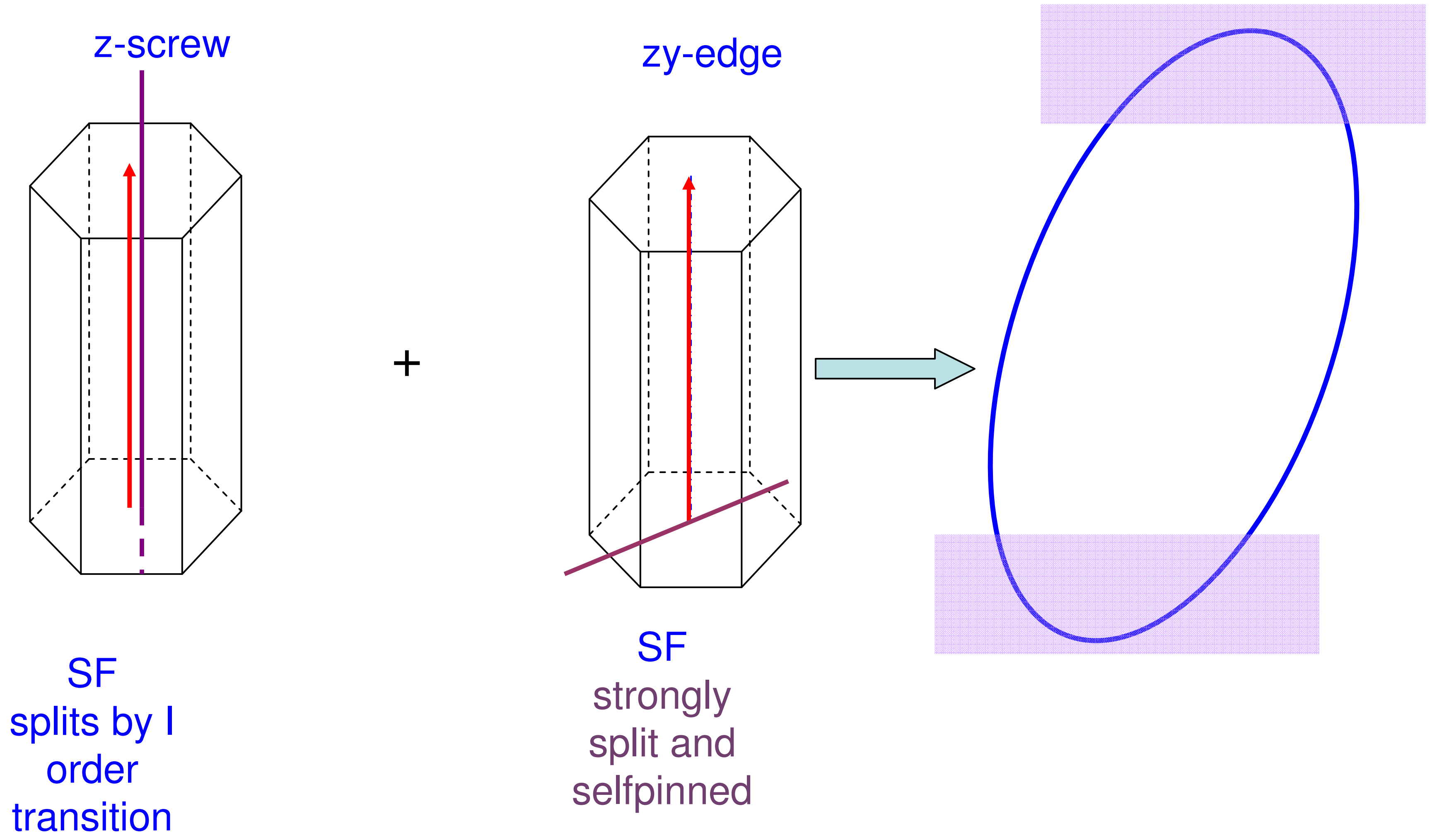
X-screw



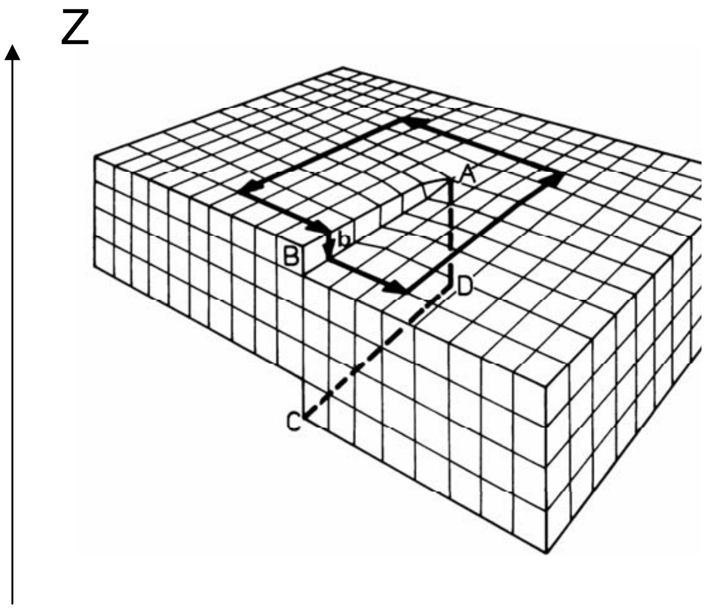


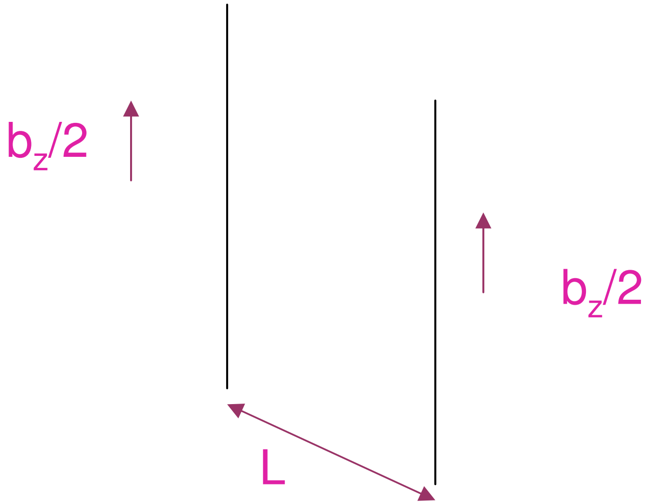
G. Soyler et al.

Fully SF loops

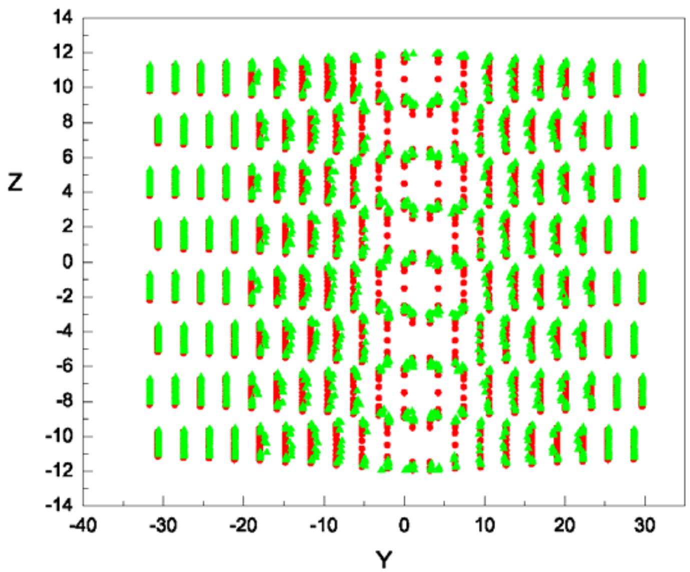


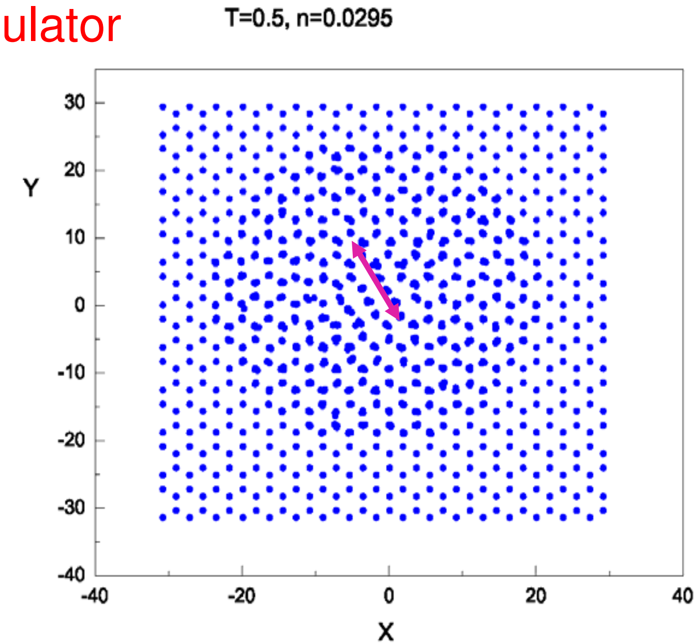
Splitting of z-screw dislocation makes it insulator

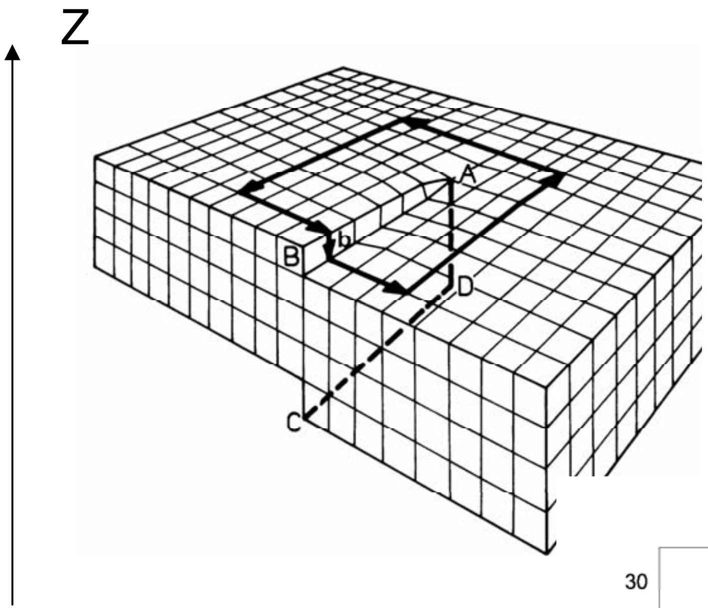


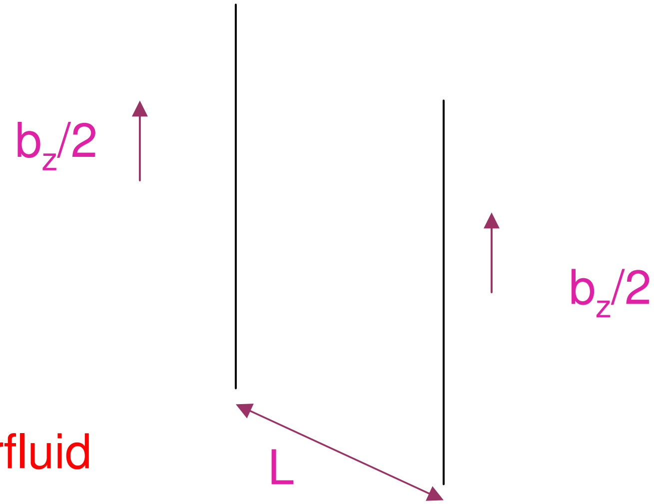


split=insulator



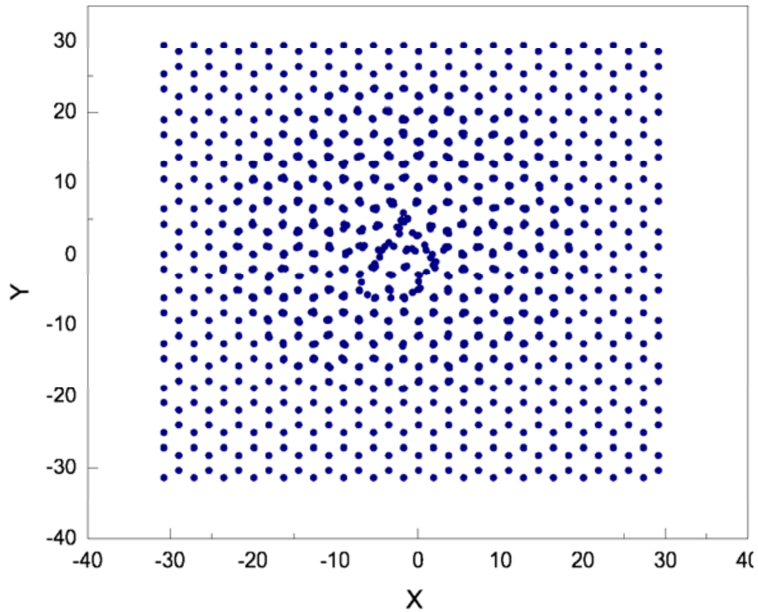




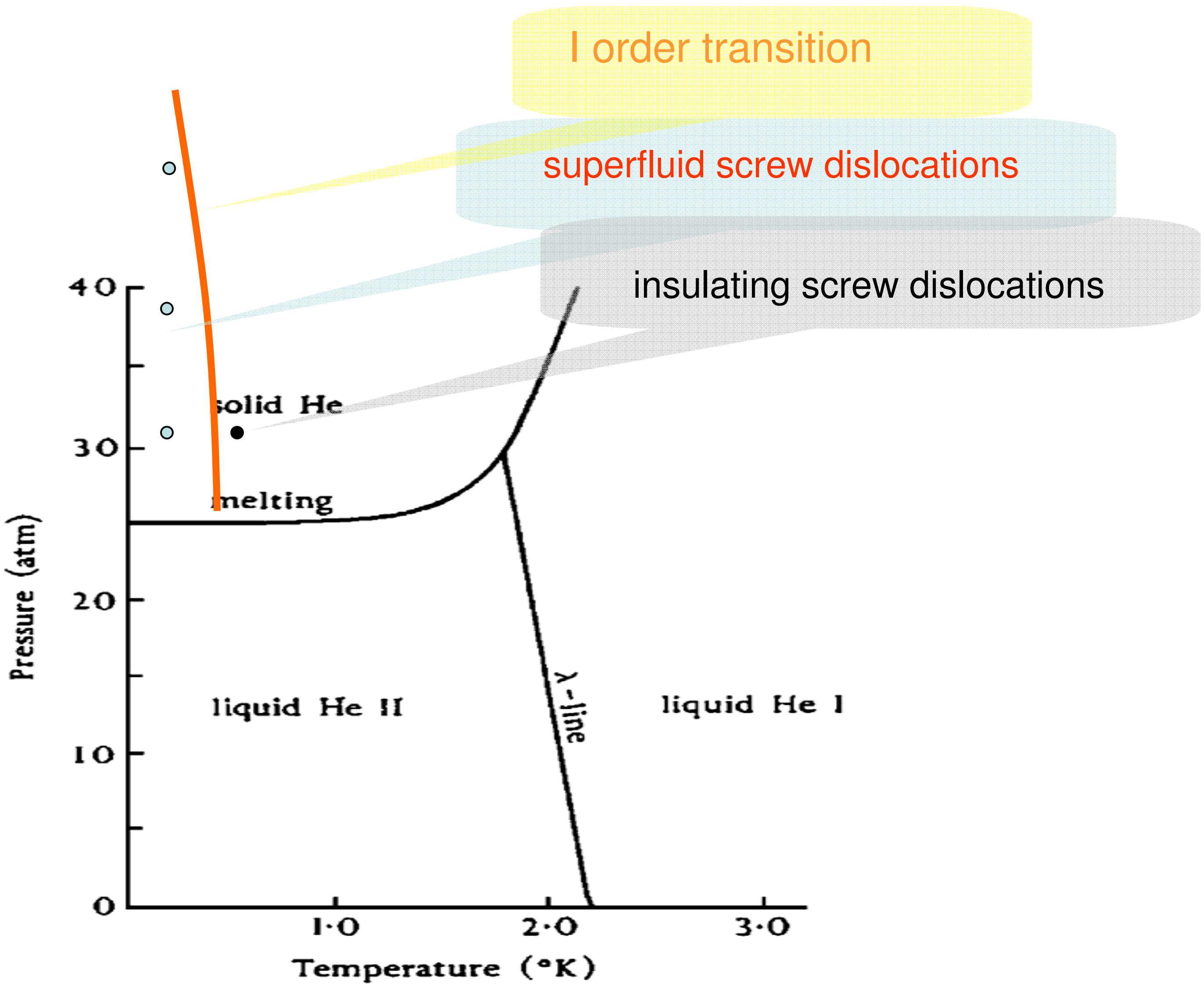


superfluid

T=0.25, n=0.0295



(Preliminary) phase diagram for dislocation SF



Strain and SF gap

$$F_{\text{int}} = (r - T_{ij}u_{ij} - T_{ijkl}u_{ij}u_{kl} - \ldots)|\psi|^2 + \ldots.$$

$$T_{xx} = T_{yy} = r_{\perp}; \qquad T_{zz} = r_{\parallel}$$

T_{ijkl} – symmetry of elastic moduli

$$|\psi|^2 \sim (-r + T_{ij}u_{ij} + T_{ijkl}u_{ij}u_{kl} + \ldots)$$

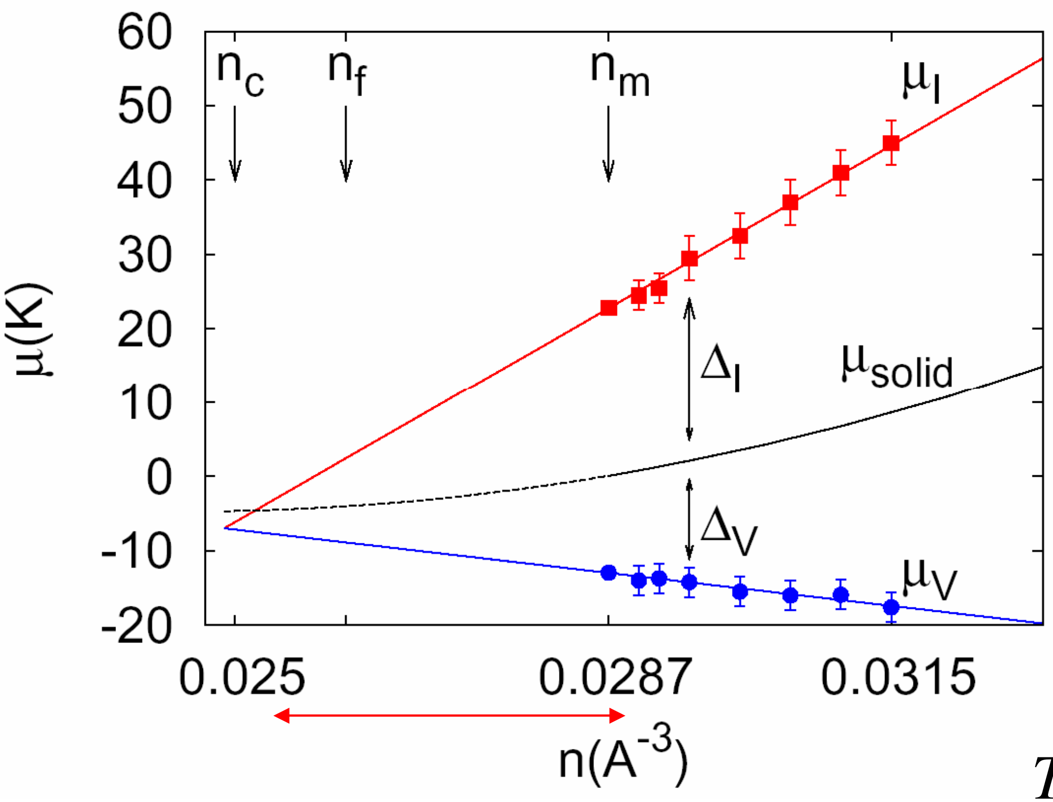
Higher order terms in strain are equally important

no proximity to superfuidity of ideal crystal (no perfect supersolid)

Density change and vacancy gap

V. M. Nabutovskii and V. Ya. Shapiro, JETP 48, 480 (1978)
S. I. Shevchenko, Sov. J. Low Temp. Phys. **13**, 61; 553 (1987)
J. Toner, PRL **100,** 035302(2008)

L. Pollet, et al, cond-mat 08053713



$$\delta n / n \approx 0.13$$

$$\delta n \approx -u_{ii} n$$

$$u_{xx} = u_{yy} = u_{zz}$$

No significant quadratic terms!!!

$$T_{zzzz} + 2T_{xxyy} + 2T_{xxxx} + 4T_{xxzz} \approx 0$$

XY-edge dislocation: Insulating

$$u_{ii} \approx \frac{b}{2\pi r}, \quad r = a,\ b = a \rightarrow \quad \delta n / n \approx 0.16$$

Splitting: $\quad b \rightarrow b/2 \rightarrow \quad \delta n / n \approx 0.08 < 0.13$

ZY-edge dislocation: marginally SF

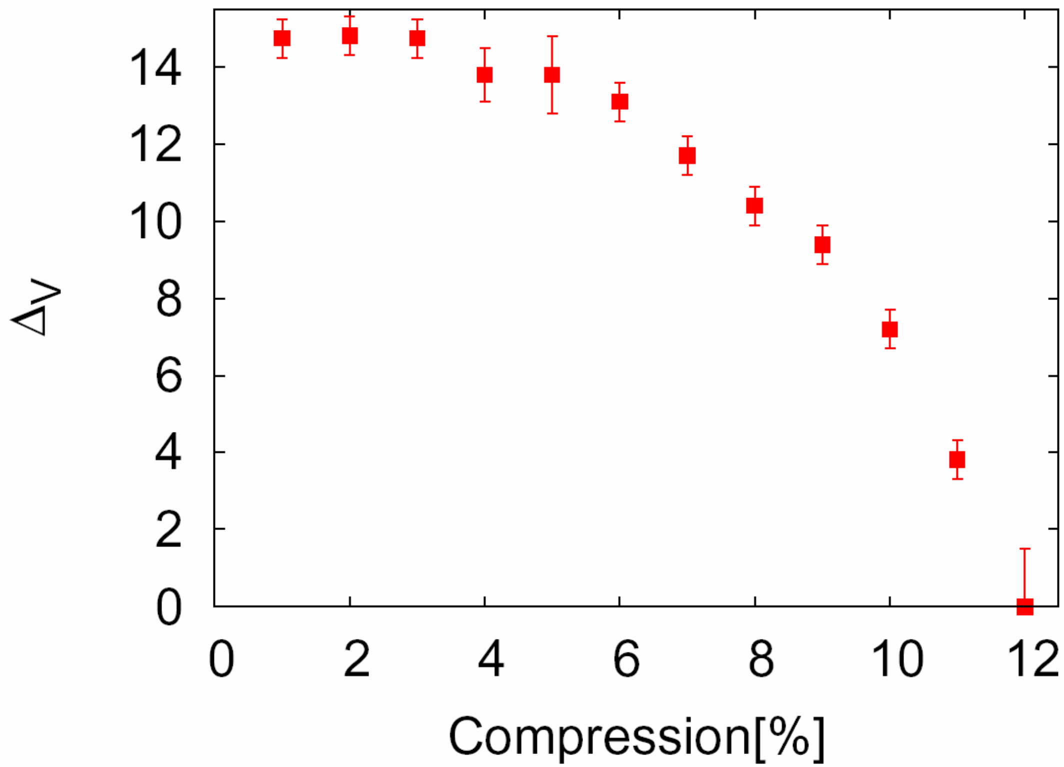
$$u_{ii} \approx \frac{b}{2\pi r}, \quad r = a,\ b = \sqrt{8/3}\,a \rightarrow \quad \delta n / n \approx 0.26$$

Splitting: $\quad b \rightarrow b/2 \rightarrow \quad \delta n / n \approx 0.13$

Anistropic compression

L. Pollet, et al, cond-mat 08053713

$$u_{xx} + u_{yy} + u_{zz} = 0$$



No linear term!

$$r_{\parallel} = r_{\perp}$$

Anistropic compression

$$|\psi|^2 \sim \left(-r+(T_{zzzz}+T_{xxyy}/2+T_{xxxx}/2-2T_{xxzz})\,u_{zz}^2\right) \sim \left(1-\frac{u_{zz}^2}{(0.12)^2}\right)$$

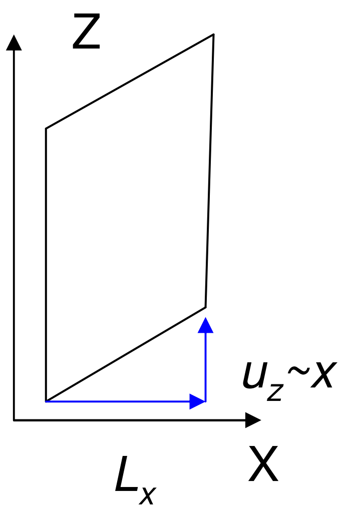
$$T_{zzzz}+2T_{xxyy}+2T_{xxxx}+4T_{xxzz} \approx 0$$

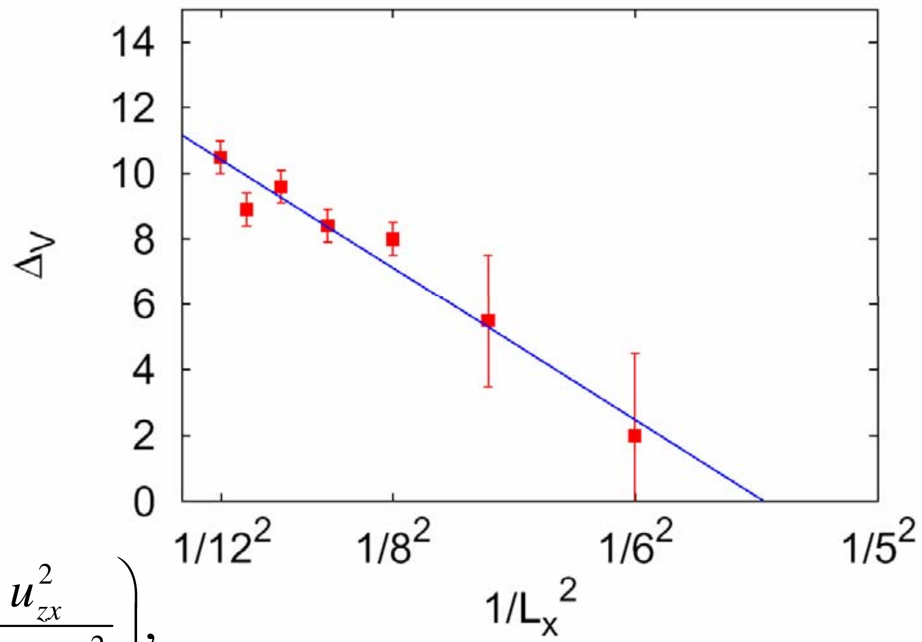
split ZY-edge is marginally SF

$$u_{zz} = \frac{b_z}{2\pi a} \approx 0.26$$

$$u_{zz}/2 \approx 0.13$$

Shear strain





$$|\psi|^2 \sim -(r - 4T_{xzxz}u_{xz}^2) \sim -\left(1 - \frac{u_{zx}^2}{(0.15)^2}\right),$$

screw dislocation: $\sqrt{u_{zx}^2 + u_{zy}^2} = \dfrac{b_z}{4\pi r} \approx 0.22, \; r = \dfrac{a}{\sqrt{3}}, \; b_z = \sqrt{\dfrac{8}{3}}a$

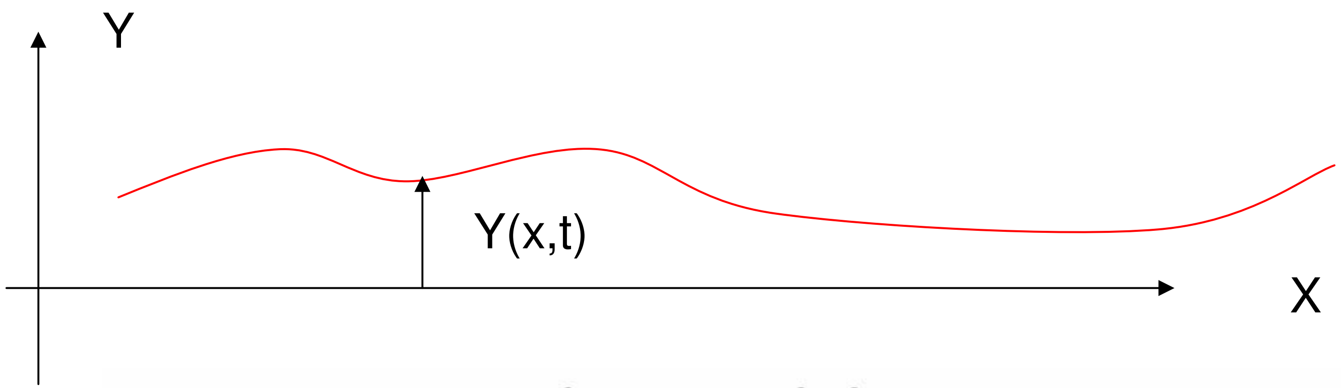
superfluid if unsplit: $|\psi|^2 \sim -\left(1 - \dfrac{(u_{zx}^2 + u_{zy}^2)}{(0.15)^2}\right) = -1 + \left(\dfrac{0.22}{0.15}\right)^2 > 0,$

insulating if split: $-1 + \left(\dfrac{0.11}{0.15}\right)^2 < 0 \;\; \rightarrow \;\; \psi = 0$

Quantum (non-)roughening and J.Day & J.Beamish experiment

J. Day & J. Beamish, *Nature* **450**, 853 (2007)

Quantum dislocation



$$\frac{S}{\hbar} = \int dx \int dt \left[\frac{m n_0 b^2}{2\hbar} \dot{Y}^2 + \frac{m n_0 b^2 V_s^2}{2\hbar} (\nabla_x Y)^2 - \frac{u_P}{\hbar b} \cos\left(\frac{2\pi Y}{b}\right) \right]$$

m – He4 mass, n_0 – density, b – Burgers vector, V_s – speed of sound, u_P – Peierls barrier

Quantum rough dislocation ⟷ Peierls barrier u_p is effectively zero at T=0

Zero point wandering

ratio *K* of phonon and kink energies becomes ~1

in He4: $$K = \frac{2\pi\hbar}{4b^4 n_0 m V_s} \approx \frac{h}{b m V_s} \approx 1$$

K – Luttinger parameter

Long-range interaction between kinks due to 3d elastic matrix

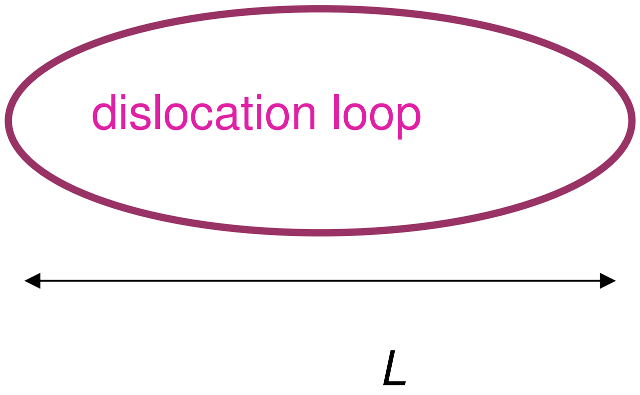
J.P.Hirth, J.Lothe, " *Theory of Dislocations*", McGraw-Hill, 1968
A. M. Kosevich, "*The Crystal Lattice: Phonons, Solitons, Dislocations, Superlattices",* Wiley, 2005

Long-range space-time interaction suppresses quantum roughening

$$U_{LR}(x,t) \approx \frac{g}{x^2+t^2}$$

$$S = \sum_{\omega,q} \{ \frac{1}{2K}[1 + g\ln\left(1+\frac{Q_0^2}{\omega^2+q^2}\right)](\omega^2+q^2)|Y_{\omega,q}|^2\} + S_{SG}, \quad g \approx 1$$

$$\int d^3r\, \dot{\vec{u}}^2 \rightarrow \int dx \dot{Y}^2 \int dydz(\nabla_y u)^2 \sim L\ln L\, \dot{Y}^2$$



$$\int d^3r\, (\nabla_x \vec{u})^2 \sim L\ln L$$

Coulomb gas mapping

$$Z = \int DY \; \exp(-S/\hbar).$$

$$Z = \sum_{n_\pm(i)=0,1,2,..,} \left(\Pi_i \frac{u_P^{n_+(i)+n_-(i)}}{n_+(i)!n_-(i)!} \right) \mathrm{e}^{-\frac{1}{2}\sum_{ij}(n_+(i)-n_-(i))U(i-j)(n_+(j)-n_-(j))}$$

$$U(x,t) \sim \sum_{q,\omega} \frac{\mathrm{e}^{i(qx+\omega t)}K}{[1+g\ln(1+\frac{Q_o^2}{q^2+\omega^2})](q^2+\omega^2)} \approx \frac{4K}{g}\ln(1+g\ln(x^2+t^2))$$

Kostrelitz-Thouless transition is destroyed for arbitrary small *g*

$$F_{\mathrm{pair}} = U(R) - \ln R^2 = 4\frac{K}{g}\ln(1+g\ln R) - \ln R^2 \to -\infty$$

Pairs are ionized into plasma state – Peierls barrier is relevant at T=0!!!

RG

$$\frac{du_P}{dS} = 2\left(1 - \frac{2K}{1+gS}\right)u_P$$

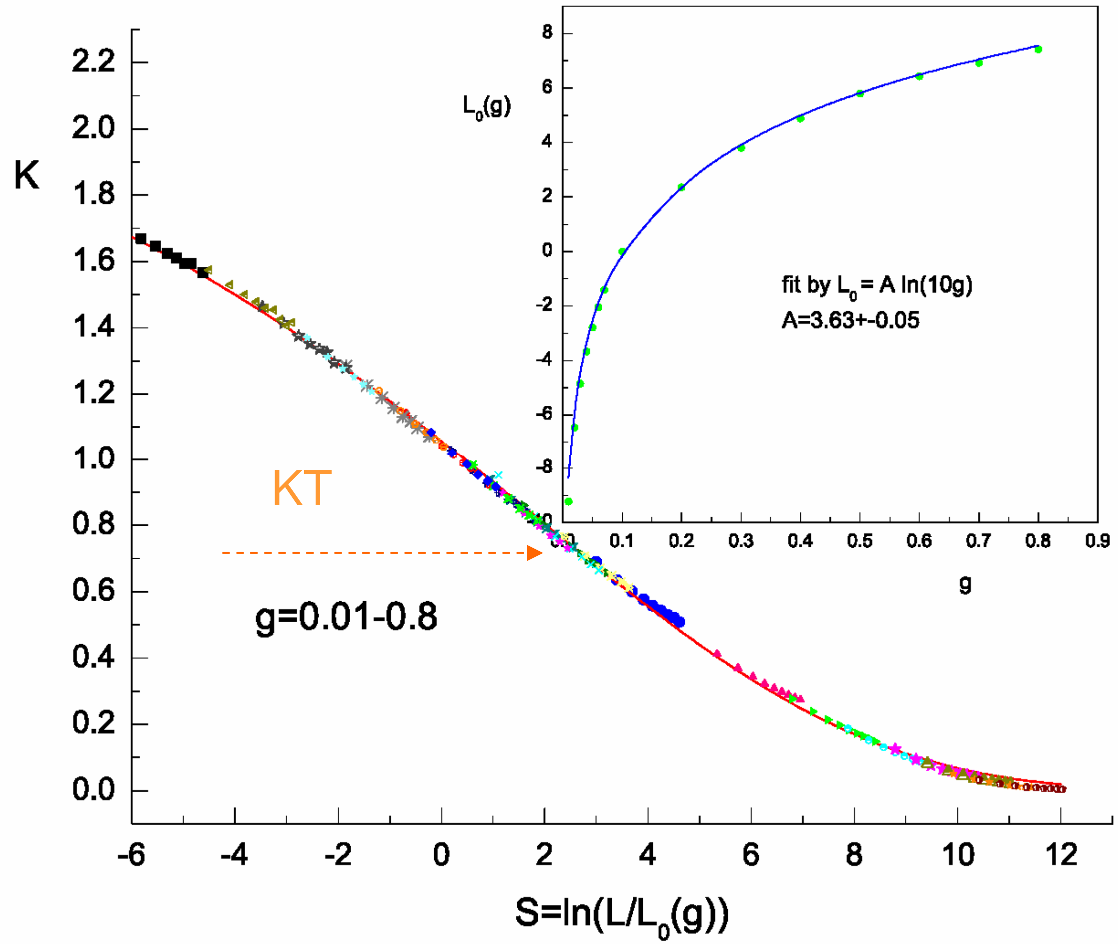
$$\frac{dK}{dS} = -\frac{K^3 u_P^2}{(1+gS)^2}$$

$$\frac{d(g/K)}{dS} = 0, \quad S \sim \ln L$$

u_p grows at large L for any g(0) and K(0)

MC simulations (of dual model) at T=0

Monte Carlo Worm algorithm (Prokof'ev&Svistunov (1998)):
http://montecarlo.csi.cuny.edu/umass/index.html



Consequences

- No quantum roughening = no quantum macroscopic wandering
- Gapped spectrum rather than sound-like (gap << kink energy)

$$\omega = \sqrt{q^2 + \Delta^2}$$

- Intrinsic hardening of shear modulus at T< gap (at pinning distances smaller than inverse concentration of thermal kinks)

$$\frac{1}{\mu} = \frac{1}{\mu_0}\left(1 + \frac{\gamma n_d}{(1 + g\ln L_p)(L_p^{-2} + n_d + \Delta^2)}\right), \quad \gamma \approx 1$$

If gap were zero: Thermal activation of He3

$$F = E_B(N_{He3} - N_1) + T(N_{\mathrm{He3}} - N_1)\ln\left(\frac{N_{\mathrm{He3}} - N_1}{eN_0}\right) + TN_1 \ln\left(\frac{N_1}{eN_{0d}}\right)$$

$E_B \approx 0.8$K binding energy of He3 to dislocation; N_{He3} -total number of He3 atoms; N_1 – total number of bound He3 atoms on dislocations; N_0 - total number of possible positions of He3 atoms in the bulk (it is the largest number); N_{0d} – number of positions at dislocations.

$$\frac{\partial F}{\partial N_1} = 0 \rightarrow N_1 = \frac{n_d}{\exp(-E_B/T) + n_d} N_{\mathrm{He3}}$$

n_d – dislocation density in units of inter-particle distance: $n_d \approx 1.3 \cdot 10^{-6}$ for $10^9 \mathrm{cm}^{-2}$ density.

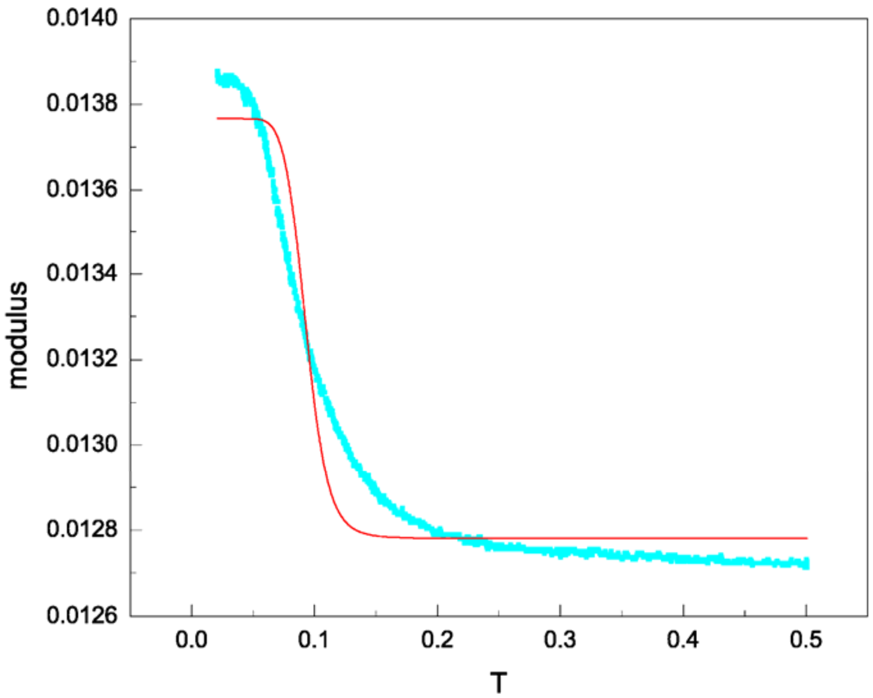
linear density of He3 in units a=1:

$$\frac{1}{L_p} = \frac{n_{He3}}{n_d + \exp(-E_B/T)}$$

L_p – pinning length

Single Arrhenius: poor fit

$$\mu(T) = \frac{\mu_0}{1 + \frac{\gamma_1}{1 + \frac{R}{\left(1 + n_d^{-1}\exp(-E_B/T)\right)^2}}}, \qquad R = \gamma_2 \frac{n_{\mathrm{He3}}^2}{n_d^3}, \qquad \gamma_{1,2} \approx 1$$



fit:

$n_d \sim 3 \cdot 10^{11} cm^{-2}$

$n_{He3} \sim 7 \cdot$ p.p.m

actual

$n_{He3} \sim 1 \cdot$ p.p.b

Finite gap (and L_p^{-1} >> soliton density)

$$\frac{1}{\mu} = \frac{1}{\mu_0}\left(1 + \frac{\gamma n_d}{(1+g\ln L_p)(L_p^{-2} + n_d + \Delta^2)}\right), \quad \gamma \approx 1$$

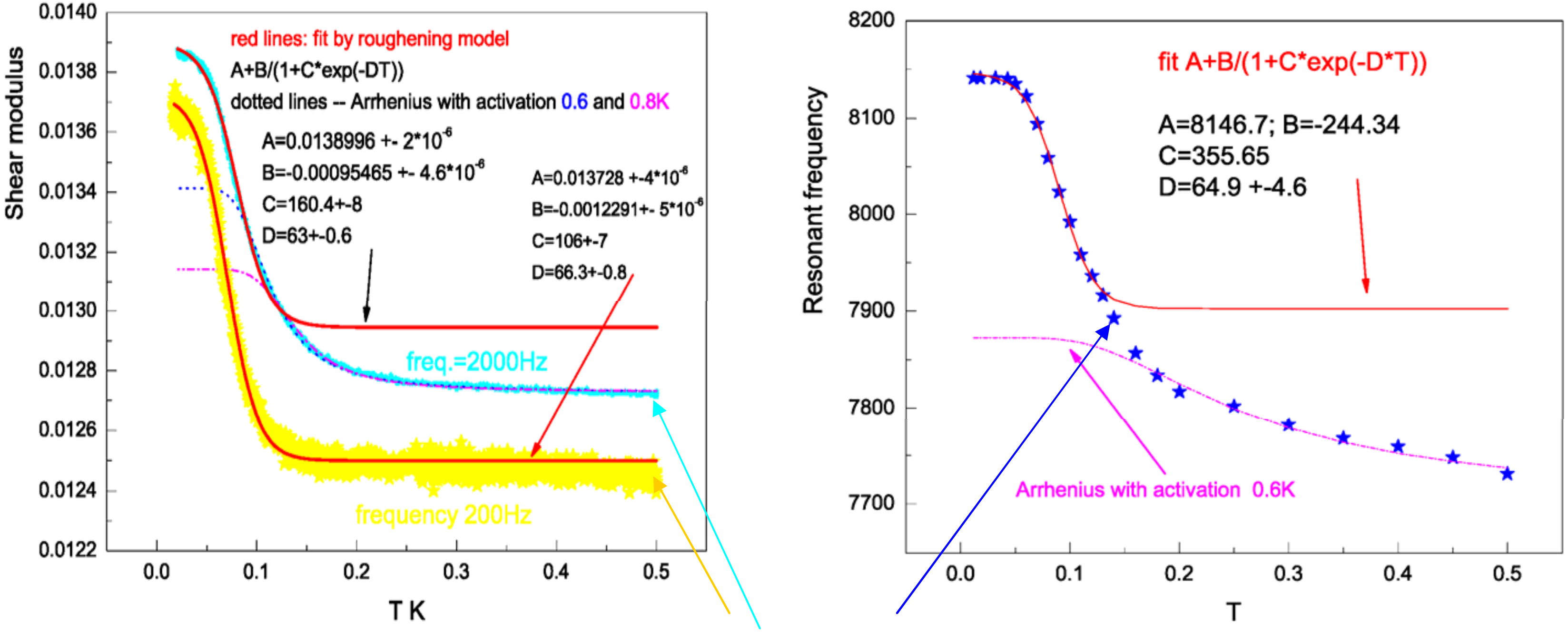
$$\cos\left(\frac{2\pi}{b}Y\right) \to \exp\left(-W_{DW}\right)\cos\left(\frac{2\pi}{b}Y\right)$$

$$\Delta \approx \exp\left(-W_{DW}/2\right)\Delta(T=0), \quad W_{DW} = 2\left(\frac{\pi}{b}\right)^2 < Y'^2 >$$

$$< Y'^2 > -\text{fluctuations of "classical" phonons} \to \quad W_{DW} \approx \frac{4\pi TK}{(1+g\ln L_p)\Delta}$$

$$\Delta(T) \approx \Delta_0 \exp\left(-\frac{2\pi K}{(1+g\ln L_p)\Delta_0}T\right)$$

Modulus hardening



data: courtesy of John Beamish, J. Day & J. Beamish, *Nature* **450**, 853 (2007)

For 1p.p.b of He3, $L_p=10^3$: $W_{DW} = D \approx 65T \rightarrow K \approx 2$ from different curves

self-consistent!

Summary

- Selfpinned SF loops (due to core splitting)
- Splitting as I order transition for Z-screw - hysteresis and metastability
- Strain criterion for SF and non-SF dislocations
- Preliminary phase diagram
- Self - pinning in the Peierls potential at low T: no quantum macroscopic wandering
- Bimodality in the modulus hardening due to Peierls gap