Stochastic effects in mesoscale materials simulations

Steve Fitzgerald

s.p.fitzgerald@leeds.ac.uk

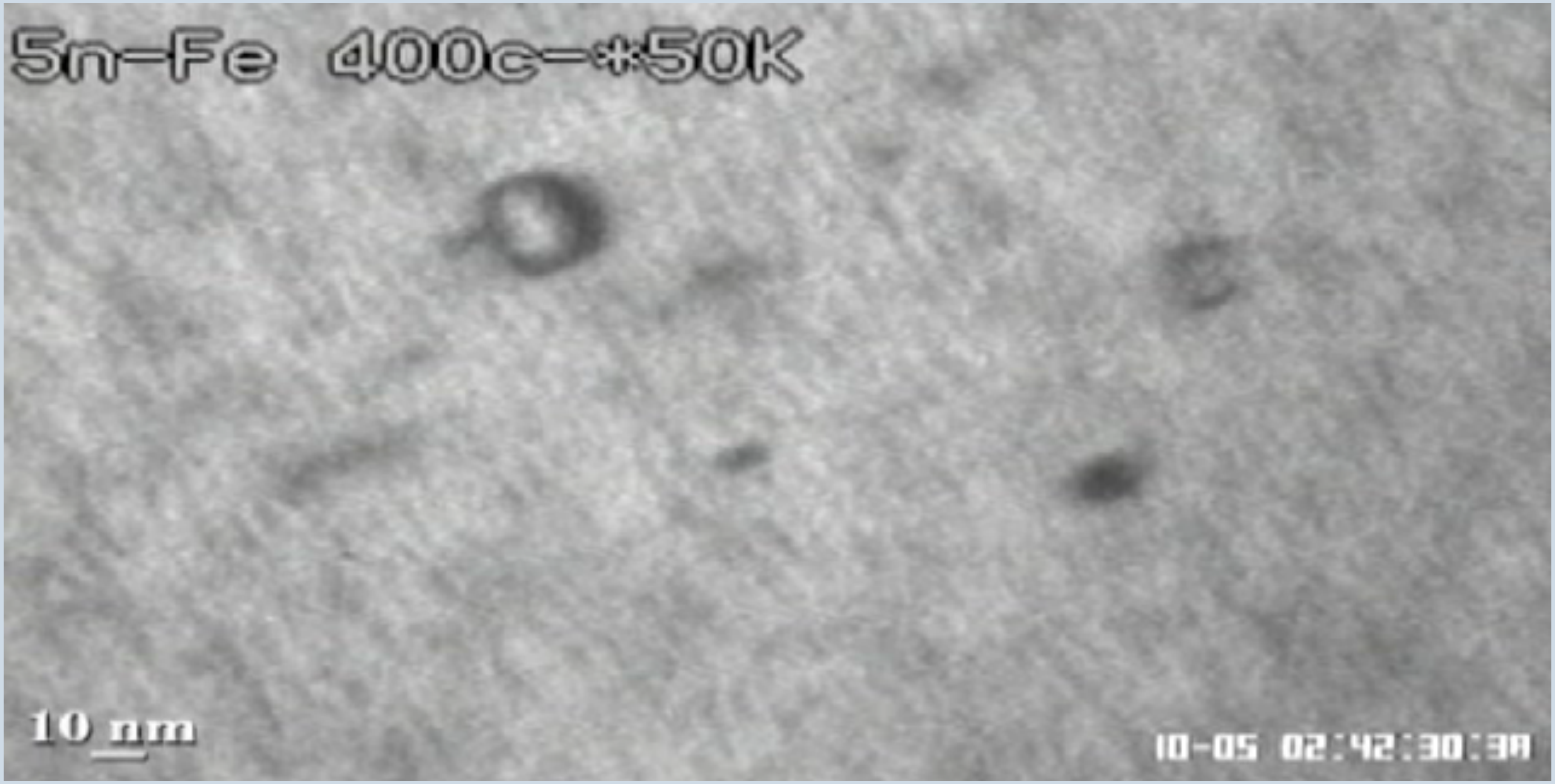
Department of Applied Mathematics

UNIVERSITY OF LEEDS

Diffusion: fluctuation and dissipation

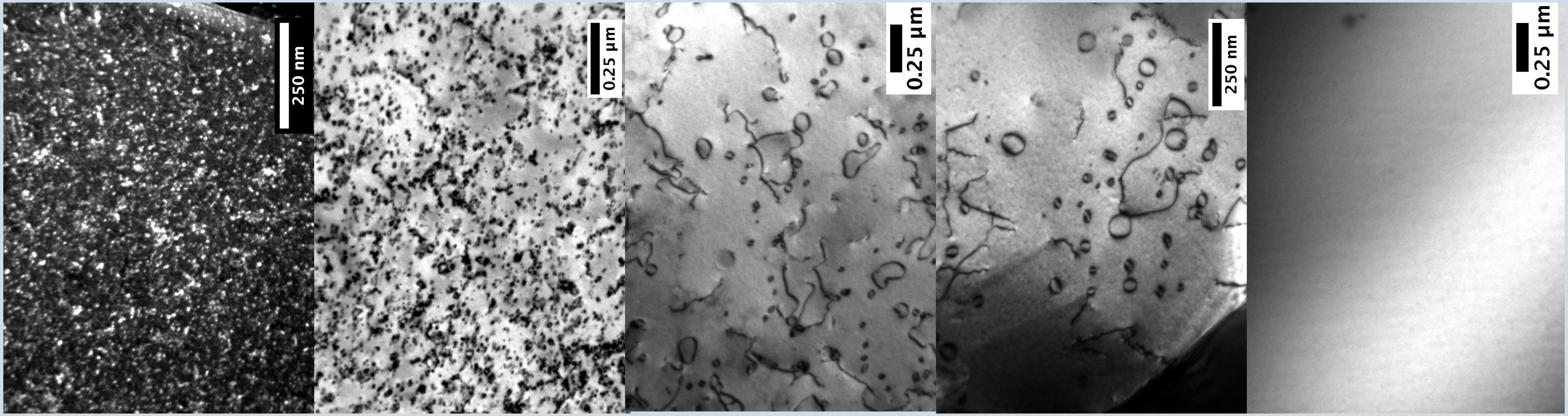
- Nuclear applications require high operating temperatures
- Irradiation drives systems away from equilibrium
- Stochastic effects govern microstructural evolution
- Dislocation motion, atomic migration is *overdamped*
- Diffusion-type behaviour
  - Mathematically, this means one time derivative, not two
- Can't have dissipation without fluctuations (Einstein)

Stochastic effects, elastic forces



Movie courtesy Prof K Arakawa, Shimane University, irradiated Fe at 400C

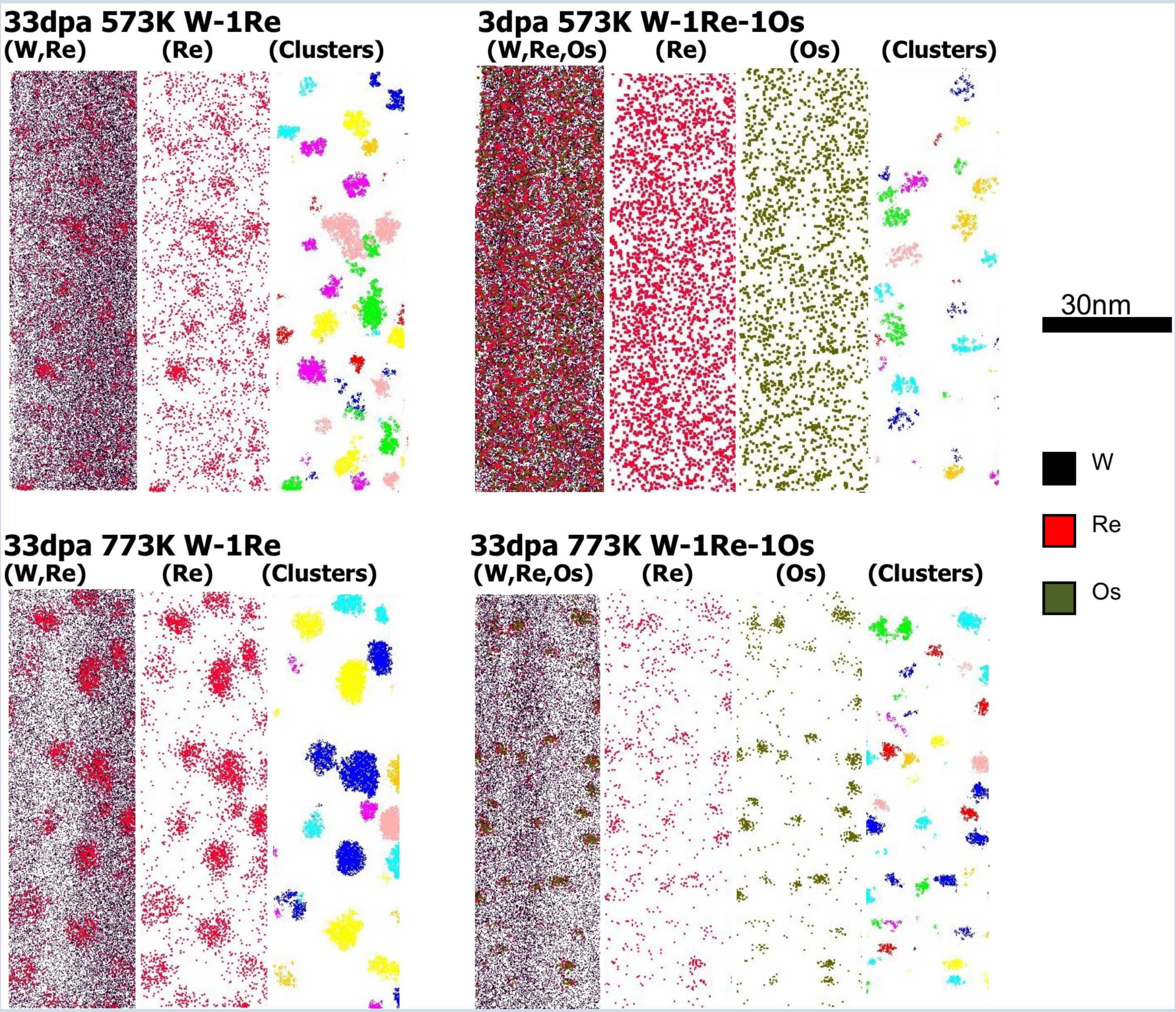
Stochastic effects, elastic forces



500°C | 800°C | 950°C | 1100°C | 1400°C

W irradiated to 1.5dpa, 500°C, 2MeV W+. 1 hour anneals
F Ferroni, P Edmondson, SPF et al Acta Mat 2014

Clustering in irradiated W-Re-Os

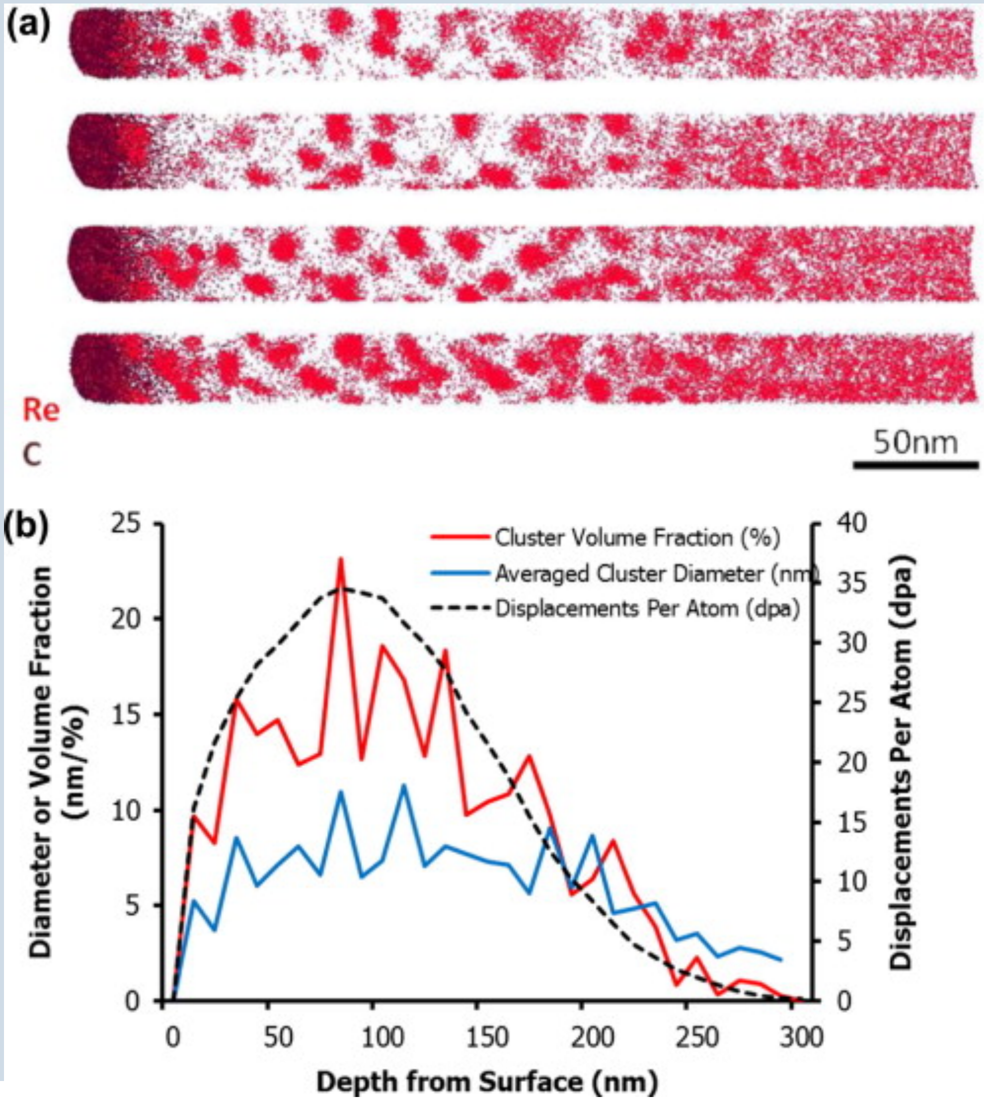


"Solute" migration mediated by vacancies and interstitials, hence enhanced by irradiation

Strongly dependent on temperature, dose

Xu et al, Acta Mat 2015

Clustering in irradiated W-Re-Os



"Solute" migration mediated by vacancies and interstitials, hence enhanced by irradiation

Strongly dependent on temperature, dose

Xu et al, Acta Mat 2015

Modelling paradigms

Atomic coordinates

- DFT* – hundreds of atoms, no free parameters, ps, 0K
- MD – millions of atoms, potential dependent, ns, finite temp.
- kMC – large length and time scales, dependent on rates (need all *a priori*)

Collective coordinates (far fewer)

- DDD – microns, milliseconds, need local rules to deal with interactions
- Langevin dynamics – large length and timescales, need phenomenological models, *no rates or rare event assumptions*

Mean field (densities and concentrations)

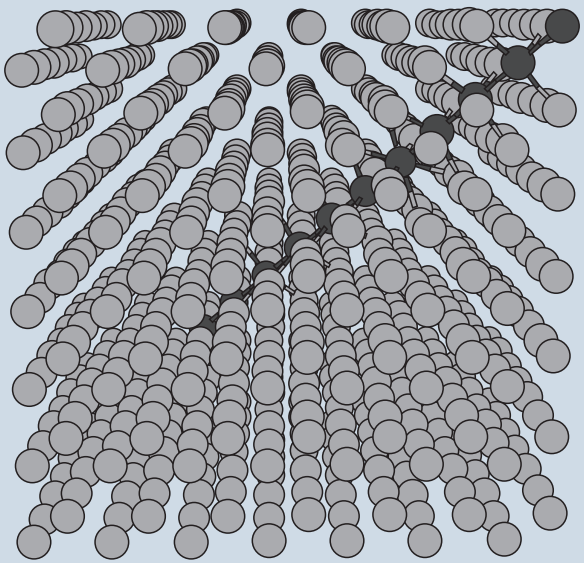
- Phase field – specify system by a few phase/conc. variables, evolve according to Cahn-Hilliard/Allen-Cahn equations

**DFT uses a density field for the electrons*

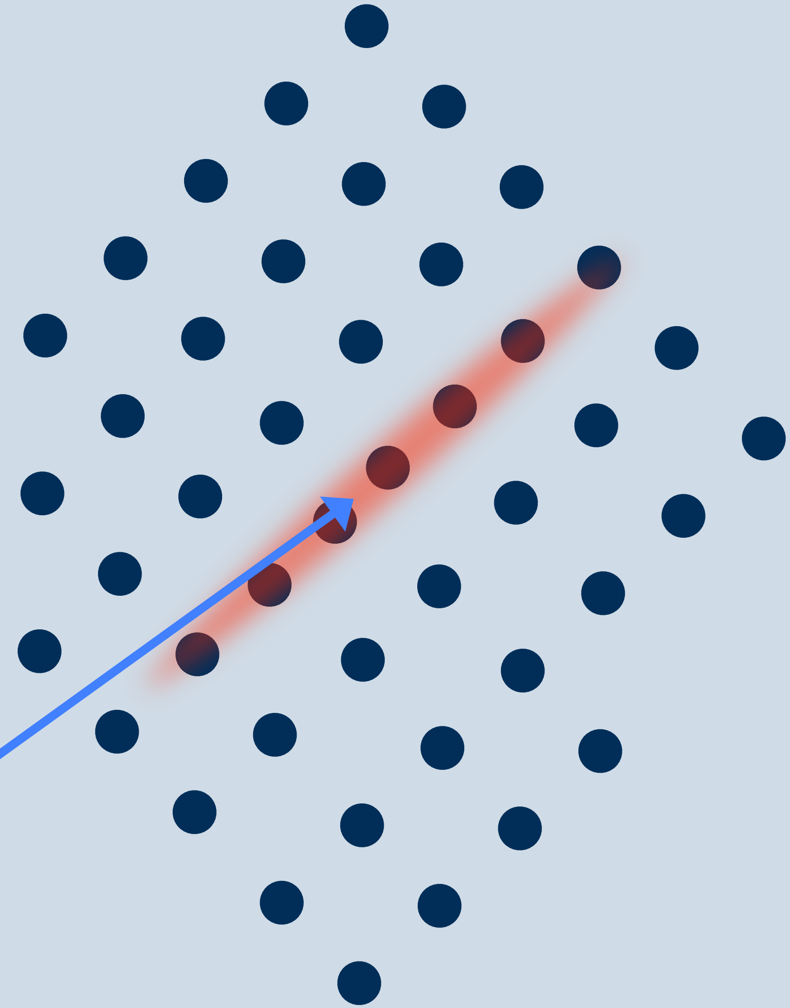
This talk

- Collective coordinates
  - » *defects, not atoms*
- Crowdions in transition metals and alloys
  - » *upscaling the mechanics of defects*
- Langevin dynamics and diffusion
  - » *a new paradigm for stochastic simulations*
- Discrete dislocation dynamics
  - » *adding fluctuations to the dissipation*
  - » *damage in thin films and microcantilevers*
  - » *nonlinear velocity reponse*

Example: <111> crowdions in bcc metals

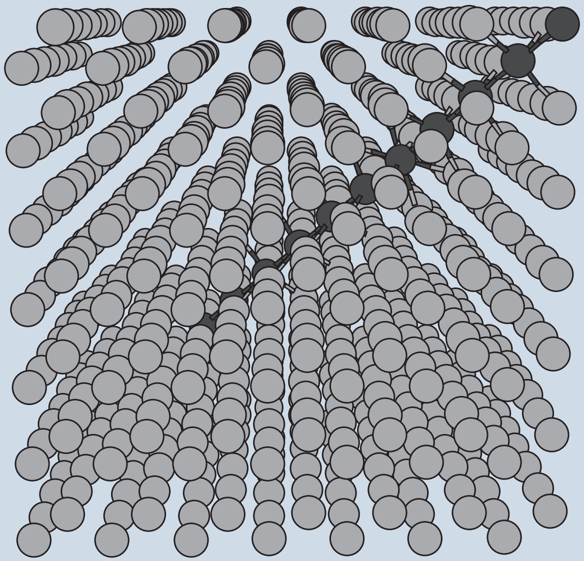


S. L. Dudarev, Phil. Mag. 2008



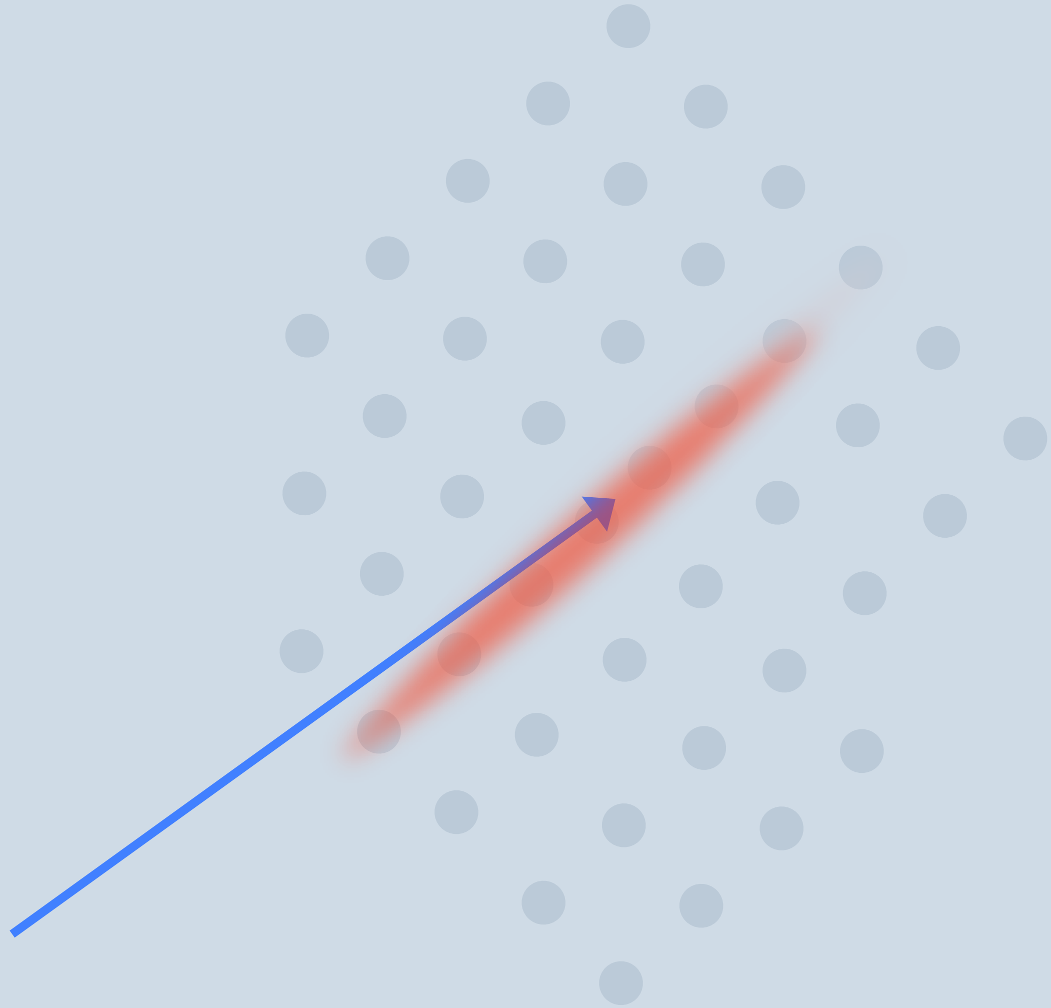
crowdion shown in red
not just one atom!

Example: <111> crowdions in bcc metals

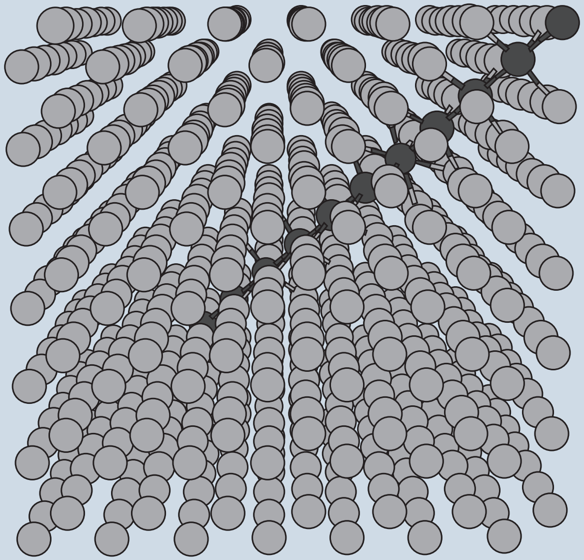


S. L. Dudarev, Phil. Mag. 2008

crowdion shown in red
not just one atom!

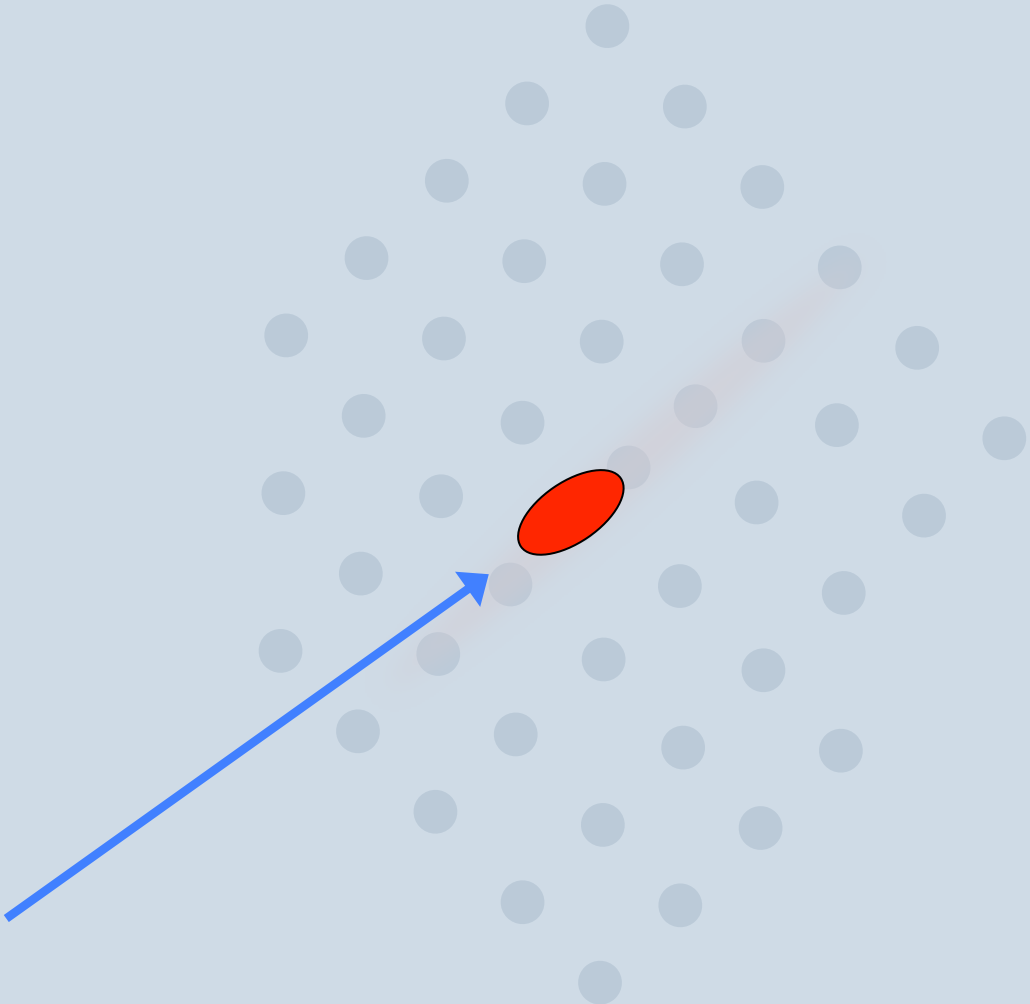


Example: <111> crowdions in bcc metals



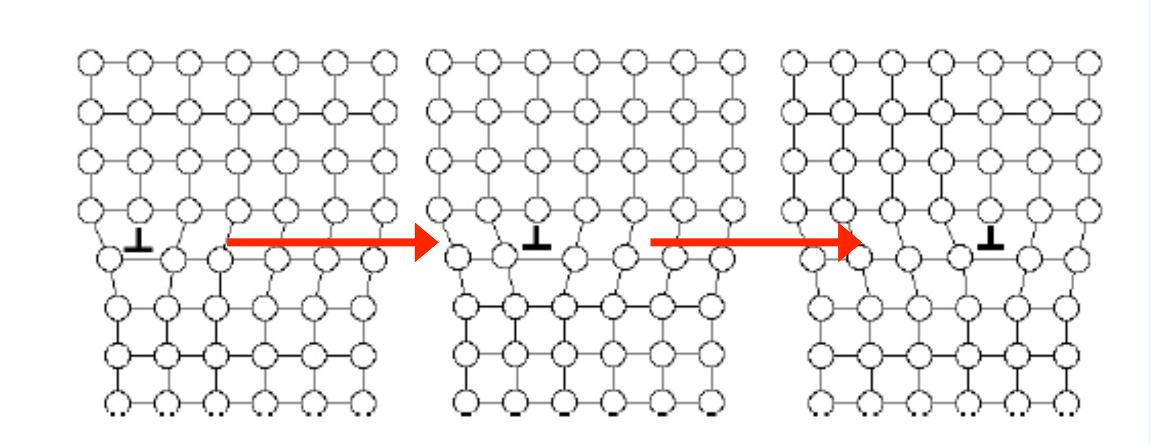
S. L. Dudarev, Phil. Mag. 2008

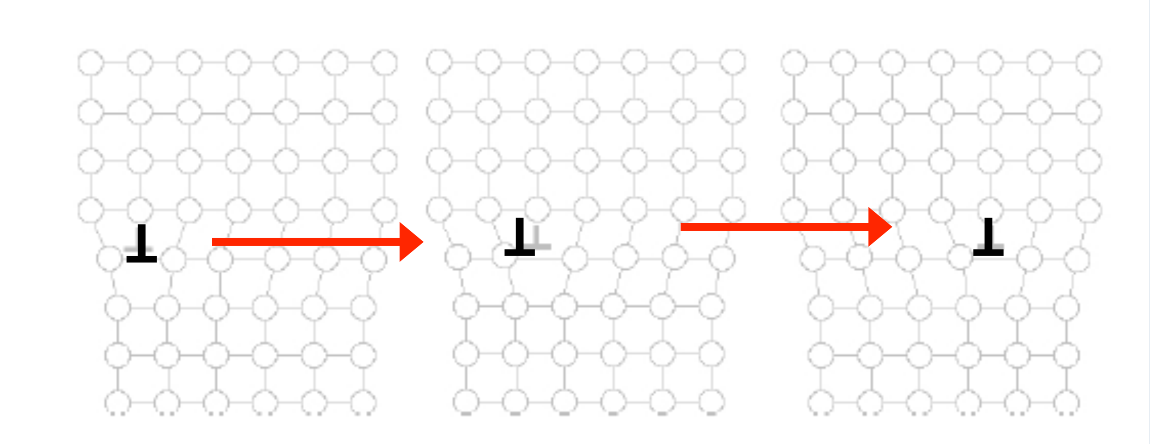
Integrate out atoms



Treat *defect* as fundamental object – point in this case

Example: Dislocations





Integrate out atoms

Treat *defect* as fundamental object – line in this case

Defect equations of motion

$$m\ddot{x} = -\nabla V(x)$$

inertia *potential gradient*

- Newton's second law
- Need a *phenomenological model* to assign effective mass and coupling to effective potential
- Deterministic
- No dissipation

Defect equations of motion

noise

$$m\ddot{x} + \gamma\dot{x} = -\nabla V(x) + \eta(t)$$

inertia friction potential gradient

- Add friction and noise, neglect inertia
- (assume particle reaches terminal velocity very fast)
- Sidesteps effective mass issue

Fluctuation – dissipation theorem

$$\gamma D = k_{\rm B} T$$

FDT

$$D = \frac{k_{\rm B} T}{\gamma}$$

$$\langle v(t) v(t') \rangle = 2D\delta(t - t')$$

Thermal velocity autocorrelation function – assume uncorrelated "white noise". This is the "D" in diffusion/Fokker-Planck equation:

$$\dot{\rho} = \left(\gamma^{-1} \left(-\nabla V \rho\right) + D\rho_x\right)_x$$

- Relates damping, fluctuations and temperature
- At low temperature and high damping, fluctuations are small
- Not so at high *T*…

Langevin dynamics

- Directly integrate stochastic equation of motion for *x(t)*

$$\gamma \dot{x} = -\nabla V(x) + \eta(t)$$

- Includes *random force* drawn from suitable distribution each timestep
- cf Ginzburg-Landau approach
  - *Also cf Allen-Cahn*

$$\Gamma \frac{\partial q}{\partial t} = -\frac{\delta E}{\delta q} + \xi$$

- Dynamics is a *gradient flow* (plus noise), no inertia
- Quasi-off lattice method

See eg Swinburne et al PRB 2013, Dudarev et al PRB 2010

Frenkel-Kontorova model for crowdions

- Few parameters (lattice spacing a, spring constant β, height of sine potential V_0, mass of atoms m)

- Lagrangian for displacement of n[th] atom $u_n(t)$:

$$\mathcal{L} = \sum_{n=-\infty}^{\infty} \left(\frac{m\dot{u}_n^2}{2} - \frac{\beta}{2} \left(u_{n+1} - u_n\right)^2 - V_0 \sin^2 \frac{\pi u}{a} \right)$$

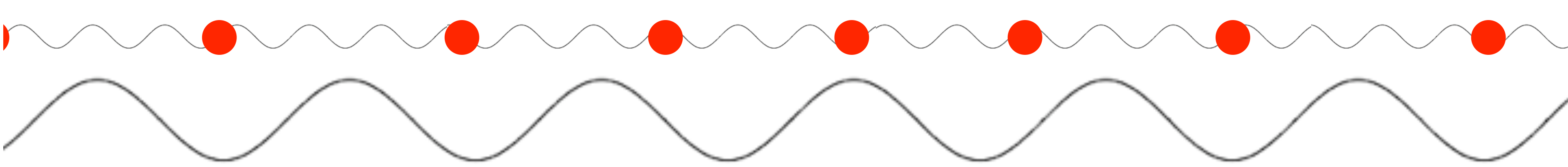
- Equation of motion (in continuum limit β term becomes a derivative, $u_n(t) \longrightarrow u(z,t)$):

$$m\ddot{u}(z,t) - \beta a^2 u(z,t)'' = V_0 \sin\left(2\pi u(z,t)/a\right)$$

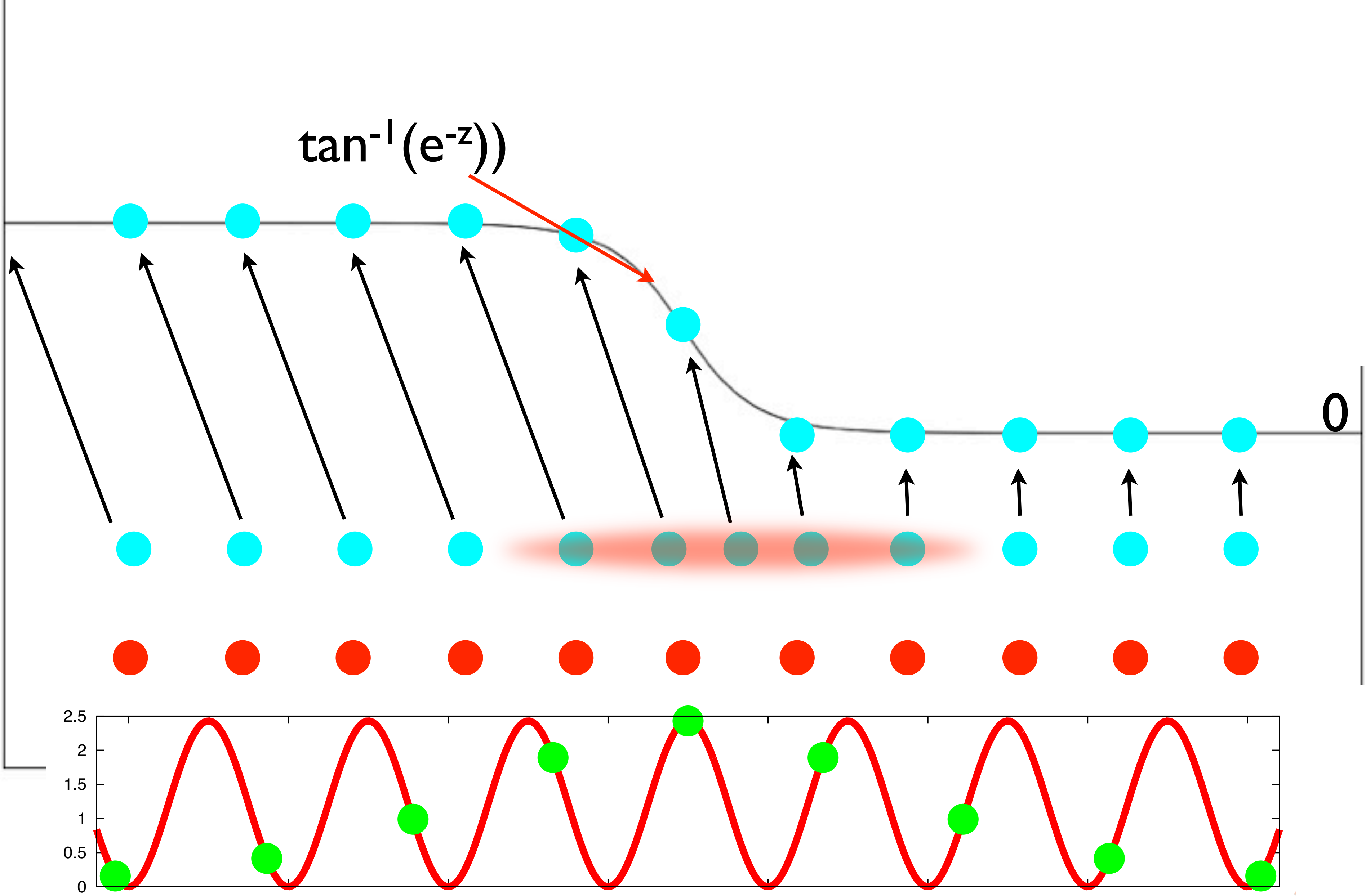
sine-Gordon equation

- Kink solution: $u = \frac{2}{\pi}\arctan\left(\exp\left[-\mu(z - Vt - z_0)\right]\right)$

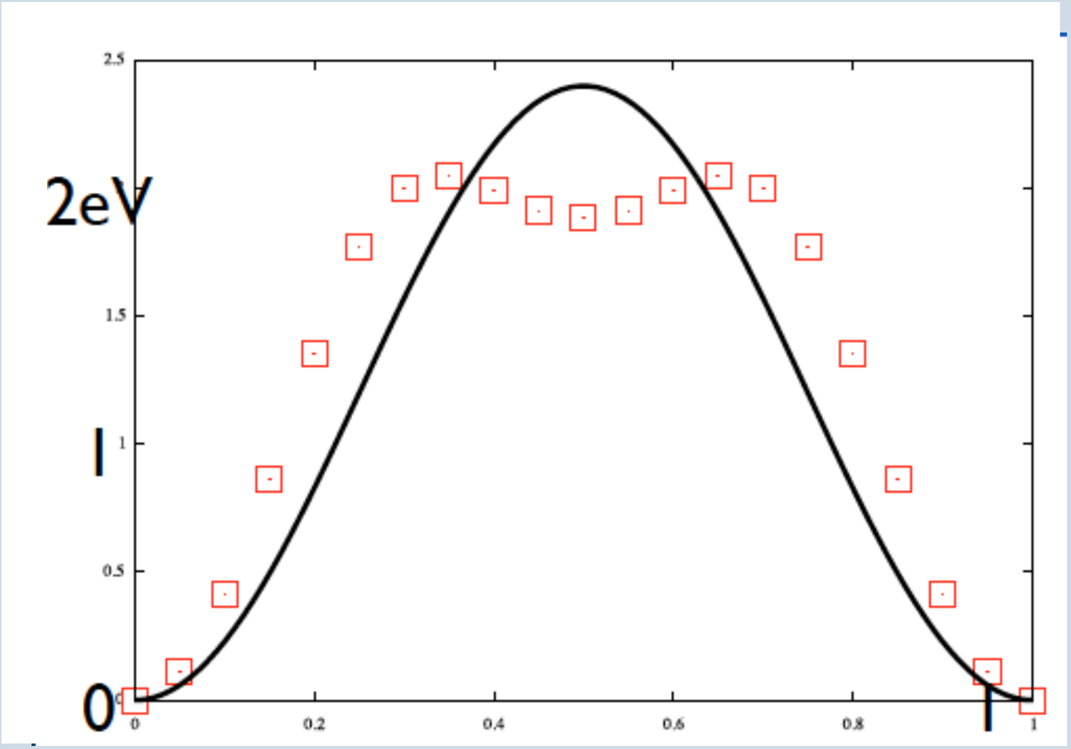
$$\mu^2 = \frac{2V_0\pi^2}{\beta a^4}$$



Displacement field “kink” solution (schematic, not to scale)

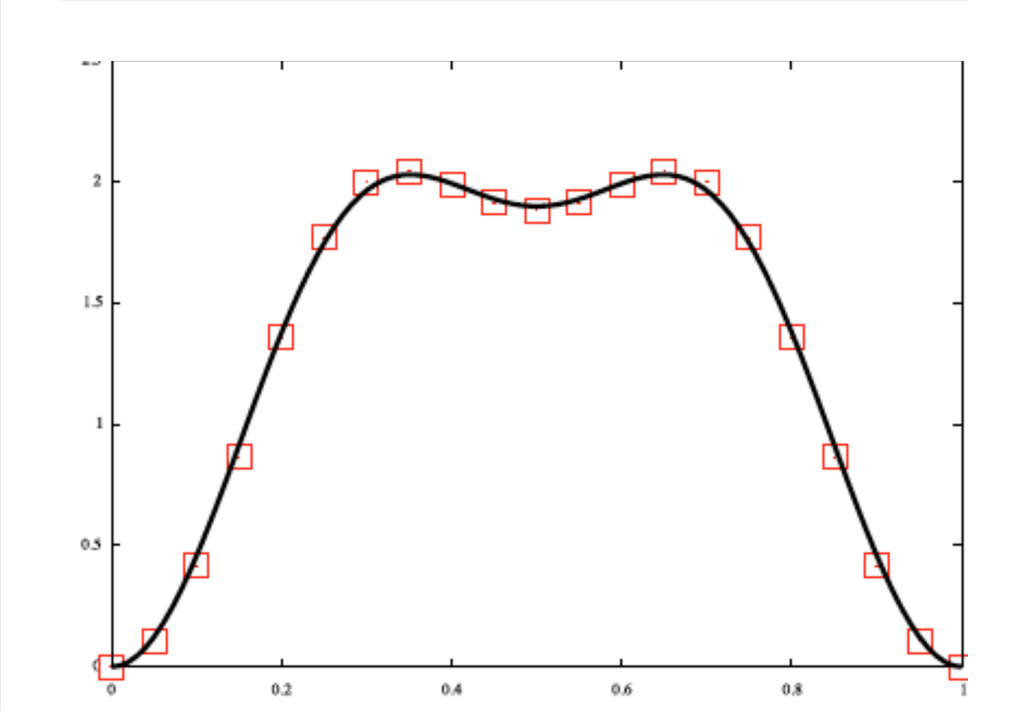


DFT calculation of V_0 for tungsten



- Not sinusoidal
- Clear local minimum
- Sine approximation can be viewed as first term in Fourier series of true potential
- Can we do better?

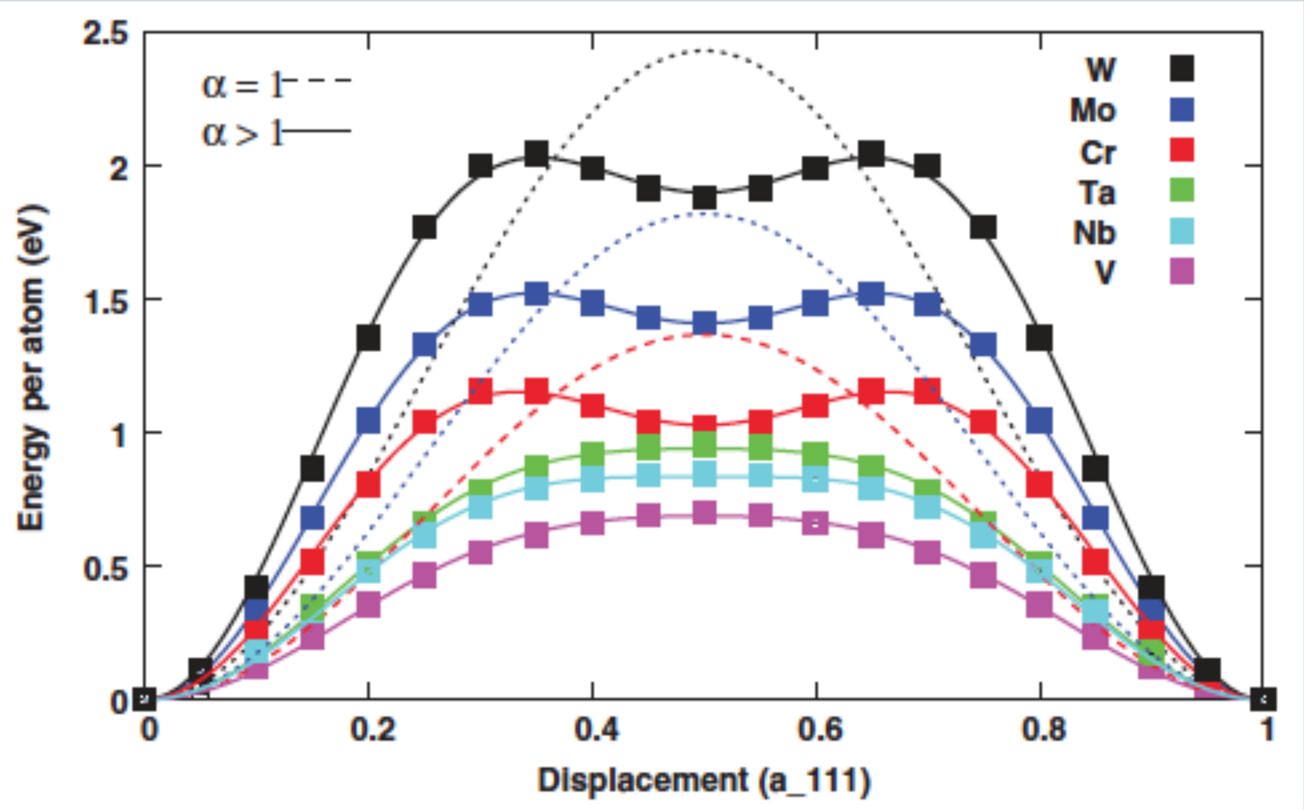
DFT calculation of V_0 for tungsten



- Yes!
- 2 parameter fit very accurate
- Captures local minimum
- Can still get an analytical form for the displacement field:

$$V_0 = \mu^2 \left(\sin^2 \frac{\pi z}{a} + \lambda \sin^2 \frac{2\pi z}{a} \right) \quad u = \frac{a}{\pi} \tan^{-1} \left(\frac{\alpha}{\sinh(\mu a (z - z_0))} \right)$$

Solution first found by Frank and van der Merwe for dislocations



Clear group-specific trend – “double-hump” most pronounced in Group VI metals

SPF and Nguyen Manh PRL 2008

Migration barriers

- *Lattice* potential ~ few eV
- What about *defect migration potential*? **Much** lower
- Soliton solution *locally* partitions energy equally between string and substrate
- So can write energy in discrete form as:

$$E = \int_{-\infty}^{\infty} \left[\frac{\beta}{2} \left(\frac{\partial u}{\partial z} \right)^2 + V(u) \right] \mathrm{d}z \longrightarrow 2 \sum_{n=-\infty}^{\infty} V(u_n)$$

$$u_n = u(z_n) = u(na - z_0)$$

Crowdion centre of mass

collective coordinate

Energy no longer indpt of z_0

Migration potential – *Peierls potential*

- Can calculate Fourier series for defect migration potential

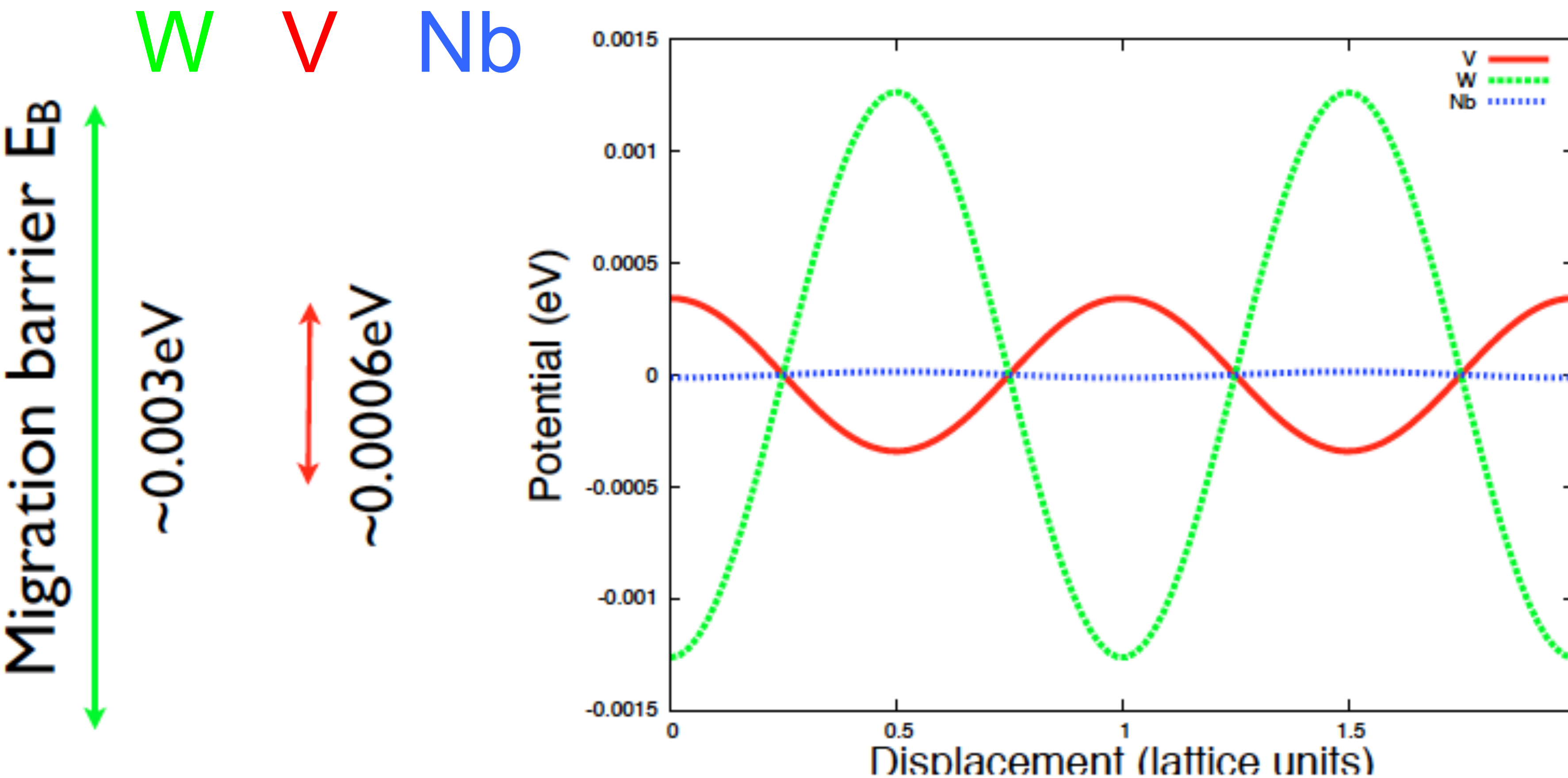
E_0 is ctm energy

$$E(z_0) = E_0 + \sum_{j=1}^{\infty} I_j \cos\left(\frac{2\pi j z_0}{a}\right)$$

$$I_j = \frac{2V_0\alpha\pi}{\mu a}\operatorname{cosech}\left(\frac{\xi\pi}{2}\right)$$
$$\times\left\{\xi\cos\left(\frac{\xi}{4}\ln\frac{q_+}{q_-}\right) - \frac{1}{\alpha\sqrt{\alpha^2-1}}\sin\left(\frac{\xi}{4}\ln\frac{q_+}{q_-}\right)\right\}$$

$$\xi = 2\pi j/\alpha\mu a, \;\; q_\pm = 1 - 2\alpha^2 \pm 2\alpha\sqrt{\alpha^2-1}$$

- Note considerable simplification for single-sine case (α = 1)

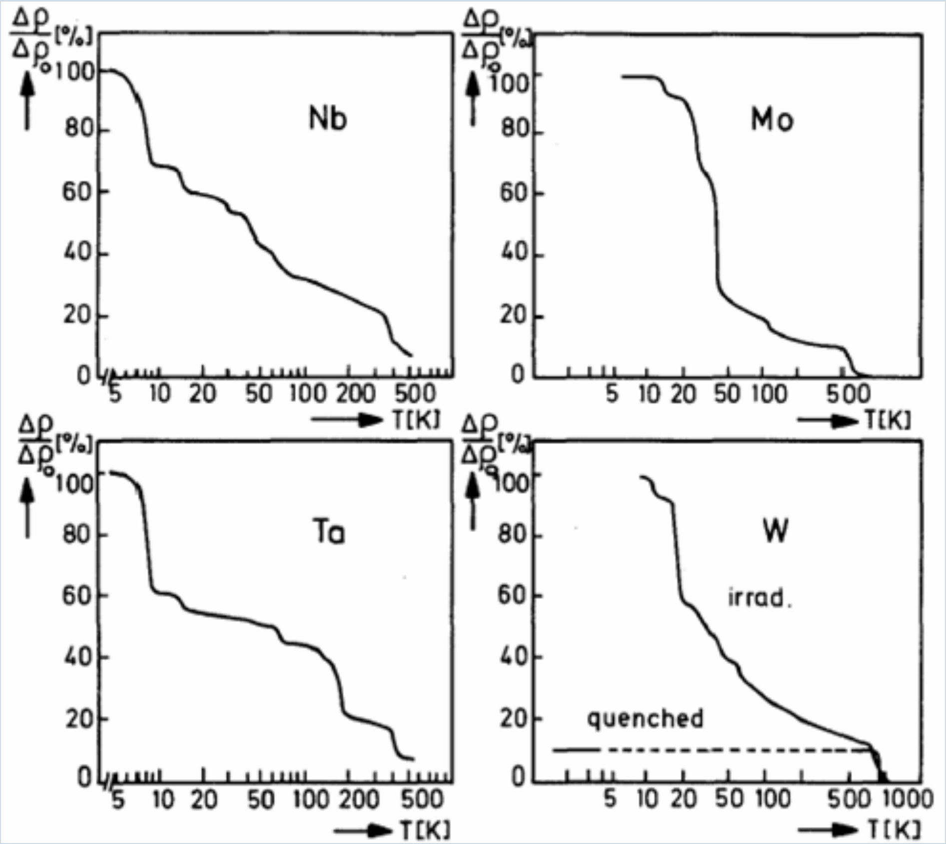


All barriers small, group 5B VERY small

(< DFT errorbar for supercell calculation of E_B)

V (group 5) shifted half period w.r.t. W (group 6)

Migration temperatures



Metal	Group	T_M (K)	E_B/k_B
V	5B	<6	~8
Nb	5B	<6	~0
Ta	5B	<6	~0
Cr	6B	~40	~100
Mo	6B	35	~30
W	6B	27	~30

Ehrhart et al in Landolt-Bornstein 1991 (resistivity recovery)

*SPF and Nguyen-Manh,
PRL 2008*

Diffusion coefficients

- Generally (eg. for kMC rates) *Arrhenius*-type law is used

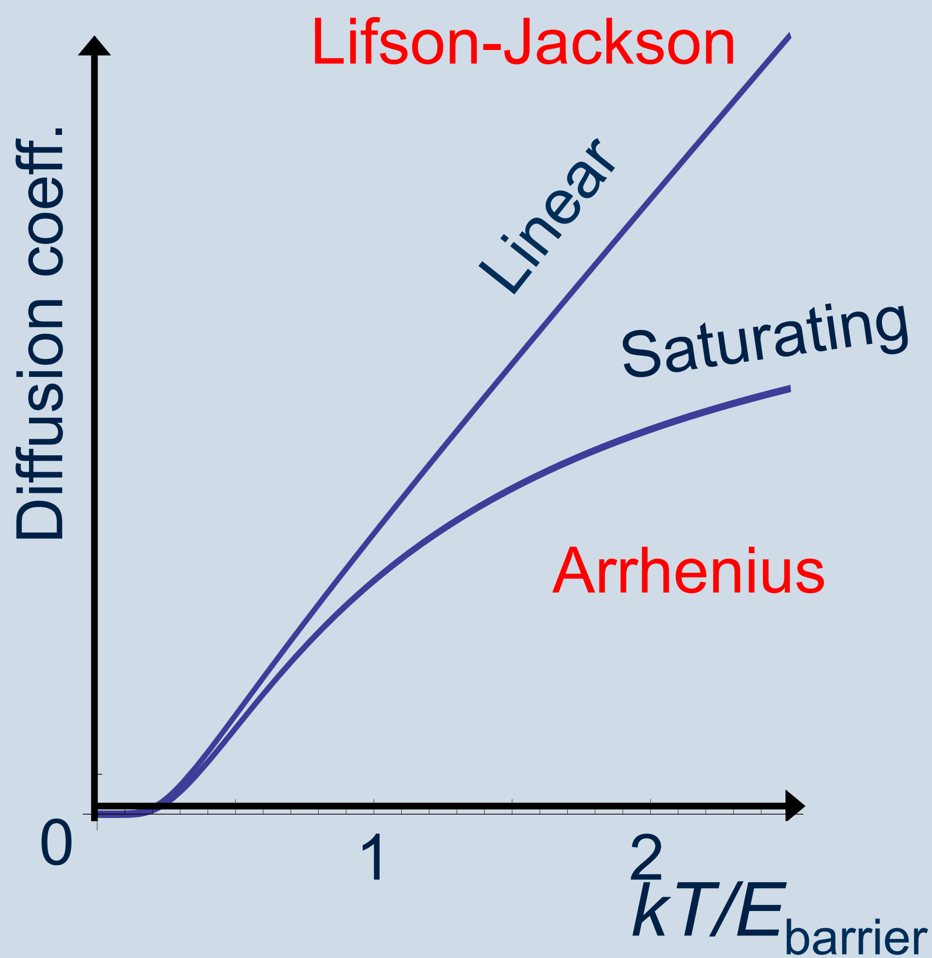
$$D = D_0 \mathrm{e}^{-E_{\mathrm{barrier}}/k_{\mathrm{B}}T}$$

- Assumes *E > kT* – "rare event escapes"
- For crowdions at all but the very lowest temperatures this isn't true
- *Lifson-Jackson* formula for diffusion in a periodic potential:

$$D \propto \frac{k_{\mathrm{B}}T}{\left(\oint \mathrm{e}^{-V/k_{\mathrm{B}}T}\mathrm{d}x\right)\left(\oint \mathrm{e}^{+V/k_{\mathrm{B}}T}\mathrm{d}x\right)}$$

- Reduces to Arrhenius when *E >> kT*
- See *Swinburne at el, PRB 2013, Risken, "The Fokker-Planck Equation"*

Effect for small barriers

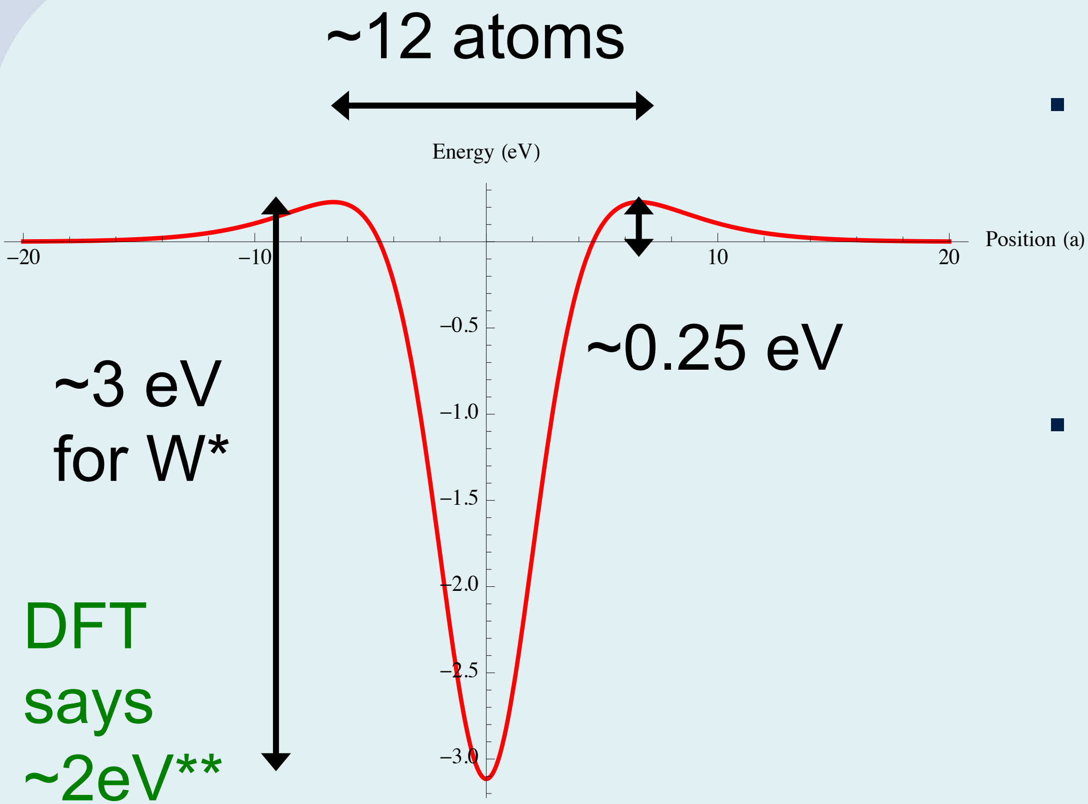


Metal	Group	T_M (K)	E_B/k_B
V	5B	<6	~8
Nb	5B	<6	~0
Ta	5B	<6	~0
Cr	6B	~40	~100
Mo	6B	35	~30
W	6B	27	~30

Ehrhart et al in Landolt-Bornstein 1991 (resistivity recovery)

Swinburne at el, PRB 2013

Crowdion pair potential (W)



- Slight barrier to overcome, but once in the well it will stay there
- *"Ostwald ripening" for loops is difficult*
  - small loops may be absorbed by larger ones, but they won't shrink much by emitting interstitials

$$V(x) = \frac{2V_0}{3\mu}\tanh\left(\frac{\mu x}{2}\right)\left(\frac{\mu x}{2}\operatorname{sech}^2\left(\frac{\mu x}{2}\right) + \tanh\left(\frac{\mu x}{2}\right)\right) - \frac{2V_0}{3\mu}$$

**assumes const μ*

*** Marinica et al JPCM 2013*

SPF, NIMB, 2014

Solutes

- Can generalize Frenkel-Kontorova model by changing one of the atoms in the string
  - change its mass, spring constant, coupling to the periodic potential

- Can derive an analytic potential

- For coupling/spring constant impurity, ie. similar mass (Re,Ta in W for example)

$$V(x) = \Delta V_0 \mathrm{sech}^2 \mu x$$

- ΔV_0 is the difference in the coupling/spring constant (they add)

- Mass impurity is (much) more complicated – future work

Braun and Kivshar, PRB 1991

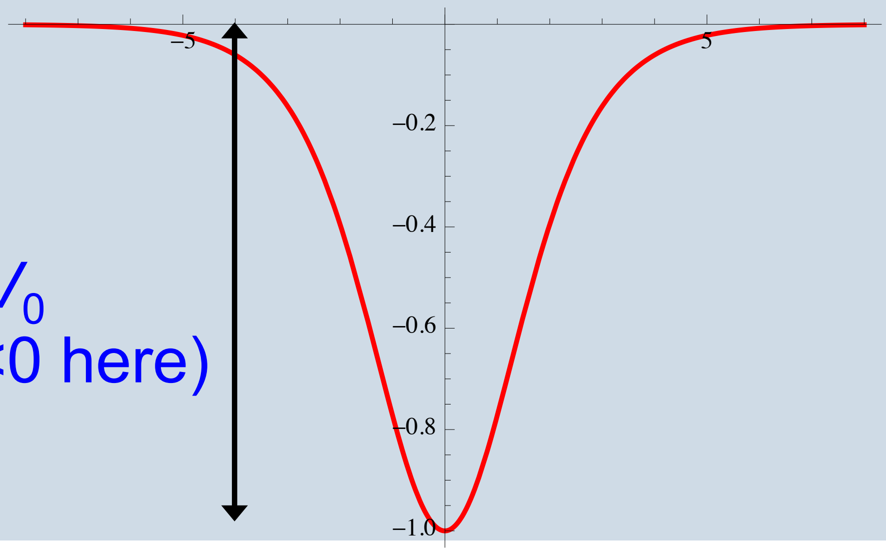
Crowdion dynamics in the FK model

- Few parameters:
  - – lattice spacing a
  - – spring constant β
  - – height of sine potential V_0
  - – mass of atoms m
  - – solute potential ΔV_0

$$\mu^2 = \frac{2V_0\pi^2}{\beta a^4}$$

$$V(x) = \Delta V_0 \operatorname{sech}^2 \mu x$$

ΔV_0
(<0 here)

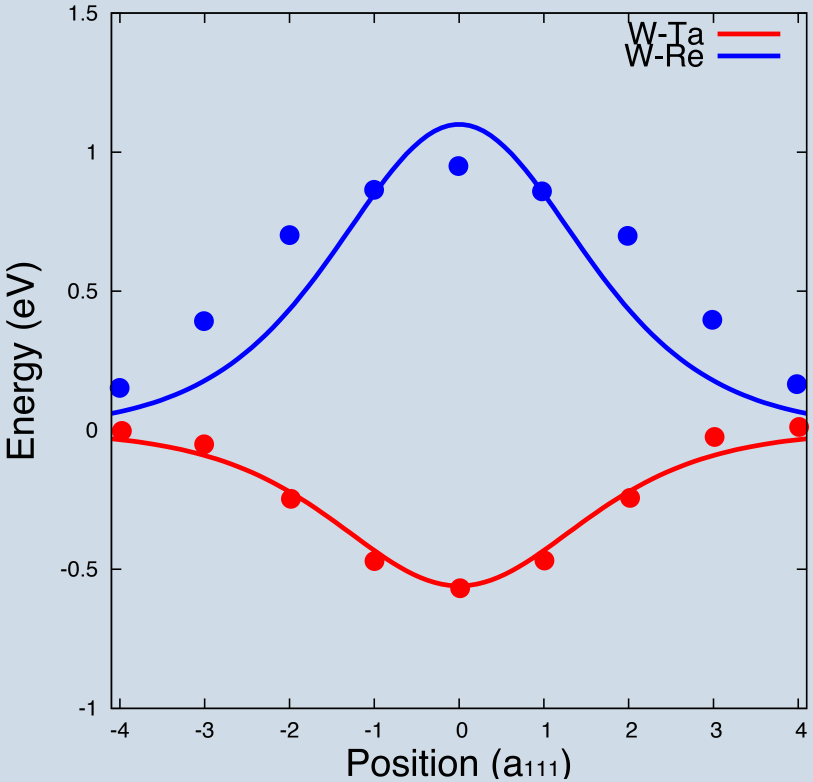


UNIVERSITY OF LEEDS

Fits to (one-parameter, μ fixed) analytic potential

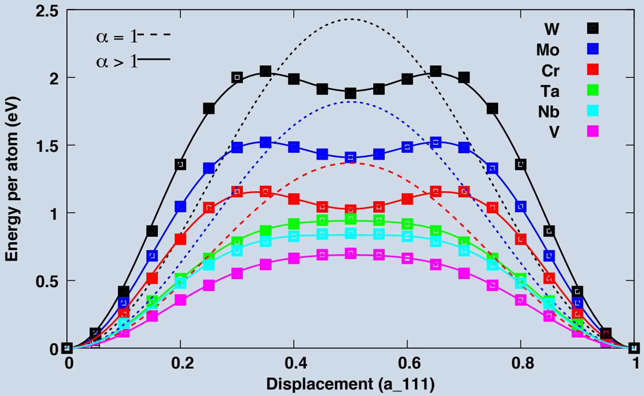
$$V(x) = \Delta V_0 \text{sech}^2 \mu x$$

NB can be attractive or repulsive, inhibits clustering either way



Ta very good, Re less so

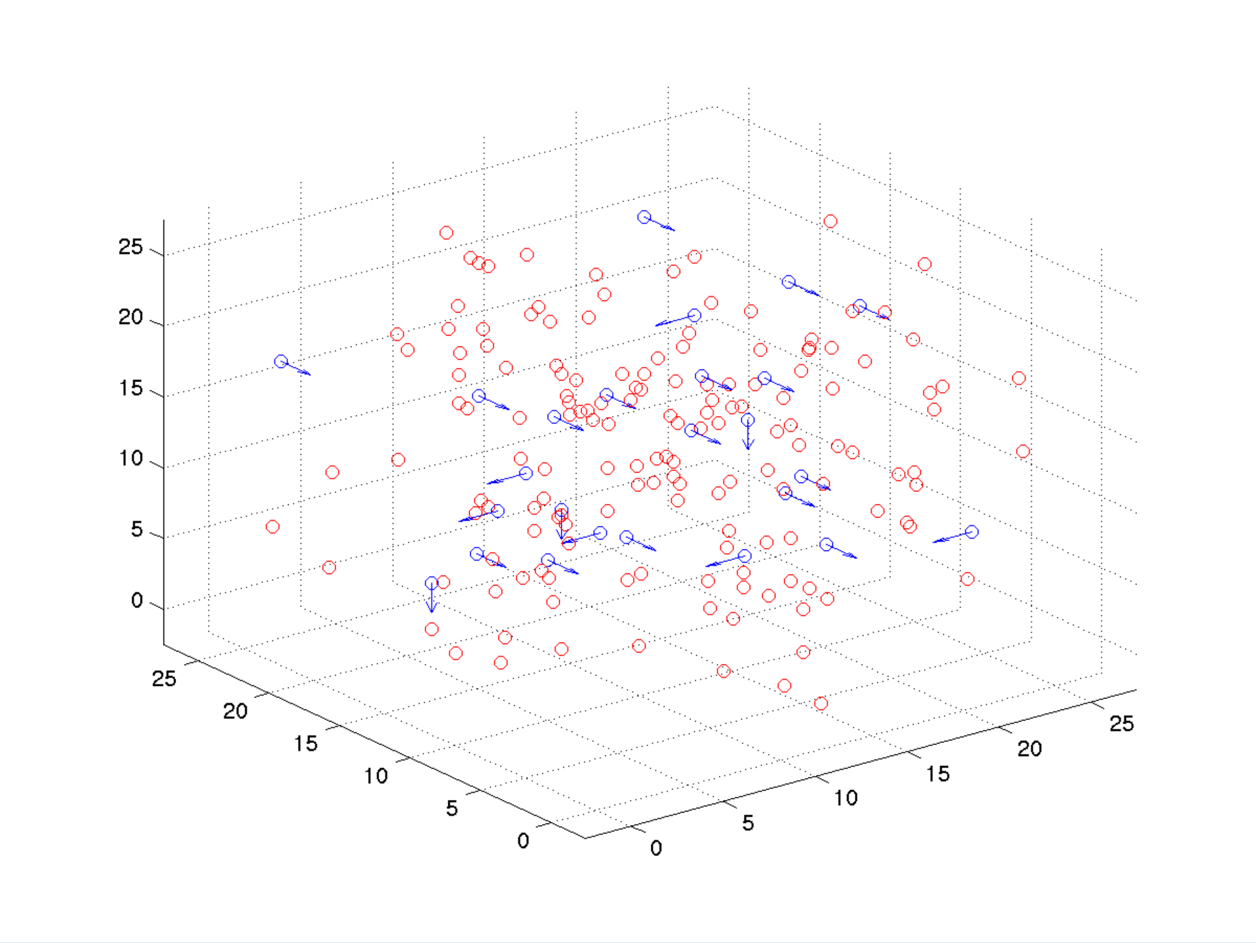
Likely to relate to the double hump lattice potential in W



SPF and Nguyen Manh PRL 2008

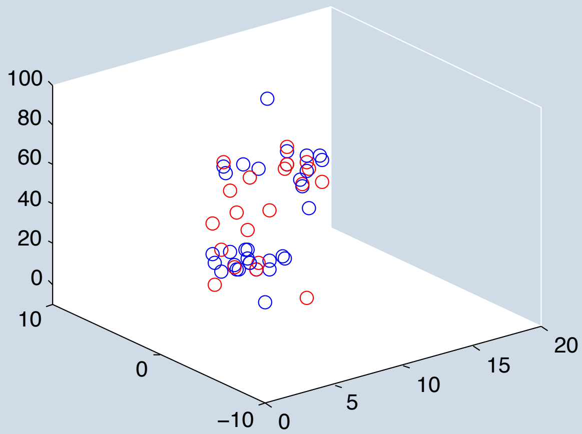
Points from DFT, Muzyk et al PRB 2011

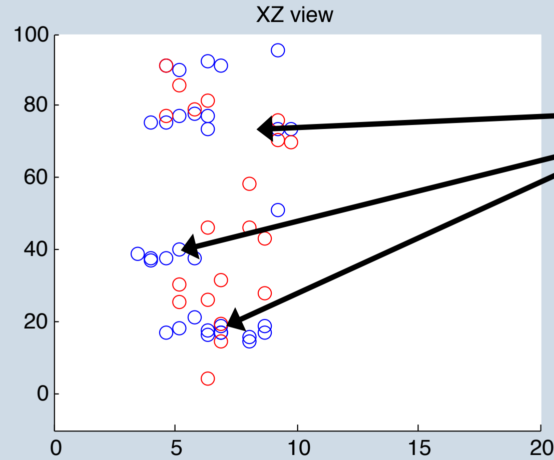
Toy simulations, “Ta in W at 1000K”



SPF, NIMB, 2014

Toy simulations, “Ta in W at 1000K”

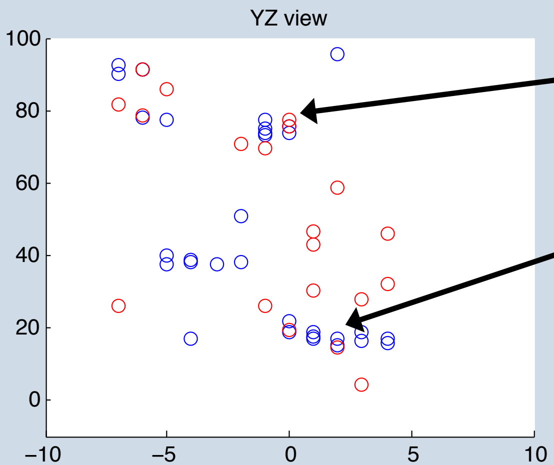




SIA clustering into nascent loops

○ crowdion

○ solute



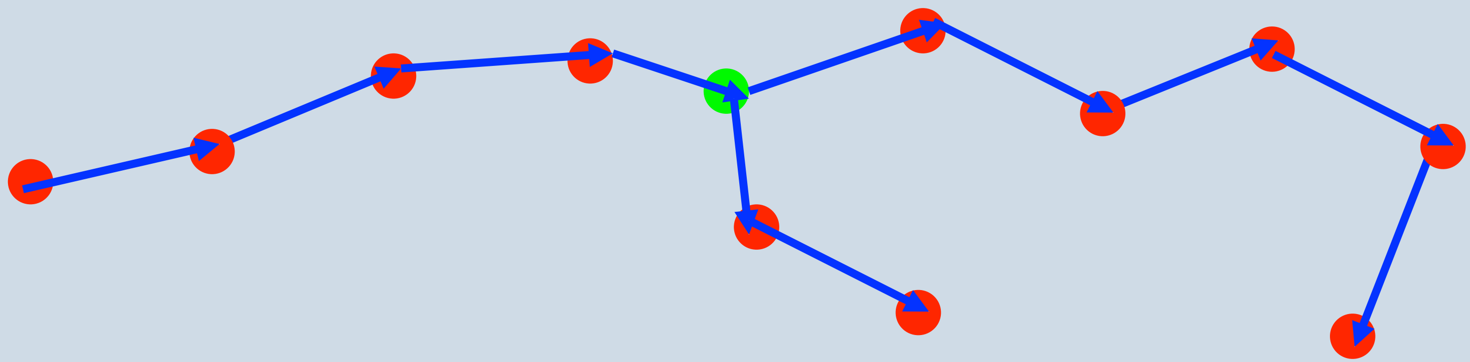
Solute pinning

- Simulations $10^{6\text{-}7}$ times cheaper than MD
- *But*: depends on accuracy of phenomenological model

SPF, NIMB, 2014

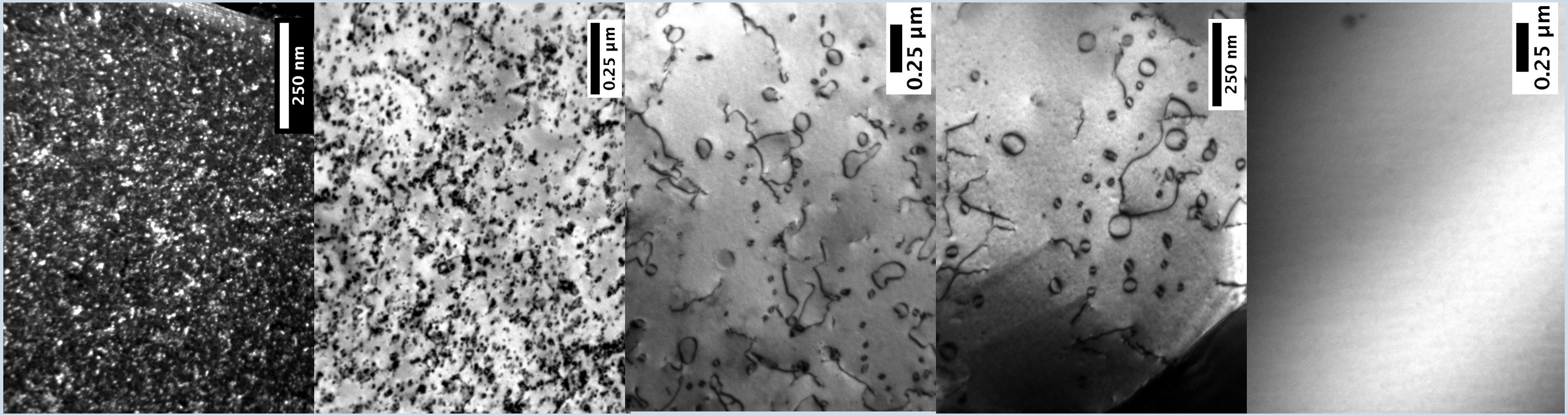
DDD simulations

- PK force calculated on dislocation segments
- Resolved into glide and climb components
- Nodes moved according to *mobility function,* $v_{\mathrm{node}} \propto F_{\mathrm{node}}$



See eg Bulatov & Cai textbook, OUP 2006

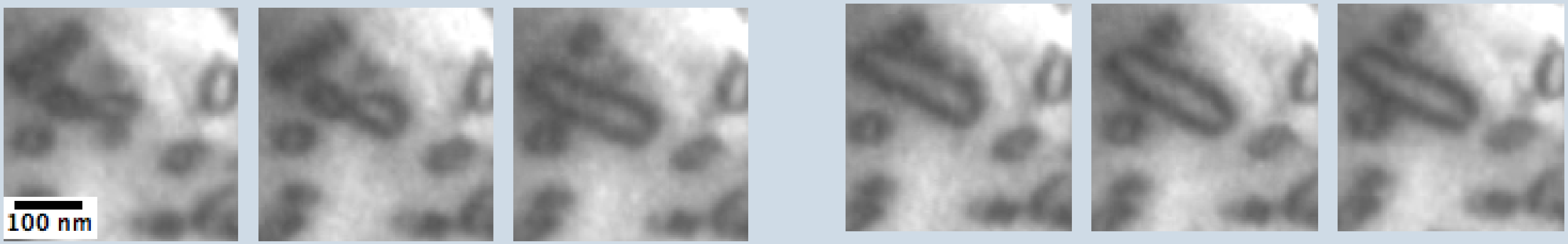
Stochastic effects, elastic forces



500°C 800°C 950°C 1100°C 1400°C

W irradiated to 1.5dpa, 500°C, 2Mev W+. 1 hour anneals
F Ferroni, P Edmondson, SPF et al submitted 2014

Loop coalescence at 1000°C



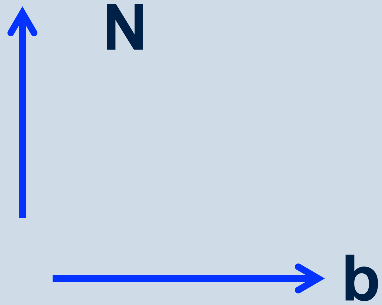
(h) t=0 (i) t=10 (j) t=34 (k) t=35 (l) t=36 (m) t=42

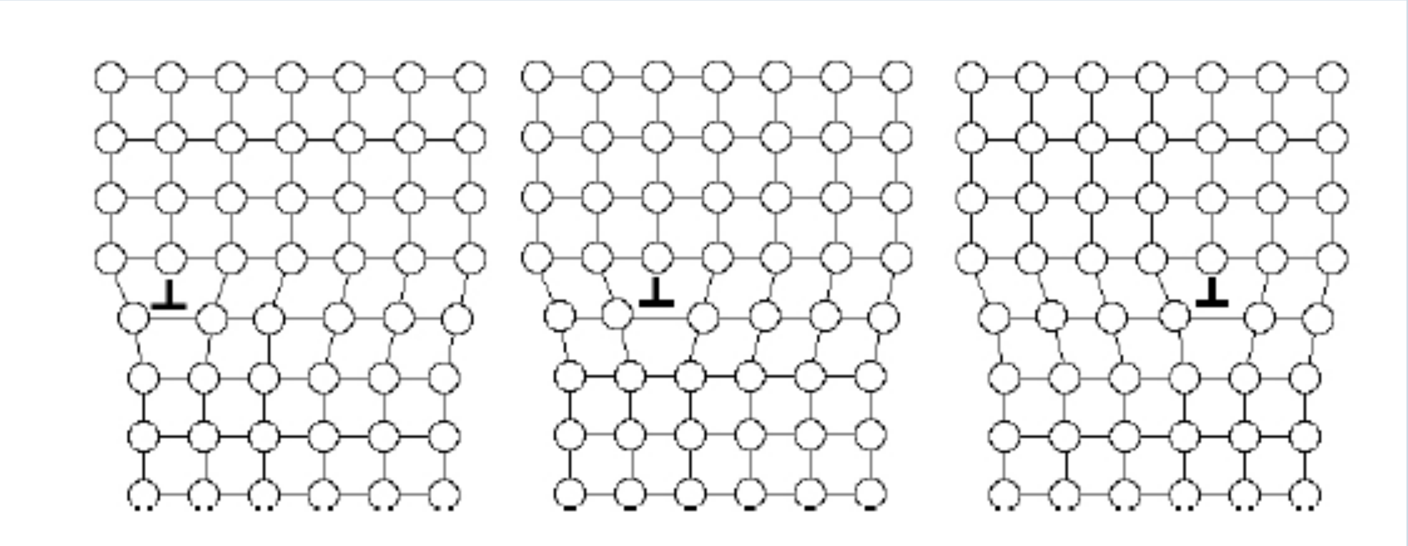
- Damage loops coarsen and coalesce
- “Finger loops” form, lead to network dislocations
- loops escape to foil surface

- Stochastic effects anneal out damage, need stochastic dynamics to quantify

F Ferroni, SPF et al submitted 2014; see also work of Jenkins, Yao, Kirk et al

Glide

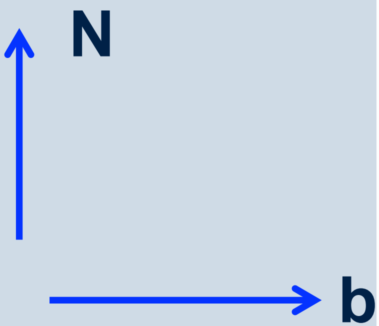




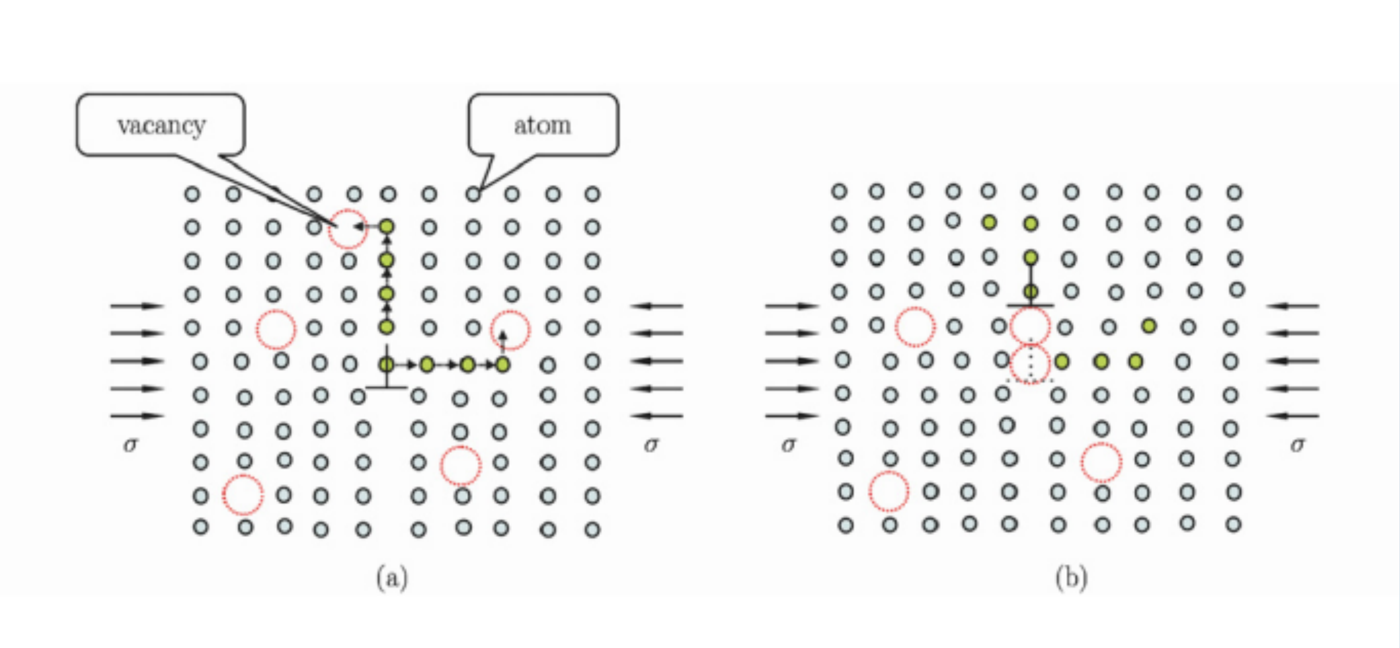
- Motion confined to glide plane
- Relatively easy, bonds break and re-form
- Above very low temperatures and applied stresses, weakly dependent on temperature

Hirth and Lothe

Climb



Gao and Cocks



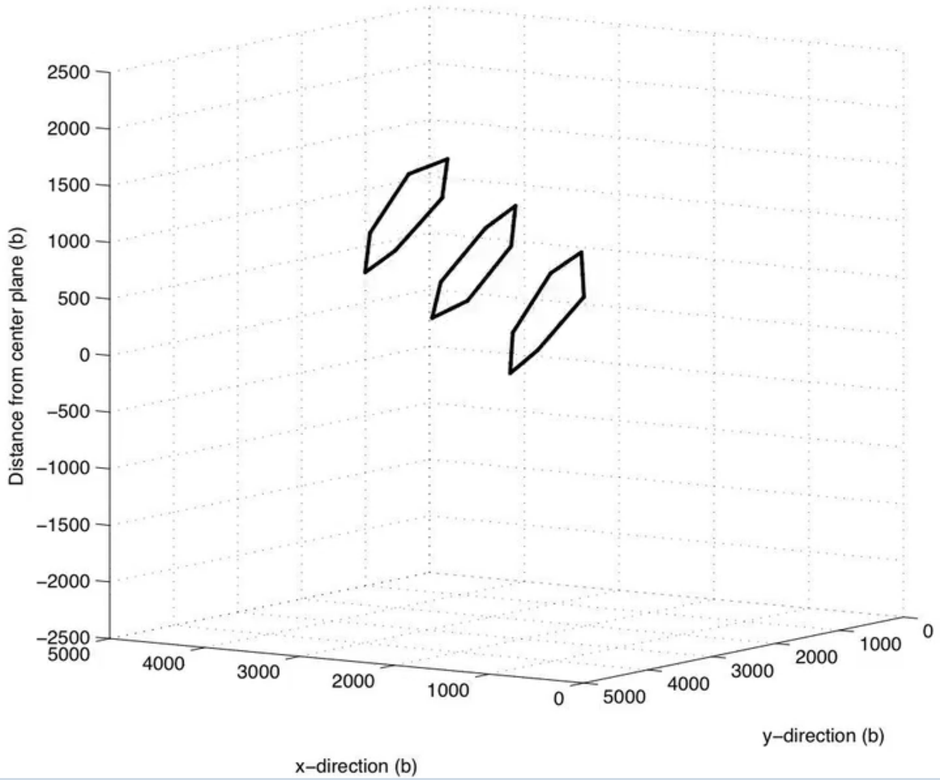
- Motion *out of the glide plane* (edge cpts only)
- Requires diffusion of point defects to and around dislocation core
- Strongly temperature dependent (via vacancy concentration and diffusivity)

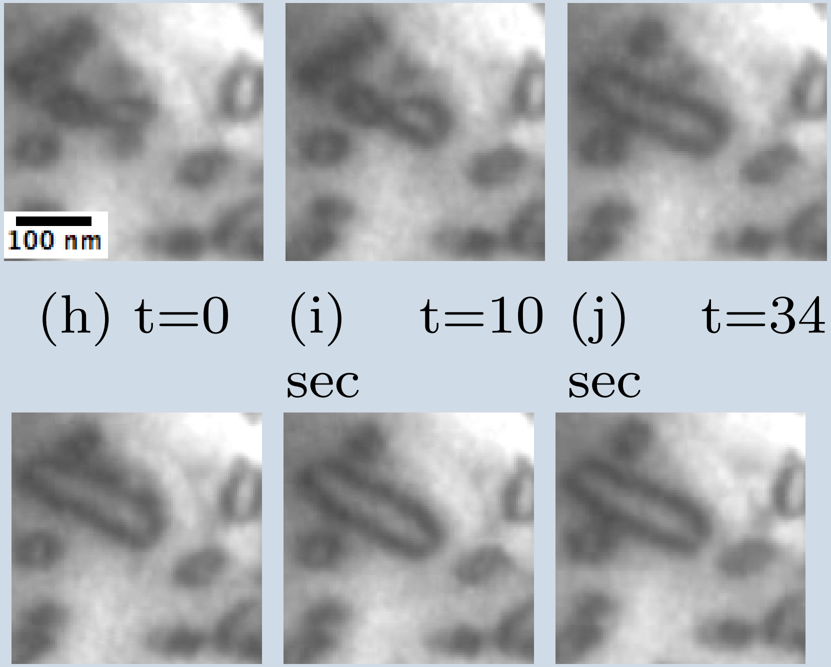
Fluctuations and dissipation for extended objects

- Dislocation drag/friction/dissipation well established
- Overdamped dynamics observed in TEM *(see eg Caillard Acta 2010)*
- Edge drag << screw drag << climb* drag
- Strong temperature dependence, esp climb
- What about fluctuations at high temperatures?
- What does the FDT look like?

**this is “mean field”, no resolution of individual vacancies*

Stochastic DDD simulations



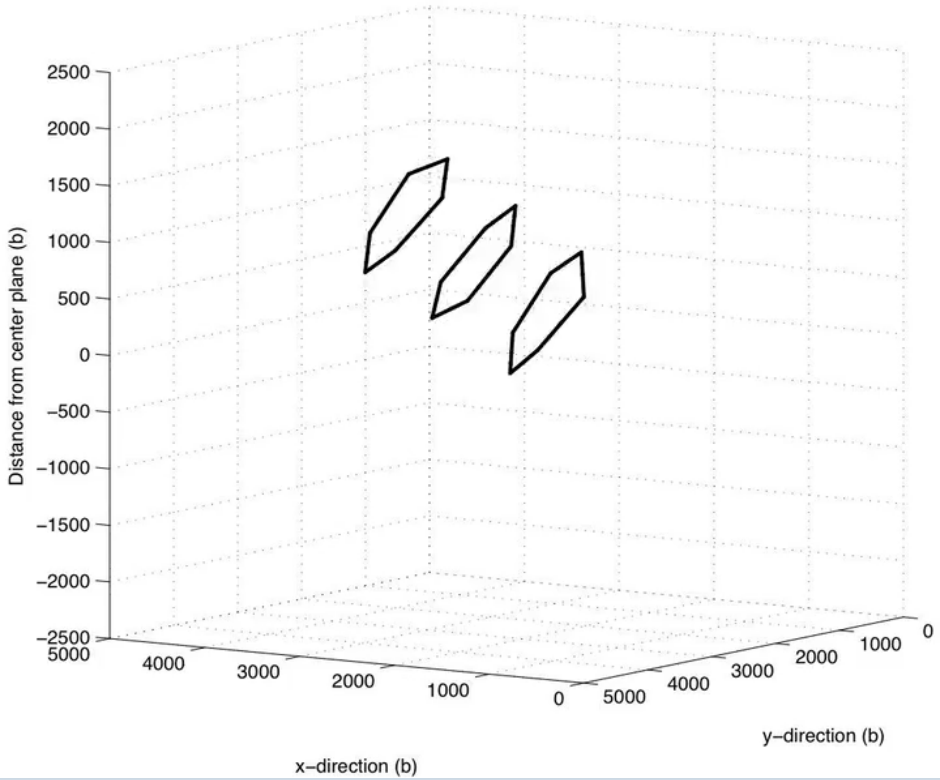


(h) t=0 (i) t=10 sec (j) t=34 sec

(k) t=35 sec (l) t=36 sec (m) t=42 sec

F Ferroni, SPF

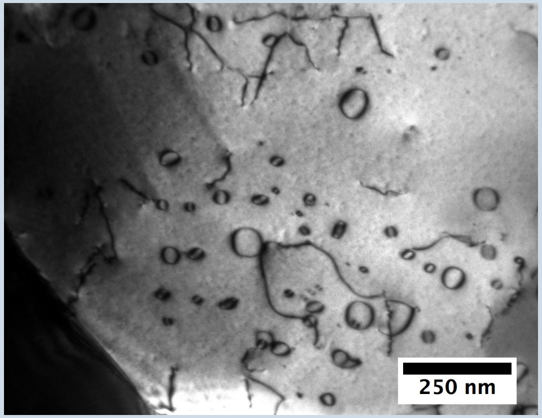
Stochastic DDD simulations



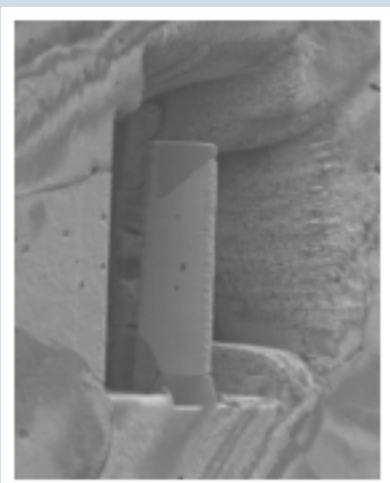
F Ferroni, SPF

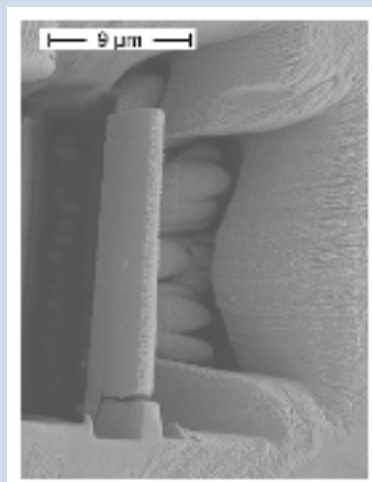
- Fast glide to form loop chains
- Slower climb & fluctuations form finger loop
- Finger loop then diffuses along glide prism
- *NB stochastic motion of loops also treated by Dudarev, Derlet et al JNM 2014*
- *Treated loops as interacting particles – collective coordinates again*
- *Captured chain formation but not coalescence*

DDD simulations of experiments



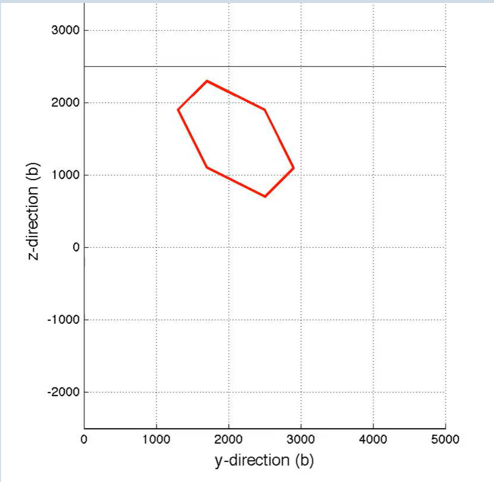
F Ferroni, SPF et al



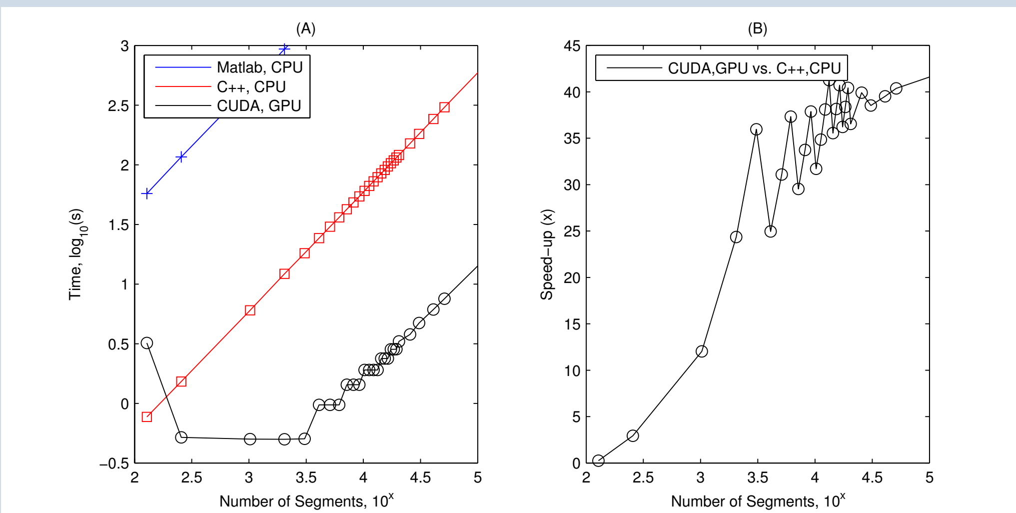


D Armstrong, S Roberts et al

- TEM foils are thin
  - loop loss to surface due to image forces
- Microcantilever mech. prop. experiments
  - size effect, disl. starvation etc
  - large body of work on this
- Need to treat free surfaces
  - spectral method for thin films
  - need FEM for 3D geometry



- Thin films: can use spectral method for images *(Weinberger, Aubry,… Cai 2009)*
- Also need virtual segments to correctly model escape-to-surface



- Use GPU code to accelerate
- 50x speed-up

Ferroni, Tarleton, SPF, MSMSE 2014, J Comp Phys 2014

GPU acceleration

NVIDIA Titan Black ~£1000

GPU acceleration

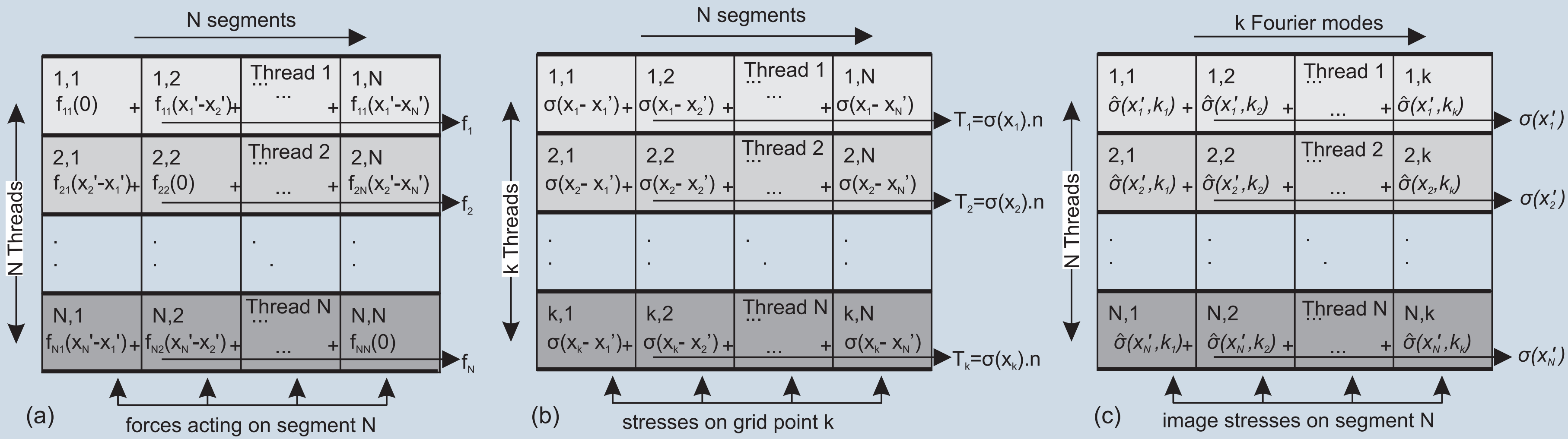
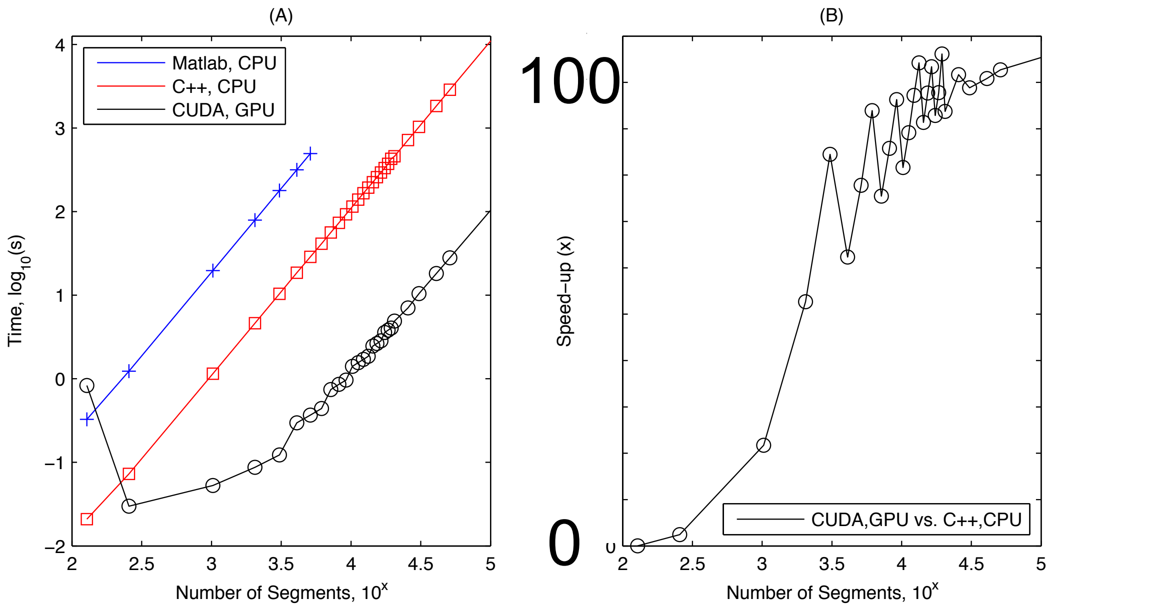


Figure 1: Parallelism of the N^2 segment interactions (a), surface traction at k grid points (b) and image stress on N segments (c).

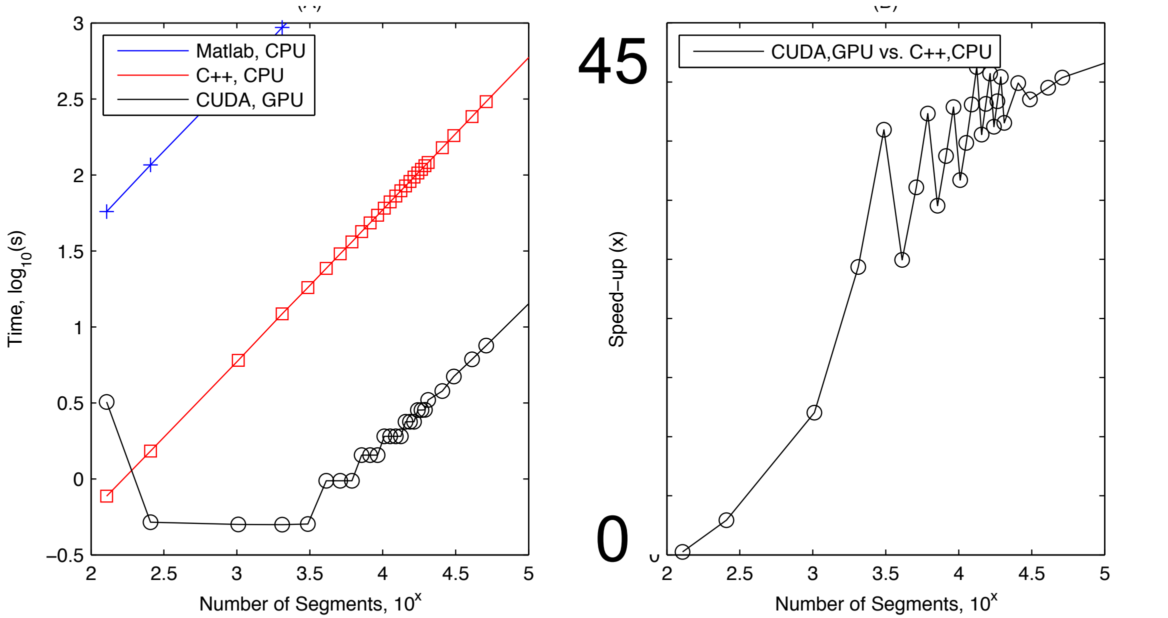
- Thin films, eg TEM foils: can use spectral method for images *(Weinberger, Aubry,… Cai 2009); more complex geometries need FEM, see Ed's talk*
- Also need virtual segments to correctly model escape-to-surface
  - Use GPU code to accelerate
  - >50x speed-up

Ferroni, Tarleton, SPF, MSMSE 2014, J Comp Phys 2014

GPU acceleration

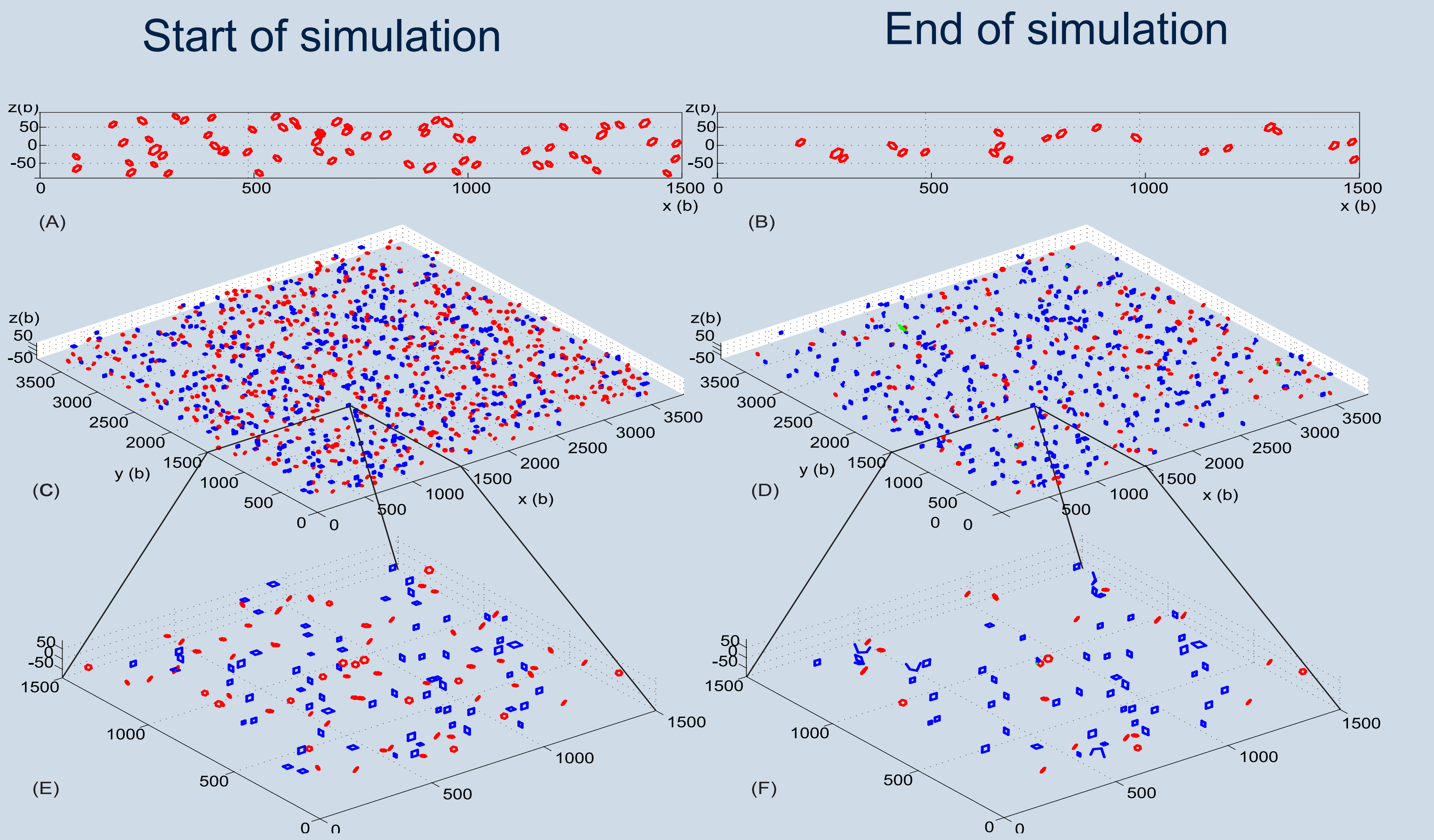


CUDA speed-up vs # of segments (seg-seg force calcs)

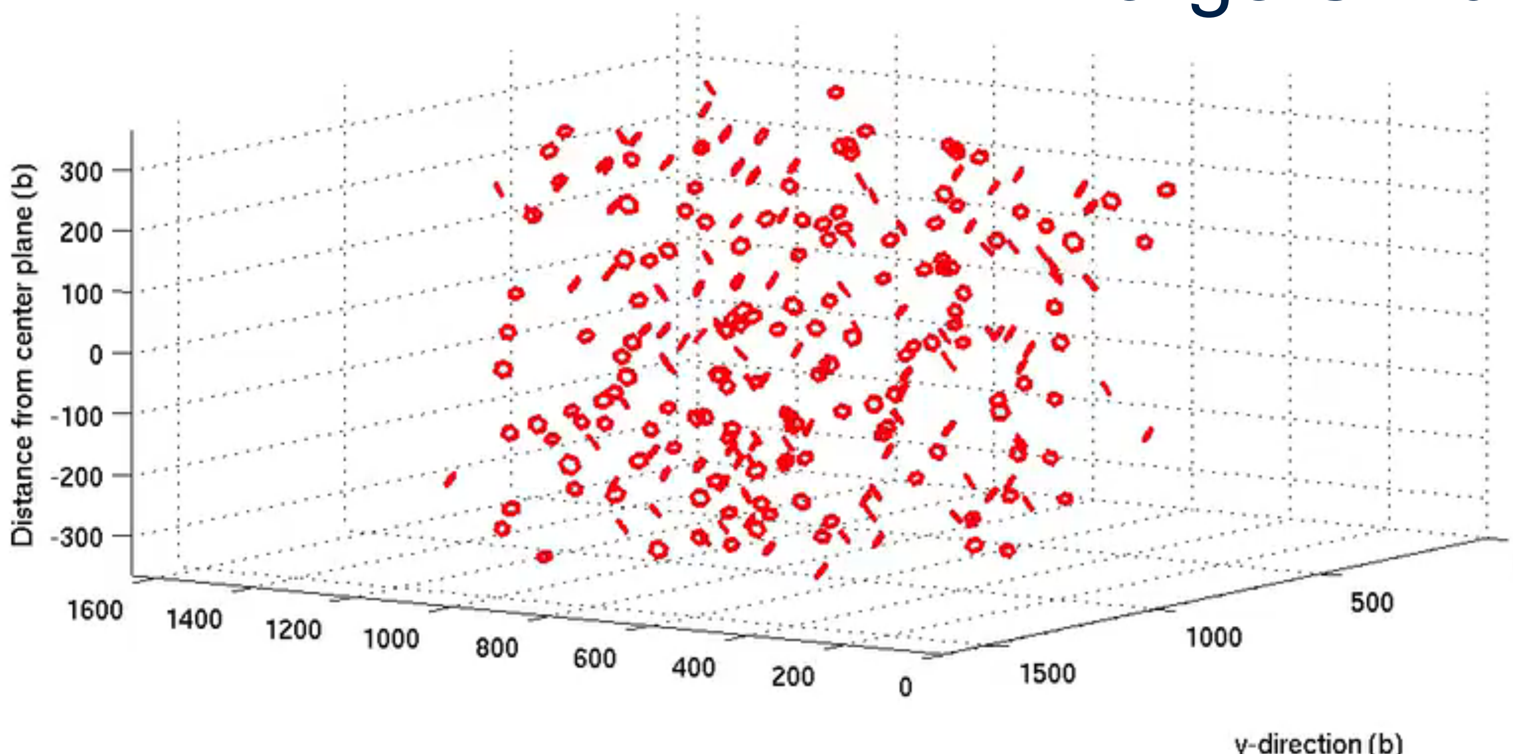


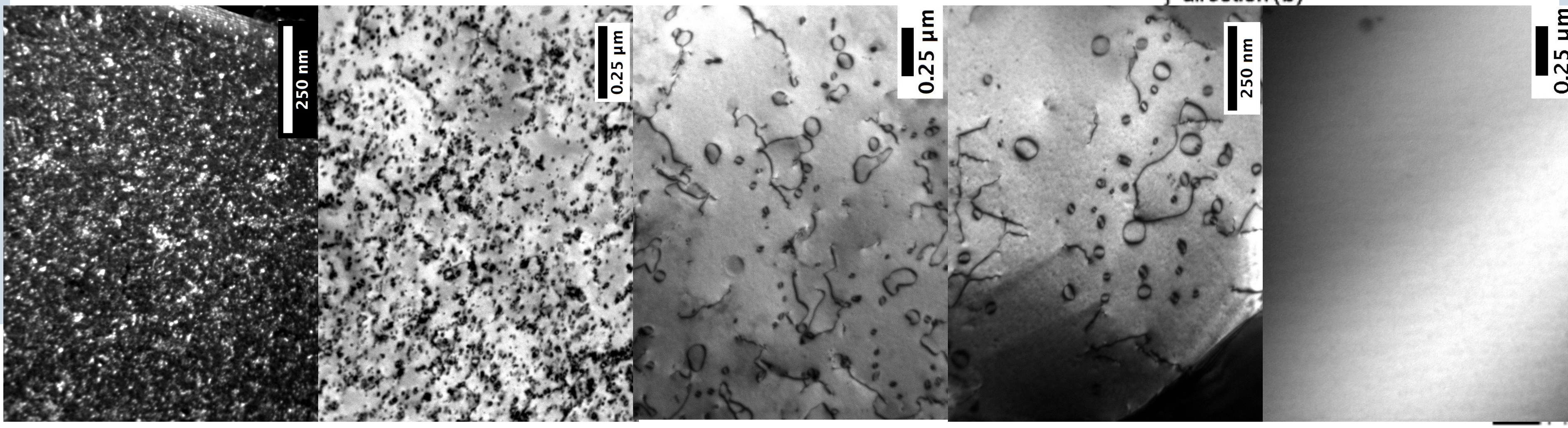
CUDA speed-up vs # of segments (image stress calcs)

Large Simulations



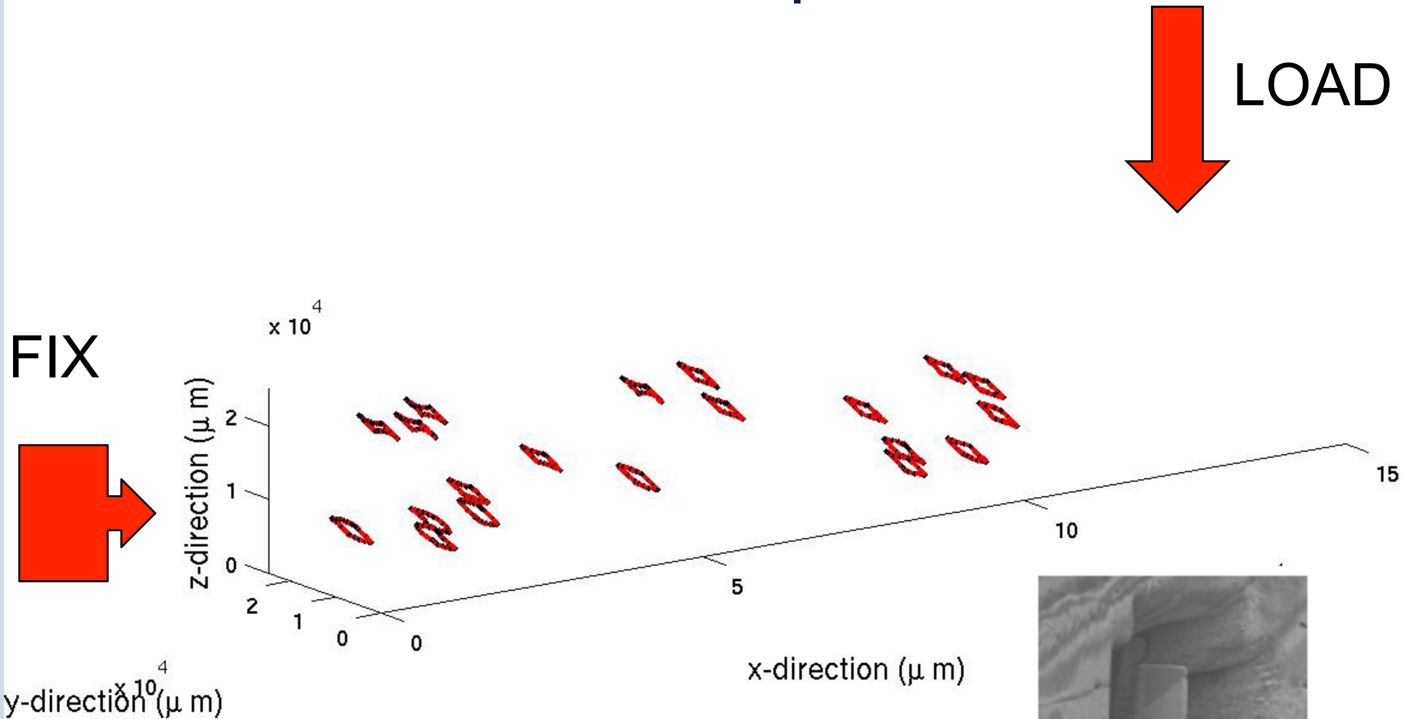
Large Simulations

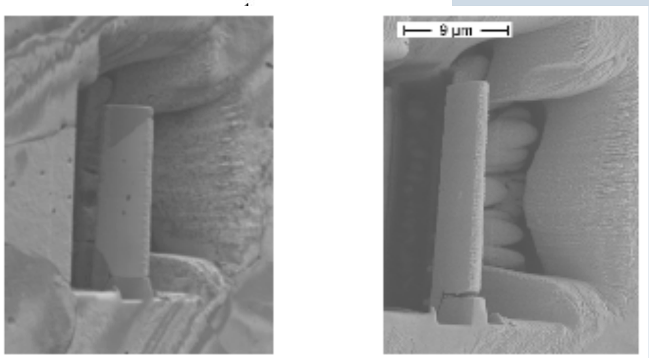




F Ferroni, SPF 2015

DDD simulations of experiments





Tarleton, Ferroni, SPF 2015

3D geometries require FEM coupling *(see also Tang, Marian, Arsenlis; Fivel et al)*

Nonlinear dislocation response

- Dislocation statics well-understood within elasticity theory
- Dynamics far less well understood
- Strongly nonlinear temperature and strain rate dependence

At low T, $v \sim \sigma^{20\text{-}40}$, at RT $v \sim \sigma^4$

See eg. Nadgornyi Prog Mater Sci 1988
Christian and Altschuler 1967
Turner and Veeland 1970

- Atomistic modelling restricted to short times and extremely high strain rates
- Discrete dislocation simulations have far greater scope, but require phenomenological input -- sometimes highly speculative, eg:

$$\text{velocity} = \boldsymbol{v} = \boldsymbol{B} \cdot \boldsymbol{\sigma} = \text{const. drag matrix} \otimes \text{stress}$$

Dislocation velocities

- Dislocation velocities measured by slip band growth technique
- Iron single crystals
- NB: caution, log-log plot!
- *Turner and Vreeland, Acta Met. 1970*

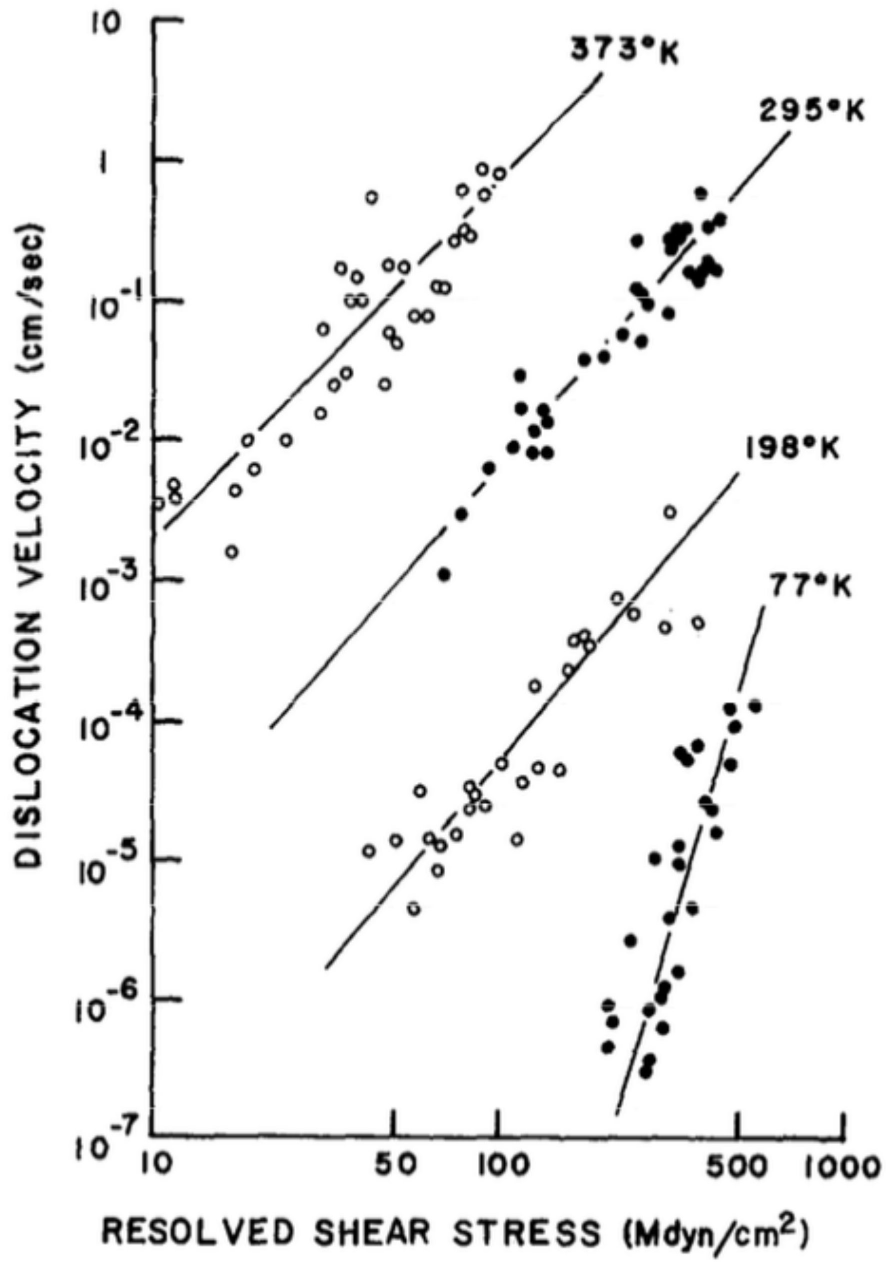
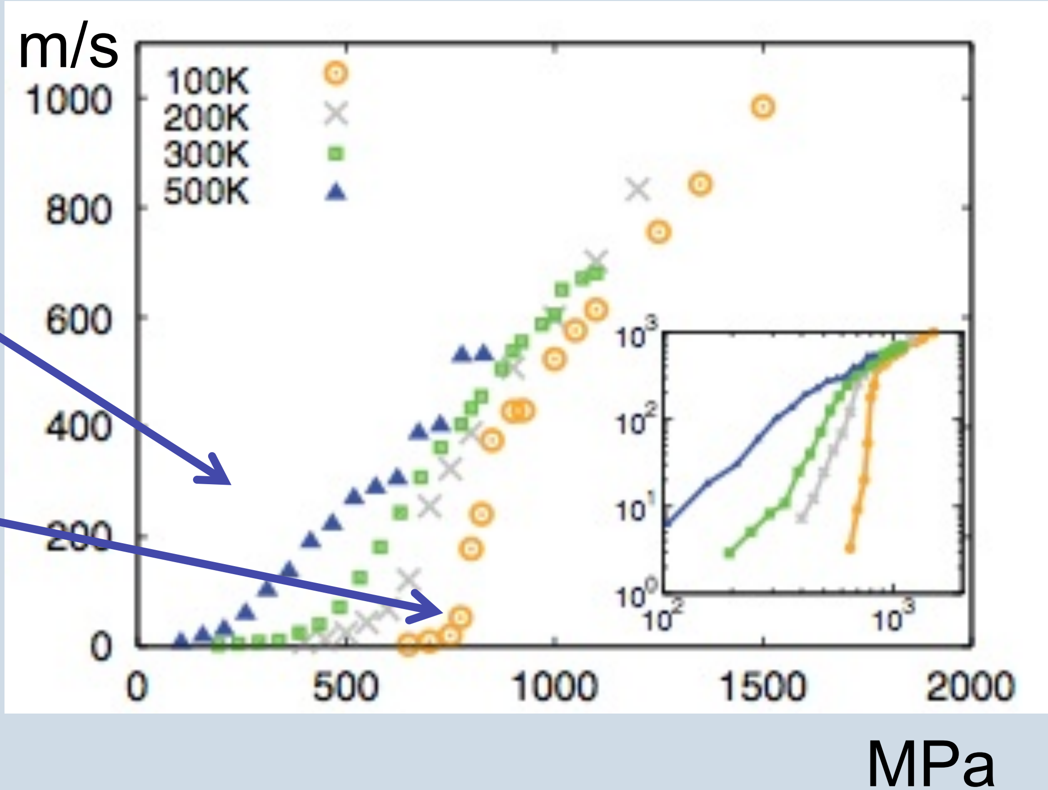


FIG. 7. Velocity of edge dislocations in iron single crystals as a function of resolved shear stress for several temperatures.

MD simulations of dislocation motion

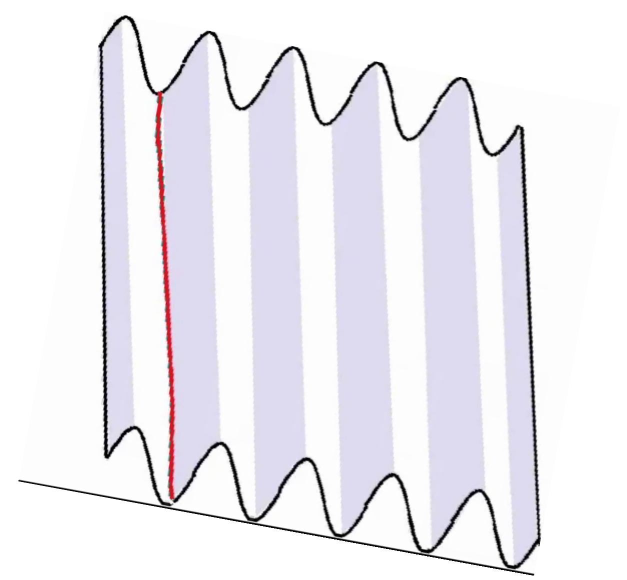
- Note nonlinearity at low stresses
- Most pronounced at lowest temperatures
- Linear results at higher stresses suggest kink nucleation no longer governing the motion

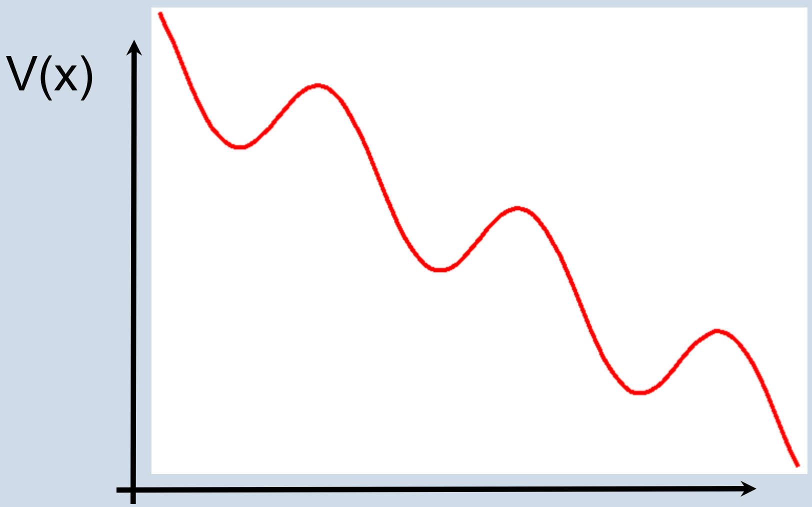


Gilbert, Queyreau, Marian PRB 2011

Kinks

- Dislocation motion appears overdamped
  - *in situ* straining experiments, dislocations stop immediately the stress is removed
- Dislocations move through "washboard" Peierls potential
- Generally accepted that this is mediated by nucleation and propagation of kinks*
- Tilt is the applied force





*See e.g. Seeger and Schiller, Hirth and Lothe, Joos and Duesbery, many others since

Kinks

- Rate of kink pair nucleation and/or propagation controls dislocation's velocity *out of equilibrium*
- Sounds simple – but it isn't.
- Experimental measurement difficult, extremely sensitive to impurities
- Guess: velocity ~ exp [$-(H_{KP} - \sigma^* V)/kT$] *Arrhenius behaviour*
  - H_{KP} is the kink pair elastic energy, ~ few eV
  - σ is the applied stress
  - V is "activation volume" ~ few $|\boldsymbol{b}|^3$
  - leads to temperature-dependent activation energy fits
- May work for high stresses, low temperatures, but not good for low stresses close to Peierls stress – creep, fracture
- Quantum effects can be important at low temperatures.

See for example Petukhov and Pokrovskii Soviet JETP 1973; Tarleton et al, Acta Mat 2008; Proville, Rodney, Marinica Nature Mat 2012

Fluctuation – dissipation theorem

$$\gamma D = k_B T$$

FDT

$$D = \frac{k_B T}{\gamma}$$

$$\mathcal{P}[\eta] \sim \mathrm{e}^{-\frac{1}{4D}\int \eta^2 \mathrm{d}t}$$

Probability distribution for Gaussian white noise (other types of noise are available!). This is the "D" in diffusion/ Fokker-Planck equation:

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2}$$

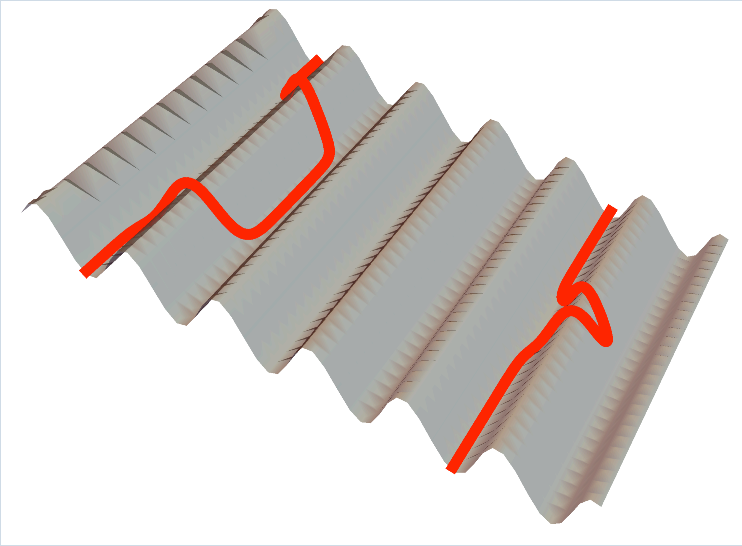
- Relates damping, fluctuations and temperature
- At low temperature and high damping, fluctuations are small
- Not so at high *T*…

Stochastic equation of motion

- Start from the Frenkel-Kontorova model/sine-Gordon equation:

$$\mathcal{L} = \frac{1}{2}\phi_t^2 - \frac{1}{2}\beta\phi_x^2 - V_0 \sin^2 \pi\phi$$

$$\rho\phi_{tt} - \beta\phi_{xx} = -V_0\pi \sin 2\pi\phi$$



- Leads to kink solutions:

$$\phi(x,t) = \frac{2}{\pi}\tan^{-1}\exp\mu(x - Vt)$$

- μ is the inverse kink width ~ (LH / RH kinks)

$$\pm\sqrt{2V_0\pi^2/\beta}$$

$$\Gamma\phi_t = \beta\phi_{xx} - V_0\pi\sin 2\pi\phi - F + \xi(x,t) = -\frac{\delta\mathcal{H}}{\delta\phi} + \xi(x,t)$$

- Add friction, driving force, random force, neglect inertia (overdamped limit) gives *Langevin equation*

- *H* is the string Hamiltonian or *energy:*

$$\mathcal{H}[\phi] = \int_{-\infty}^{\infty} \left(\frac{1}{2}\beta\phi_x^2 + V(\phi) \right) \mathrm{d}x$$

- Integral of elastic (first term) plus potential (second term)

$$V(\phi) = V_0 \sin^2 \pi\phi - F\phi$$

- Simplest option for the noise is uncorrelated Gaussian white noise, with correlation function

$$\langle \xi(x,t)\xi(x',t')\rangle = 2D\delta(x-x')\delta(t-t')$$

- and distribution $$\mathcal{P}[\xi] \propto \exp -\frac{1}{4D}\int\int \xi(x,t)^2 \mathrm{d}x\mathrm{d}t$$

- D is the noise strength and $D = \Gamma k_B T$ by the fluctuation-dissipation theorem

- Rearrange Langevin equation to $$\Gamma\phi_t + \frac{\delta\mathcal{H}}{\delta\phi} = \xi(x,t)$$

- Substitute for ξ leads to …

$$\mathcal{P}[\phi] \propto \exp -\frac{1}{4D}\int\int\left(\Gamma\phi_t + \frac{\delta\mathcal{H}}{\delta\phi}\right)^2 \mathrm{d}x\mathrm{d}t$$

$$\equiv \exp -\frac{1}{4D}\mathcal{S}[\phi]$$

← *Onsager-Machlup action S*

- Distribution for *φ(x,t)* ! (I have glossed over some details here)
- Rate of transition from metastable well to stable one given by:

$$\sum_{\text{paths }\phi_i} \mathrm{e}^{-\mathcal{S}[\phi_i]/4D} = \int \mathcal{D}\phi\,\mathrm{e}^{-\int(\Gamma\phi_t - \beta\phi_{xx} + V'(\phi))^2/4D}$$

- where the sum/integral is taken over all configurations *φ* that satisfy the initial and final conditions

$$\int \mathcal{D}\phi\, \mathrm{e}^{-\int (\Gamma\phi_t - \beta\phi_{xx} + V'(\phi))^2/4D}$$

- This object is possibly infinite, and is awkward to define rigorously
- It is the stat. mech. analogue of the Feynman path integral for the quantum mech. matrix element
- The integrand $\left(\Gamma\phi_t + \frac{\delta\mathcal{H}}{\delta\phi}\right)^2$ is the analogue of the *Lagrangian*
- In the weak noise limit, the integral will be dominated by *φ*s which satisfy the Euler-Lagrange equations

$$\left(\Gamma\partial_t + \beta\partial_x^2 - V''(\phi)\right)\left(\Gamma\phi_t - \beta\phi_{xx} + V'(\phi)\right) = 0$$

$$V(\phi) = V_0 \sin^2 \pi\phi - F\phi$$

$$\left(\Gamma\partial_t + \beta\partial_x^2 - V''(\phi)\right)\left(\Gamma\phi_t - \beta\phi_{xx} + V'(\phi)\right) = 0$$

- Two solutions: ϕ^- satisfying $\Gamma\phi_t^- - \beta\phi_{xx}^- + V'(\phi^-) = 0$
- (noiseless equation of motion)
- ϕ^+ satisfying $\Gamma\phi_t^+ + \beta\phi_{xx}^+ - V'(\phi^+) = 0$
- Like the noiseless equation of motion, but with the potential flipped
- Motion *against the barrier* – controls the escape rate, and hence the kink pair nucleation rate.
- cf *instantons* in quantum field theory *(G t'Hooft, S Coleman, …)*

Bray et al, PRB 1990

- KP nucleation rate given by

$$\exp -\frac{\mathcal{S}[\phi^+]}{4D}$$

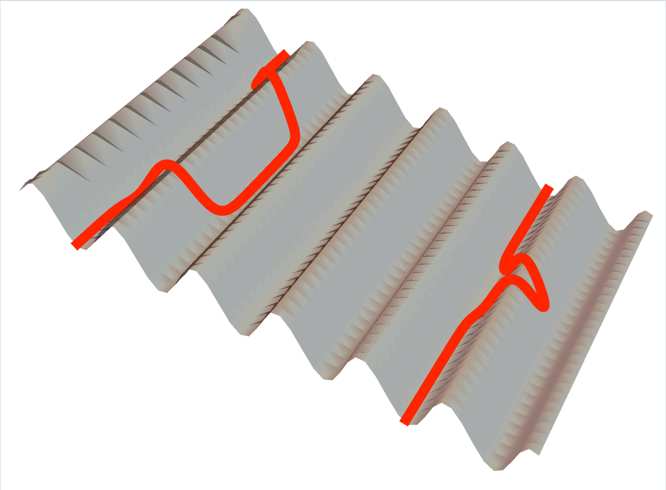
- But what is ϕ^+ ? Do we need to solve that horrible equation to find it?

- Luckily no:

$$\begin{aligned}\mathcal{S}^+ &= \int \mathrm{d}t \int \mathrm{d}x \left(2\Gamma\phi_t^+\right)^2 \\ &= 4\Gamma \int \mathrm{d}x \int_{\mathrm{min}}^{\mathrm{saddle}} \mathrm{d}\phi^+ \frac{\delta\mathcal{H}}{\delta\phi^+} \\ &= 4\Gamma \left(\mathcal{H}[\phi^+_{\mathrm{saddle}}] - \mathcal{H}[\phi^+_{\mathrm{min}}]\right) .\end{aligned}$$

- *S*$^+$ is the saddle point action, max energy configuration

- cf particle escaping from a well



At low F, it will be a well-separated kink pair, at high F it will be a small bump

Bray et al 1990

- For the saddle, need to find φ that maximizes

$$\mathcal{H}[\phi] = \int_{-\infty}^{\infty} \left(\frac{1}{2}\beta\phi_x^2 + V(\phi) \right) \mathrm{d}x$$

- Use Euler-Lagrange equations for *H[φ]*

$$\beta\phi_{xx} = +V'(\phi); \quad \frac{1}{2}\beta\phi_x^2 = V(\phi); \quad \beta\phi_x = \pm\sqrt{2\beta V(\phi)}.$$

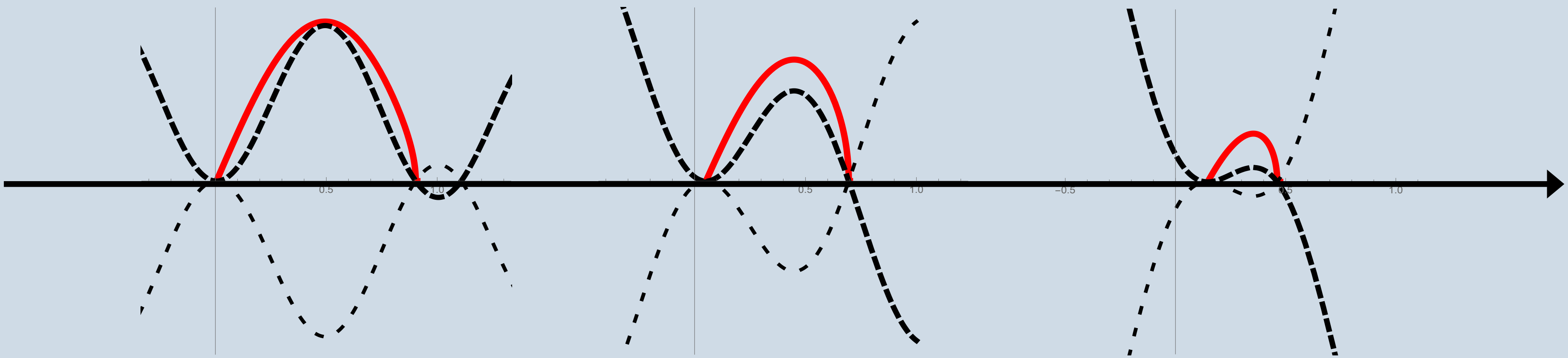
- which lets us write

$$\begin{aligned} \mathcal{H}^* &= \int_{-\infty}^{\infty} \left(\frac{1}{2}\beta\phi_x^2 + V(\phi) \right) \mathrm{d}x = \int_{-\infty}^{\infty} \beta\phi_x \frac{\mathrm{d}\phi}{\mathrm{d}x} \mathrm{d}x \\ &= 2 \int_{\phi_0}^{\phi_1} \sqrt{2\beta V(\phi)} \mathrm{d}\phi. \end{aligned}$$

- and finally velocity ~

$$\exp -\frac{\mathcal{S}[\phi^+]}{4D} = \exp -\frac{\mathcal{H}^*}{k_B T} = \exp -\frac{2}{k_B T}\int_{\phi_0}^{\phi_1}\sqrt{2\beta V(\phi)}\mathrm{d}\phi$$

- Integrals taken between two zeros of *V;* area under red curves
- Exact as far as potential concerned, works for $0 < F < \sigma_P$



- *F* small *F* medium *F* large

SPF, Scientific Reports 2016

- A simple formula velocity = fct. (stress) would be nice for eg implementation in DDD simulations.

- At small stresses, saddle configuration should be a well-separated kink pair:

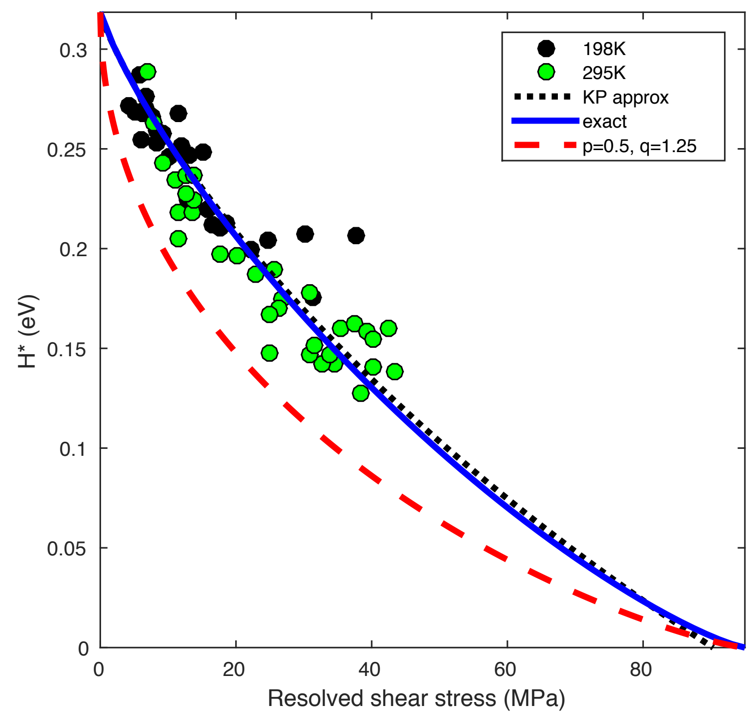
$$\phi = \frac{2}{\pi}\tan^{-1} e^{-\mu(x-R/2)} + \frac{2}{\pi}\tan^{-1} e^{\mu(x+R/2)} - 1$$

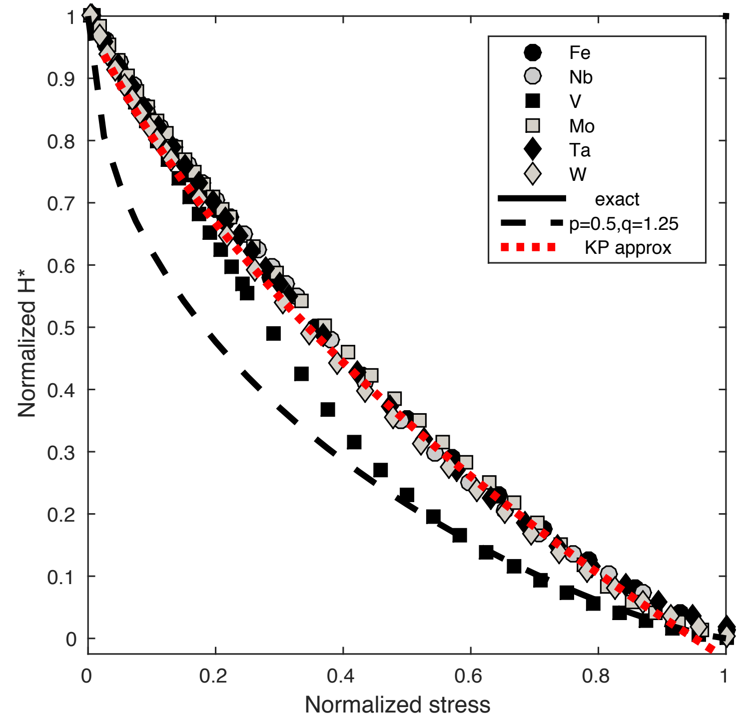
- Insert this in *H*, maximize over *R*, gives

$$\mathcal{H}^*_{\mathrm{KP}} = \sqrt{\frac{\beta V_0}{2\pi^2}}\left(8 - \mathcal{F} - \mathcal{F}\ln\left(\frac{16}{\mathcal{F}}\right)\right) \qquad \mathcal{F} = F/V_0$$

- This is where the wild nonlinearity comes from: $\exp -\frac{\mathcal{H}^*}{k_B T}$

has no power series at small *F*.





- Left: exact formula (red) and KP approximation (black dashed) fitted to *H** extracted from data for edge dislocation velocities in Fe *(Turner and Vreeland 1970)*
- Right: DFT-based calculation for some bcc metals of *H** *(Dezerald et al 2015)*

Dashed line: $\left(1-(F/V_0)^{0.5}\right)^{1.25}$

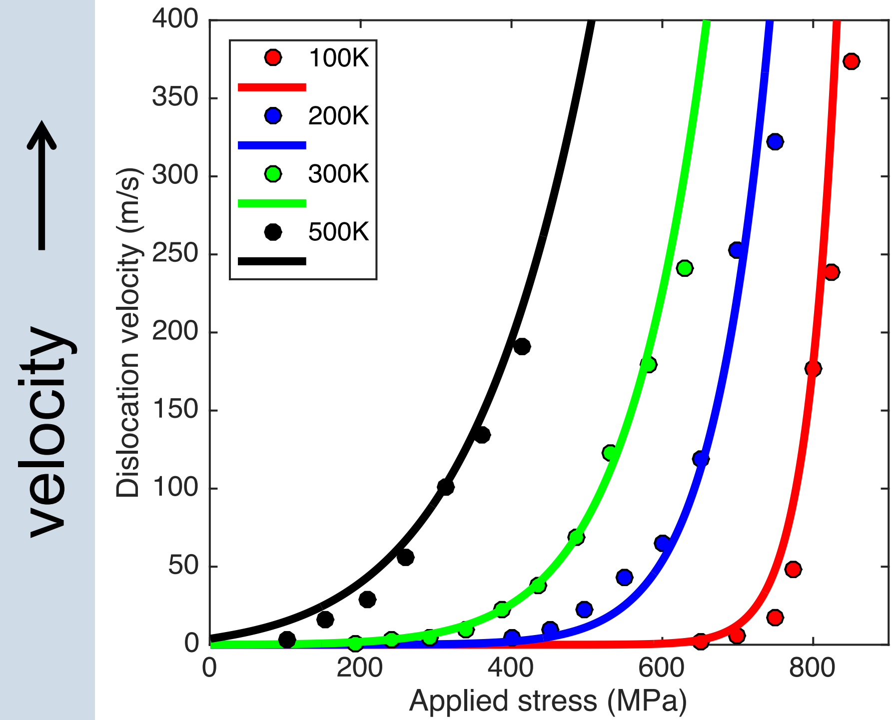
Right: fit of

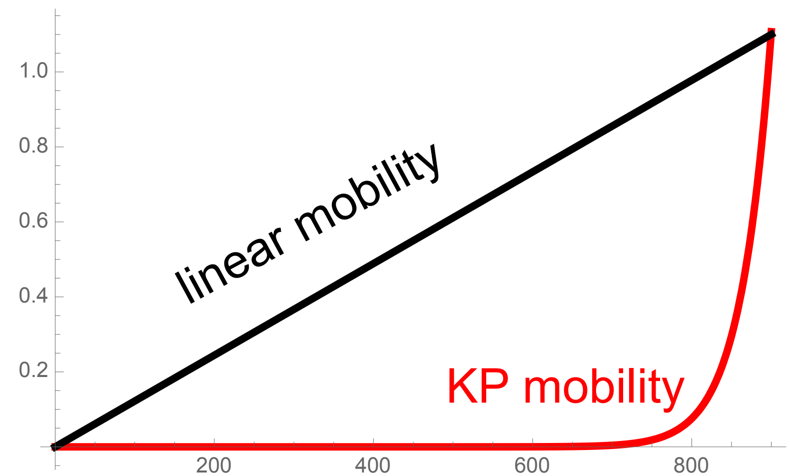
$$A \exp - \frac{\mathcal{H}^*}{k_B T}$$

to MD velocities *(Gilbert et al 2011)*

Screw dislocations in Fe

Power law isn't appropriate – looks more like a threshold





Fe, 100K

Conclusions and acknowledgments

- Mesoscale modelling is crucial to bridge the gap in understanding between micro and macro
- Capabilities increasing all the time
- Plenty of room in the middle!
- Thanks to Francesco Ferroni, Ed Tarleton, Daniel Thompson, Dave Armstrong, Steve Roberts and the MFFP group at Oxford; Sergei Dudarev, Duc Nguyen Manh, Tom Swinburne at CCFE

FDTN FUSION DOCTORAL TRAINING NETWORK
arc advanced research computing
EPSRC Engineering and Physical Sciences Research Council
CCFE CULHAM CENTRE FOR FUSION ENERGY