Defects, singularities and waves

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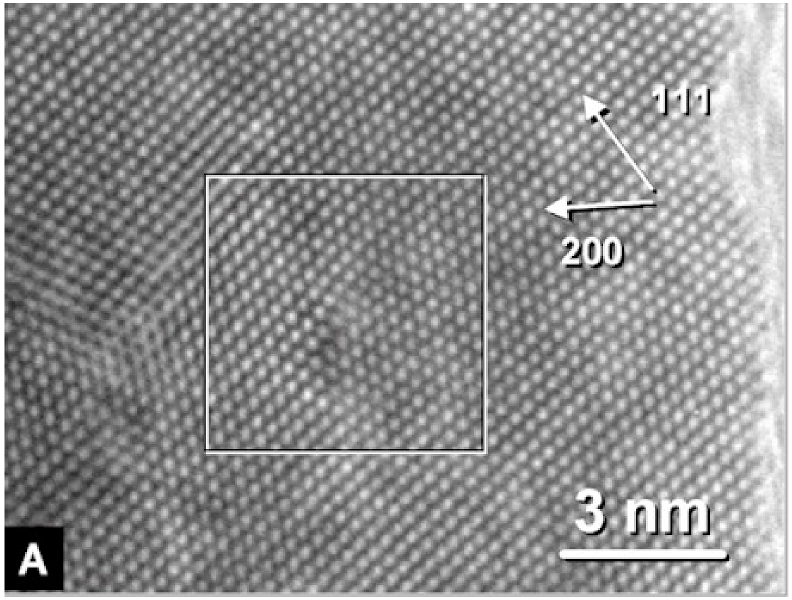
Outline

1. Defects in crystals.
2. Line singularities in elasticity.
3. Periodized discrete elasticity models.
4. Nonlinear waves in lattices.
5. Bifurcation theory for nucleation.
6. Bifurcation theory for depinning.
7. One dimensional waves.
8. Conclusions and perspectives.

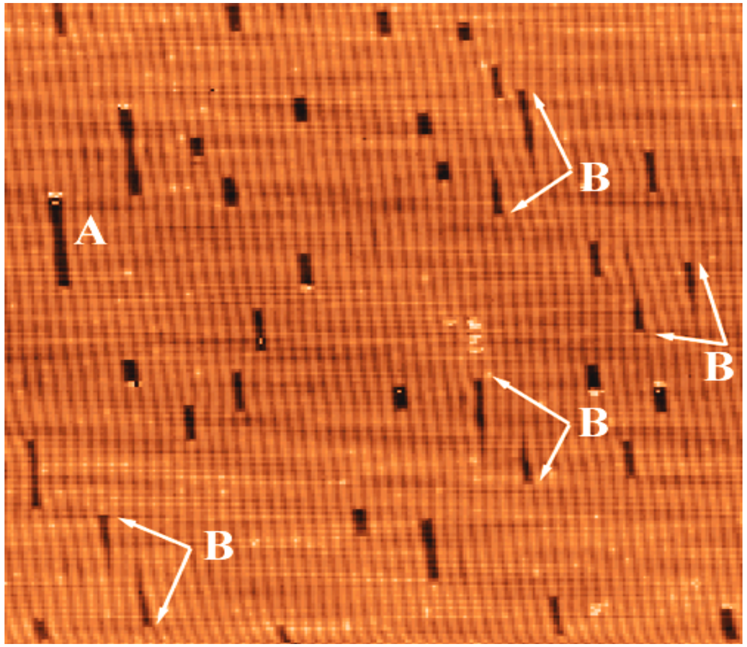
1. Defects in crystals

Dislocations: Defects supported by curves

Edge dislocation



Radiation and radiactive waste
Management group, Michigan
HRTEM, UO_2



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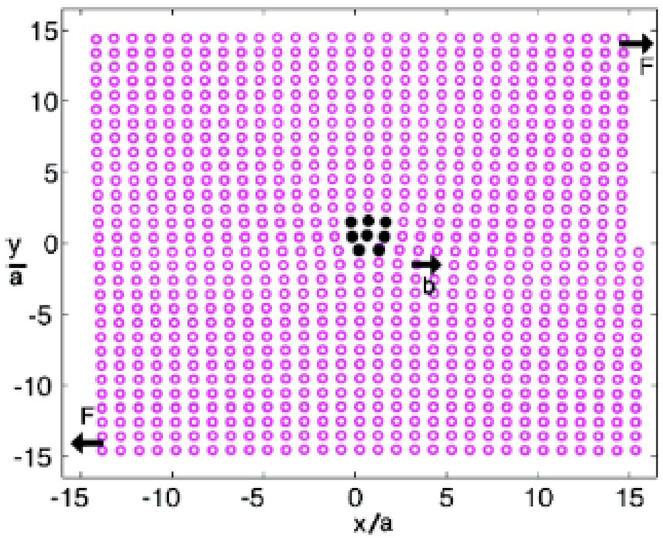
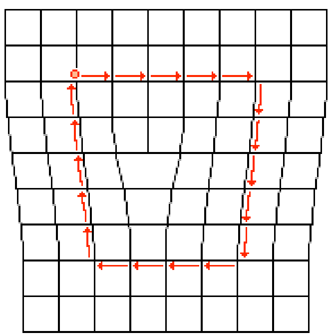
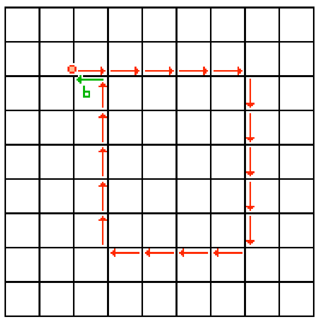
STM, Au

Edge dislocation
(dislocation line // τ points out of the page)

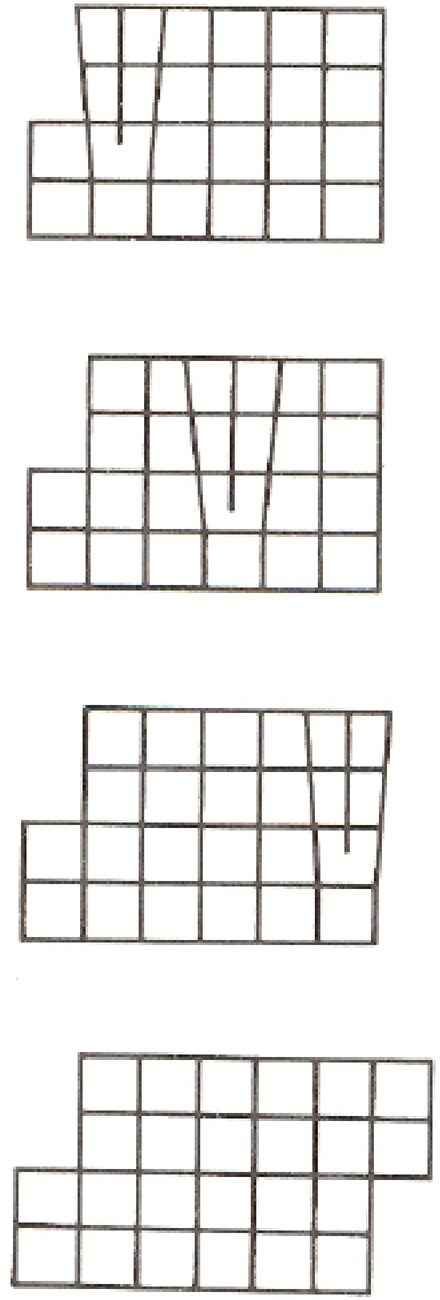


b ⊥ τ: Glide plane spanned by b and τ





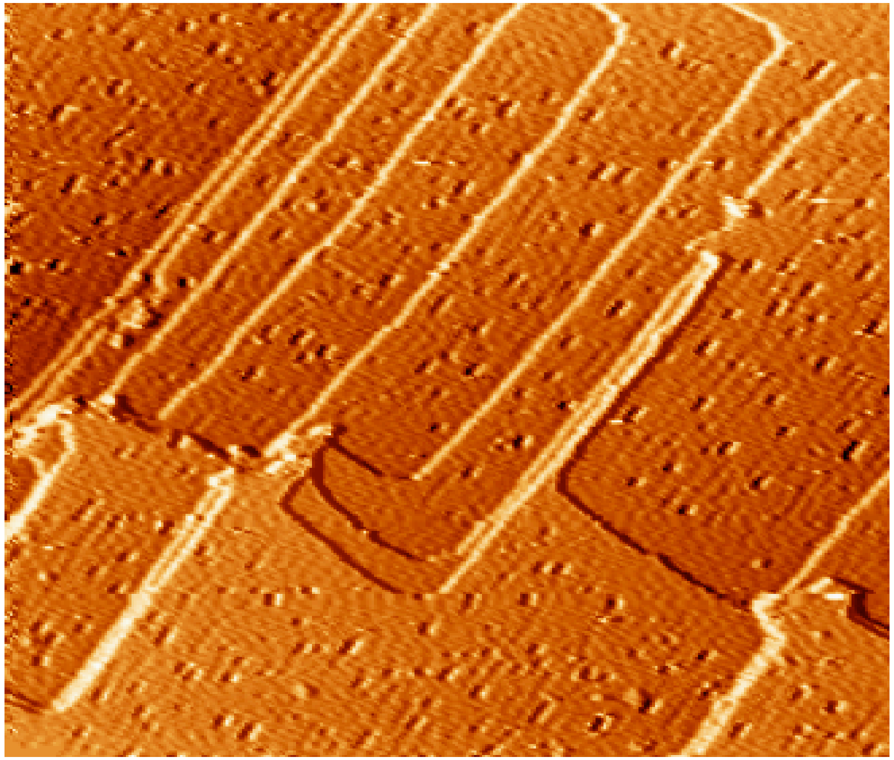
Burgers circuit   Same in undistorted lattice



Screw dislocation:

(glide plane includes b and any other crystal direction)

Burgers vector b || τ



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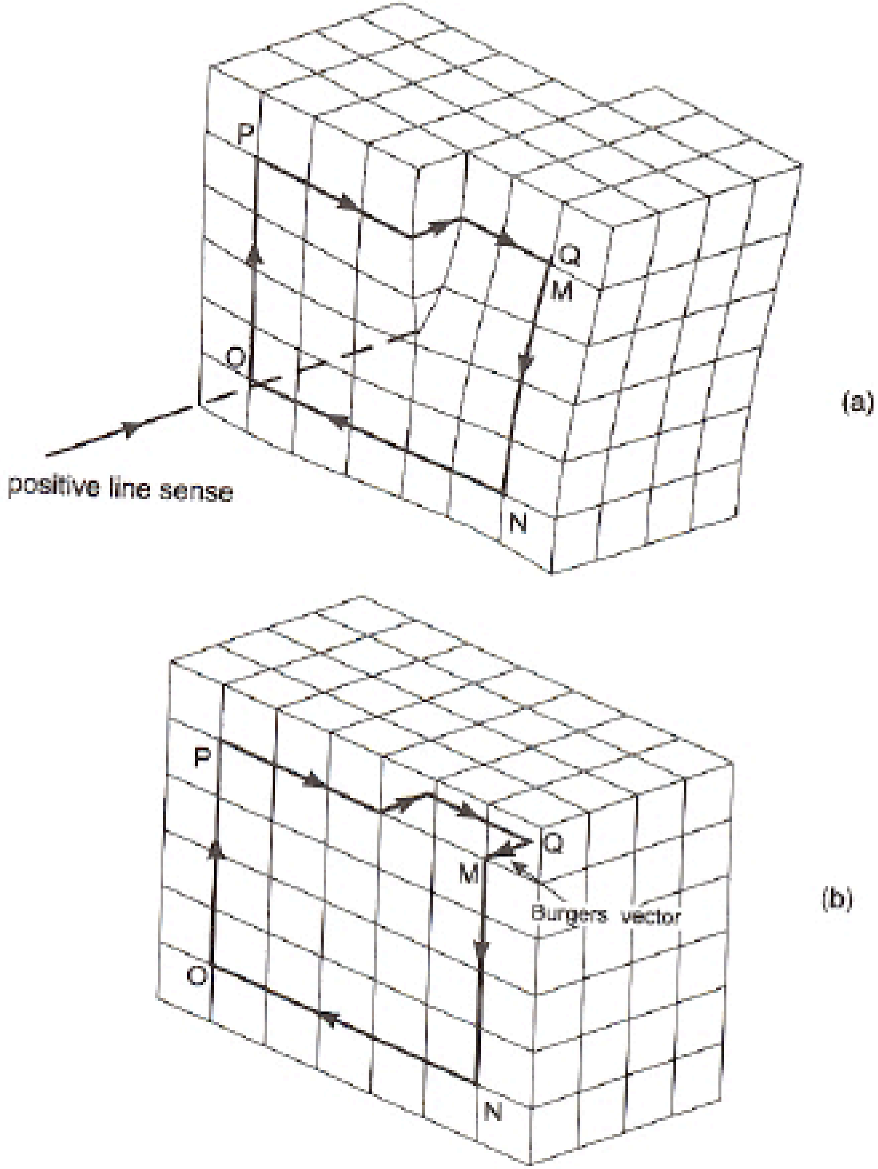
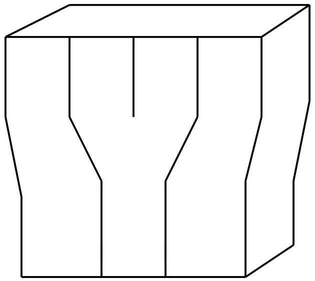


• Dislocations control the mechanical properties of crystals (strength, plastic deformation, growth rate…) and distort their optoelectronic properties.

• How can they be controlled to improve the properties of materials (semiconductors and metals)?

• What is the simplest mathematical framework to understand dislocation motion, nucleation and interaction?

2. Line singularities in elasticity



Continuum limit

u Displacement $u_{tt} - \mathrm{div}[\sigma(u)] = \delta_\Gamma$

Navier equations +
Dirac sources supported by
lines representing dislocations

Given a dislocation line, solve

$$\mathrm{div}[\sigma(u)] = \delta_\Gamma$$

- $\nabla u \sim 1/r$, r = distance to dislocation core
  $\rightarrow$ linear elasticity breaks down at core.
- u describes atomic arrangement far from core (far field), core structure remains unknown.

- u_{tt}- $\operatorname{div}[\sigma(u)] = \delta_\Gamma$ **gives no information on defect motion, the singularities do not move.**

Reason: the motion and nucleation of dislocations is controlled by the lattice structure, which regularizes the singularity. Spatial discreteness cannot be neglected.

- **Line singularities in the equations of elasticity (dislocations)**

~ Line singularities in Euler equations (vortex lines)

- **Vortices move in any direction in response to infinitesimal perturbations whereas dislocations only move in the directions of the principal crystallographic planes and when the force in such direction surpasses a threshold.**

- **The equations of elasticity are the equivalent of Euler equations whereas atomic models are the equivalent of Navier-Stokes.**

3. Periodized discrete elasticity

- Need of linear nearest neighbour models
  · reproducing lattice structure and bonds
  · with cubic, hexagonal… elasticity as continuum limit

They remove the singularity and produce static defects

Which combination of neighbours yields anisotropic elasticity?

- Need of nonlinearity to restore crystal periodicity, allow change of neighbours and defect motion

Which nonlinearity? A periodic function

Frank-Van der Merve, Proc. Roy. Soc., 1949, Crystal growth
Suzuki, PRB 1967, Lomdahl - Srolovich 1986, Ariza-Ortiz, ARMA 2005, Carpio - Bonilla, PRL 2003, PRB 2005 Dislocations
Marder, PRL 1993, Pla et al, PRB 2000 Crack propagation

Top down approach → Simple cubic crystal

Displacement $u_i(x_1,x_2,x_3,t)$, i=1,2,3

Stress $\sigma(x,t)$, Strain $\varepsilon(x,t)$

$$\sigma_{ij} = c_{ijkl}\,\varepsilon_{kl},\ \varepsilon_{kl} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right)$$

Potential energy

$$\frac{1}{2}\int c_{ijkl}\,\varepsilon_{ij}\varepsilon_{kl}$$

Navier equations

$$\rho\frac{\partial^2 u_i}{\partial t^2} - \sum_{j,k,l}\frac{\partial}{\partial x_j}\left(c_{ijkl}\frac{\partial u_k}{\partial x_l}\right) = f_i, \quad i = 1,2,3$$

Displacement $u_i(l,m,n,t)$, i=1,2,3

Discrete strain $\varepsilon(l,m,n,t)$

$$\varepsilon_{ij} = \frac{1}{2}\left[g(D_j^+ u_i) + g(D_i^+ u_j)\right]$$

Potential energy

$$\frac{1}{2}\sum_{lmn} c_{ijkl}\,\varepsilon_{ij}\varepsilon_{kl}$$

Discrete equations

$$m\frac{d^2 u_i}{dt^2} - \sum_{j,k,l} D_j^-\left[c_{ijkl}\,g(D_l^+ u_k)\,g'(D_j^+ u_i)\right] = f_i$$

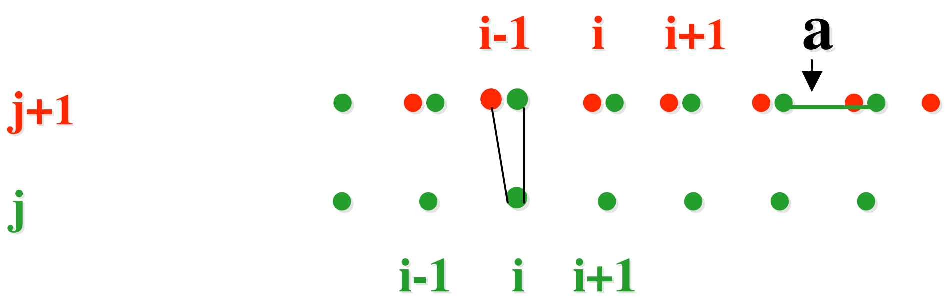
g periodic (period=lattice constant), normalized by g´(0)=1

$D^+_{j,}$ D^-_j forward and backward differences in the direction j

$D^+_2\, u_1(l,m,n) = u_1(l,m+a,n) - u_1(l,m,n)$

$D^-_1\, u_3(l,m,n) = u_3(l,m,n) - u_1(l-a,m,n)$

- The crystal lattice is a minimizer and a stable equilibrium
- Invariant by the relevant crystal symmetries
- Nonlinearity is irrelevant out of the cores of defects (g(x)~x, x small)
- Anisotropic elasticity is recovered in the continuum limit
- Simplest correction to linear elasticity allowing for defect motion
- The periodic function g avoids relabelling neighbours and restores the periodicity of the crystal

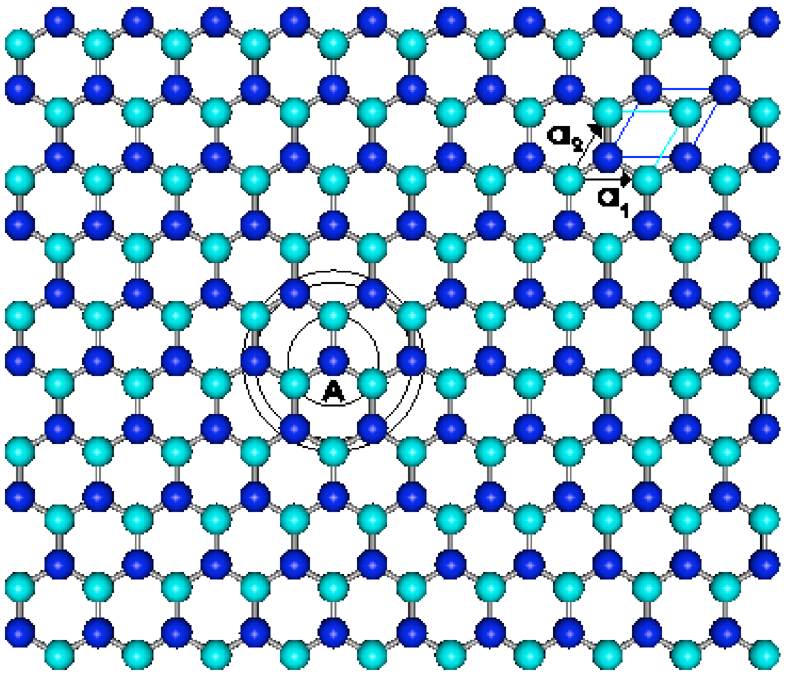


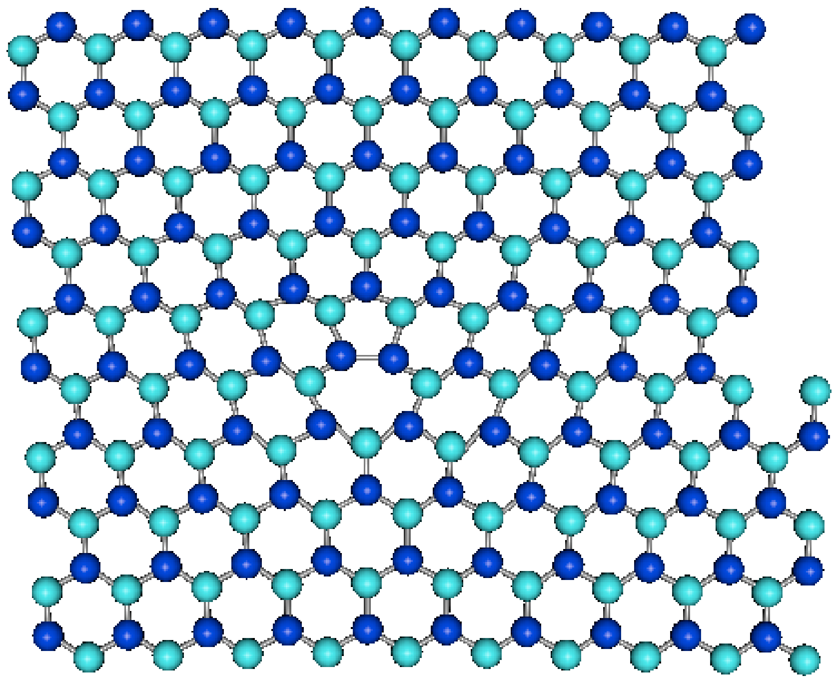
$$u_{i-1j+1}= u_{ij+1}-a$$

$$g(u_{i-1j+1}-u_{ij})=g(u_{ij+1}-u_{ij})$$

- Crystals with a few defects moving along principal crystallographic planes

It extends to 3D bcc (Fe), fcc (Cu), zinblenda (GaAs), diamond (Si) or 2D graphene lattices





The periodic function g is calibrated to produce thresholds for motion near measured values.

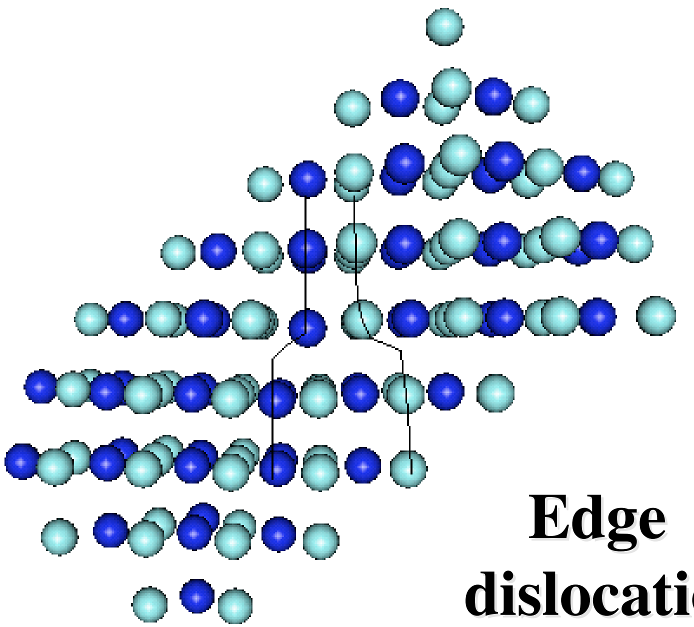
4. Nonlinear waves in lattices

4.1. Static dislocations

Strategy: 1) Compute the adequate singular solution of the Navier equations (displacement far field).

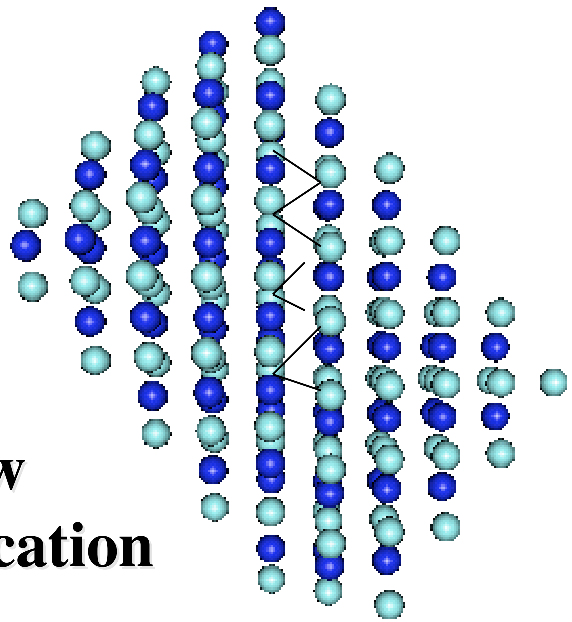
2) Use it as initial and boundary data in the damped discrete model and let it relax to a static solution as time grows.

3) Rigorous existence results.



Edge dislocation

Screw dislocation



Class of functions S: sequences $(u_1(l,m,n), u_2(l,m,n), u_3(l,m,n))$ in $(Z^3)^3$ behaving at infinity like singular solutions of Navier equations, with a Dirac mass supported on the dislocation line as a source.

Static dislocations: solutions of $D^-_j(c_{ijkl}\, g(D^+_l u_k) g'(D^+_j u_i))=0$ in the class of functions S. Two options:

a) Minimize the energy on S:

$$1/2 \ \sum c_{ijkl} \big(g(D^+_l u_k)+g(D^+_k u_l)\big)/2 \ \big(g(D^+_j u_i)+g(D^+_i u_j)\big)/2$$

b) Compute the long time limit of the overdamped equations:

$$u_i{}' - D^-_j(c_{ijkl}\, g(D^+_l u_k) g'(D^+_j u_i)) = f_i, \quad i=1,2,3$$

in S using the singular solution of Navier eqs. as initial datum.

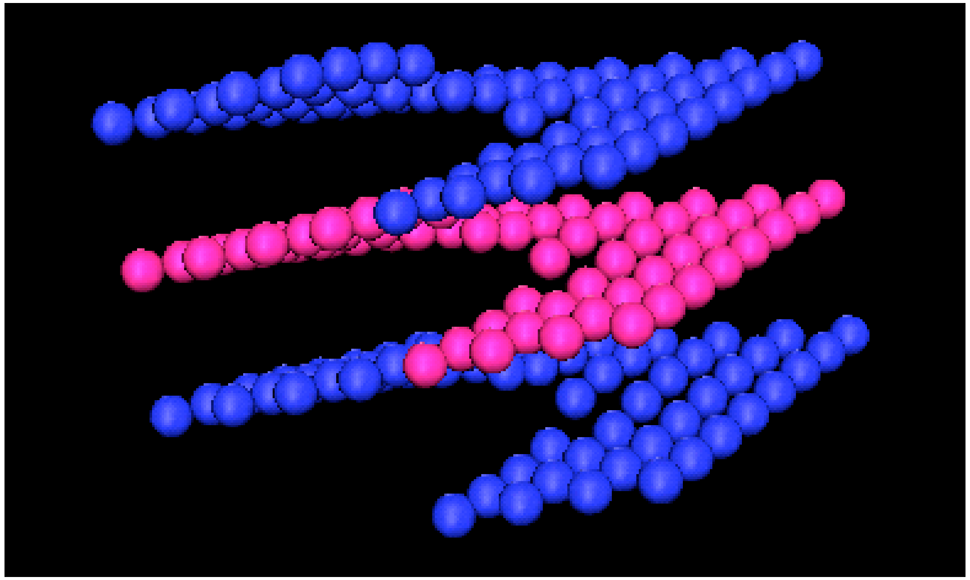
The spatial operator is ‘elliptic’ near that solution.

Outcome: Shape of the dislocation core.

Threshold for motion: the spatial operator stops being elliptic (change of type).

4.2. Moving dislocations: traveling waves

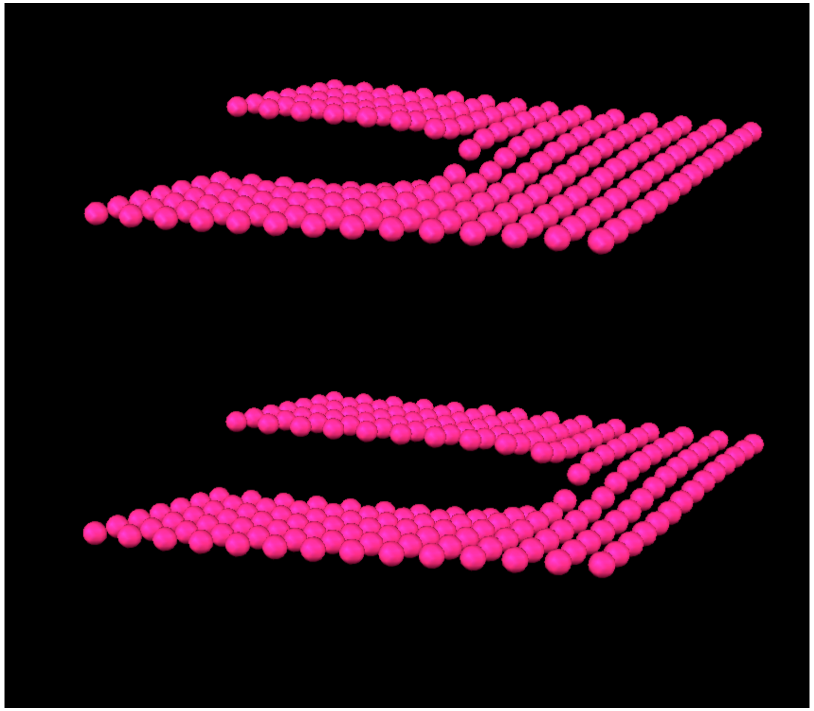
Screw dislocations



$(i,j,k+w_{ij})$

F

b



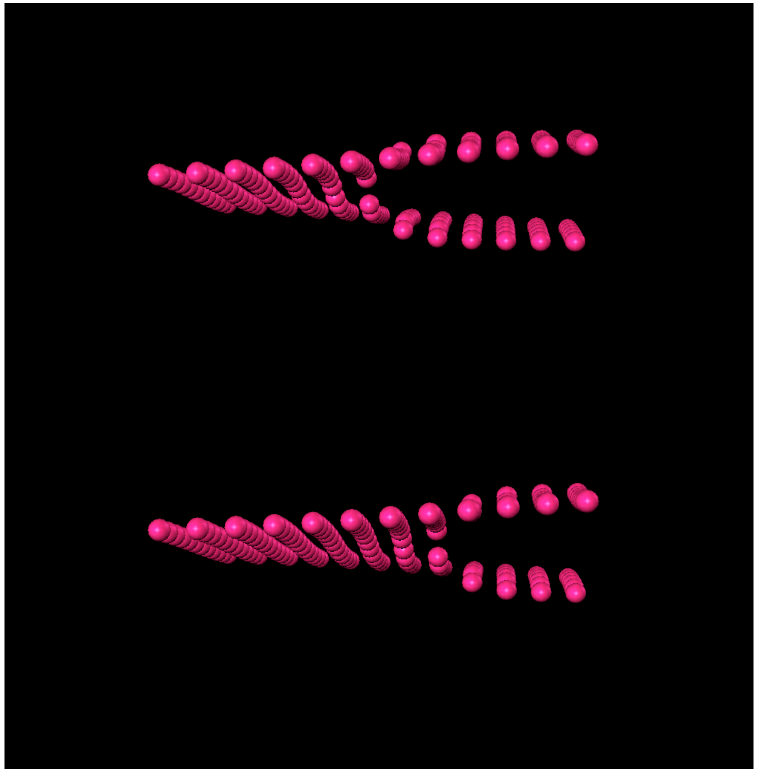
F

glide

Traveling edge dislocation

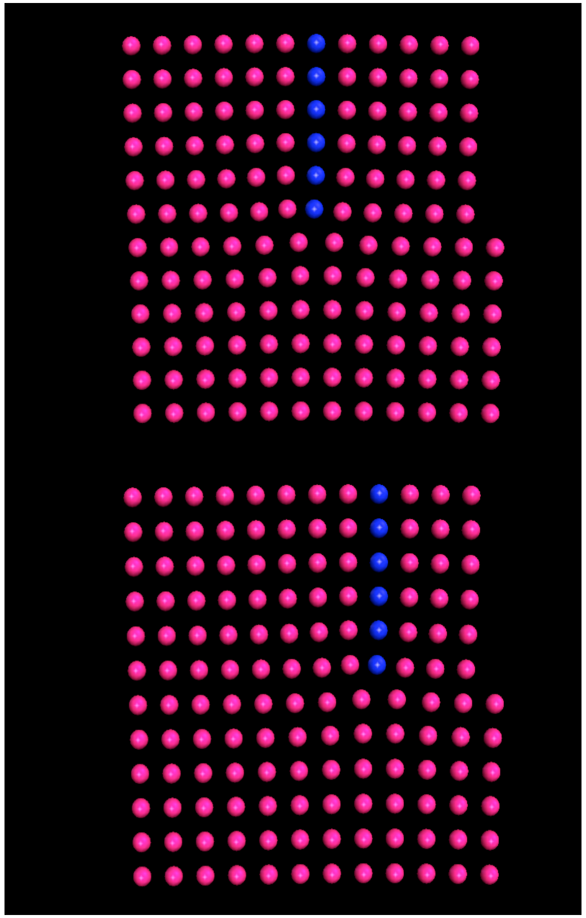
Displacement

$u_{ij}(t)=u(i-ct,j)$



Deformed lattice $(i+u_{ij}, j+v_{ij})$

$F \rightarrow$



$\leftarrow F$ $\underline{b}$

Interaction of dislocations → Interaction of nonlinear waves

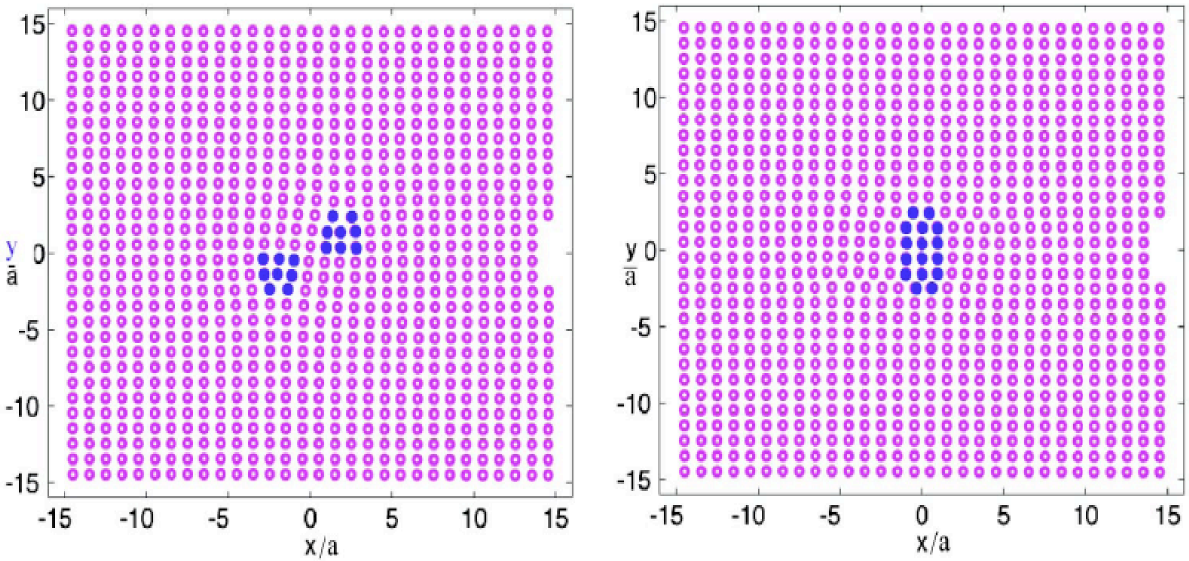


FIG. 9. (Color online) Attraction of opposite-sign edge dislocations leading to formation of a dislocation loop.

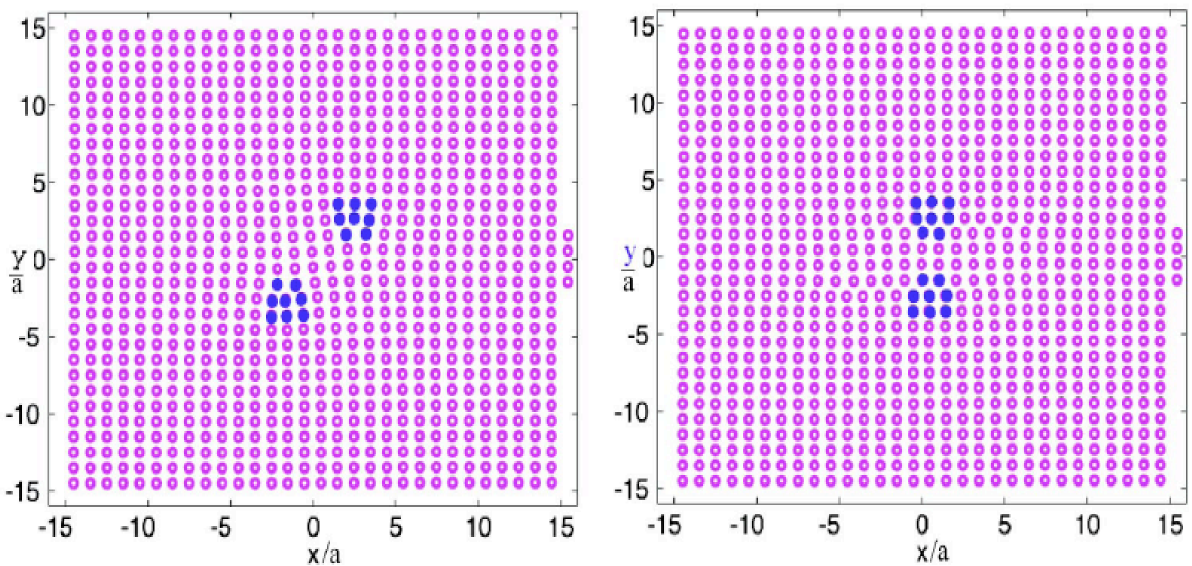


FIG. 10. (Color online) Attraction of opposite-sign edge dislocations leading to formation of a dislocation dipole.

Variational formulation:

$$\min_{1=\int dx\, \Sigma_{n,p} |\underline{u}_x|^2 (x,n,p)} \quad 1/2 \int dx\, \Sigma_{n,p}\, c_{ijkl}\, \varepsilon_{kl}(x,n,p)\, \varepsilon_{ij}(x,n,p)$$

$$\varepsilon_{kl} = \frac{1}{2}\left(g(D^+{}_l u_k) + g(D^+{}_k u_l)\right)$$

Properties of the energy? Restrictions on g?
(non convex) (periodic)

Friesecke-Wattis (1994)

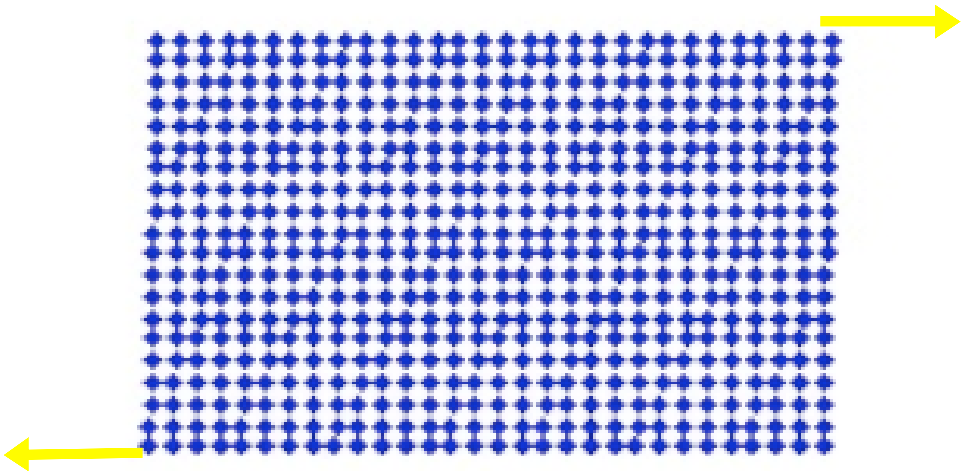
$$m\, u_n'' = -V'(u_{n+1} - u_n) - V'(u_{n-1} - u_n)$$

V´ superlinear, concentrated compactness

5. Bifurcation theory for nucleation

Why are defects nucleated?

A shear force of strength F is applied in the x direction to a perfect lattice.



Numerical continuation: Start with perfect lattice, increase F

(Plans-Carpio-Bonilla, EPL, 2008)

Assumptions: 2D cubic lattice, only displacements in the x direction are relevant

3D $\longrightarrow$ 2D   vector $\longrightarrow$ scalar   sin(x) $\longrightarrow$ x

$$m\, u_{ij}'' + \alpha\, u_{ij}' = (u_{i+1,j} - 2u_{ij} + u_{i-1,j}) + A\,[\sin(u_{i,j+1} - u_{ij}) + \sin(u_{i,j-1} - u_{ij})]$$

$u_{ij}/2\pi$: displacement of atom (i,j) along the x axis

A: stiffness ratio,

m: inertia over damping ratio

Continuum limit: scalar elasticity $u_{xx} + A\, u_{yy} = 0$.

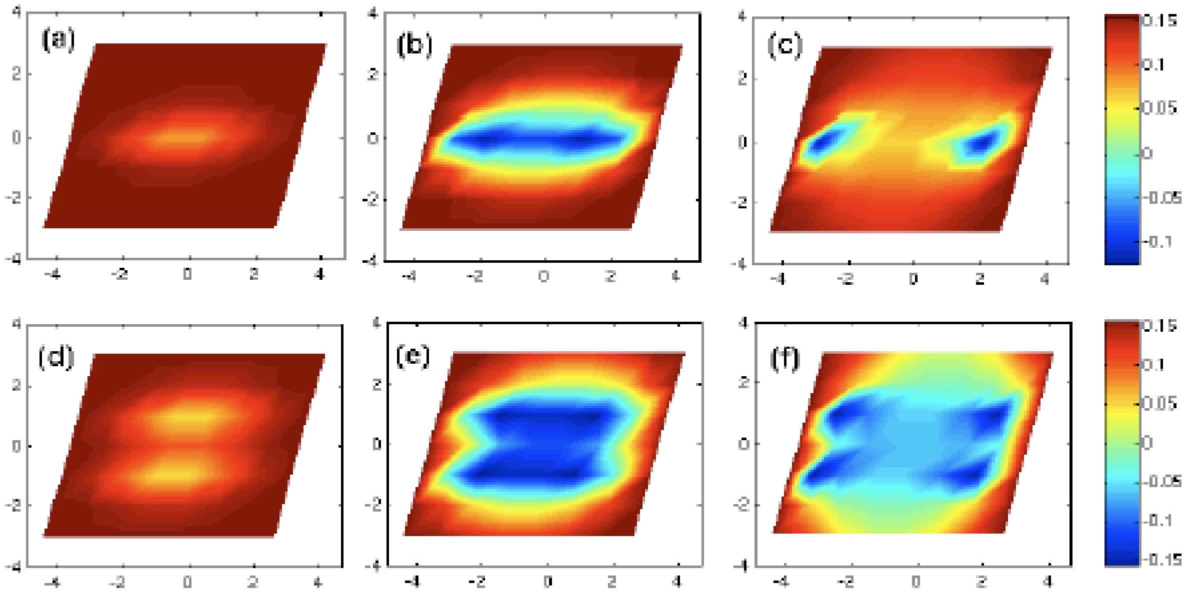
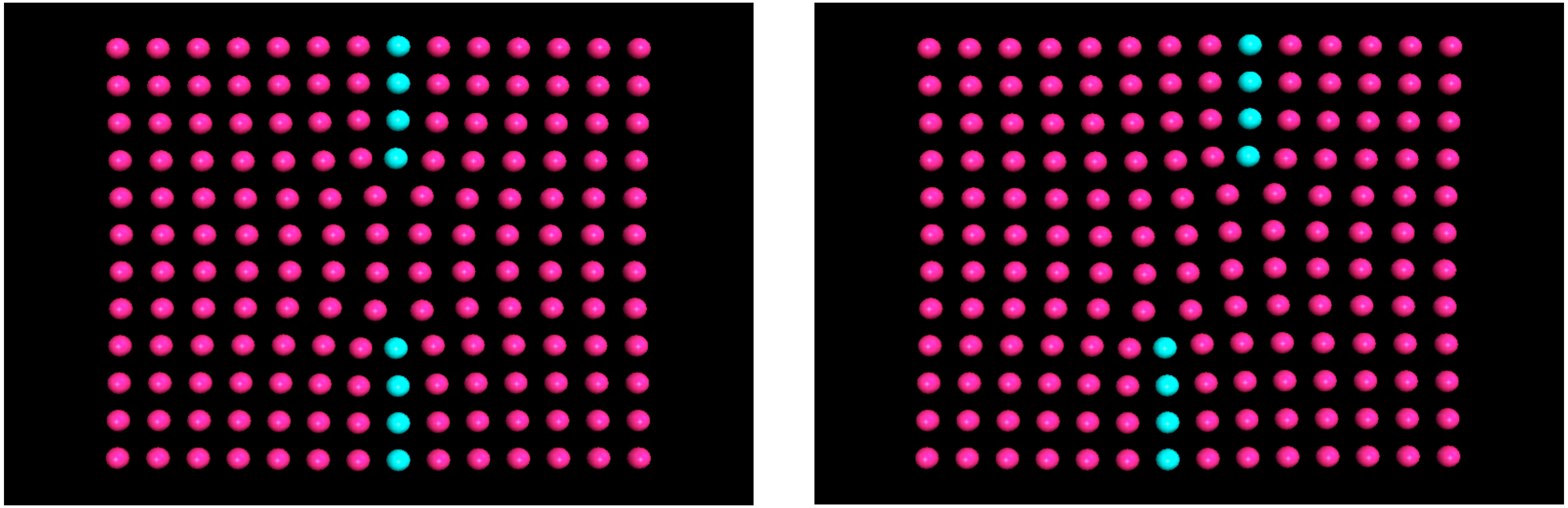


Figure 3: Upper panel from left to right: Snapshots of the strain $2e_{12}$ at times (a) 280.8, (b) 282.9, (c) 377.8 for the evolution towards BR1 with ramping time $t_r = 85$ ($c = 3.047 \times 10^{-3}$). Lower panel from left to right: Same at times (a) 302.4, (b) 304.7, (c) 393.0 for the evolution towards BR2 with ramping time $t_r = 100$ ($c = 2.59 \times 10^{-3}$). $F_f = 0.259$.

Nonlinear shear strain $2\varepsilon_{12}(i,j) = \sin(u_{i,j+1} - u_{ij})$ ($\sim \partial u/\partial y$)

Moving strain-stress concentrations

Different patterns depending on the way F is increased



Moving stress concetrations correspond to nucleation and splitting of edge dislocation dipoles

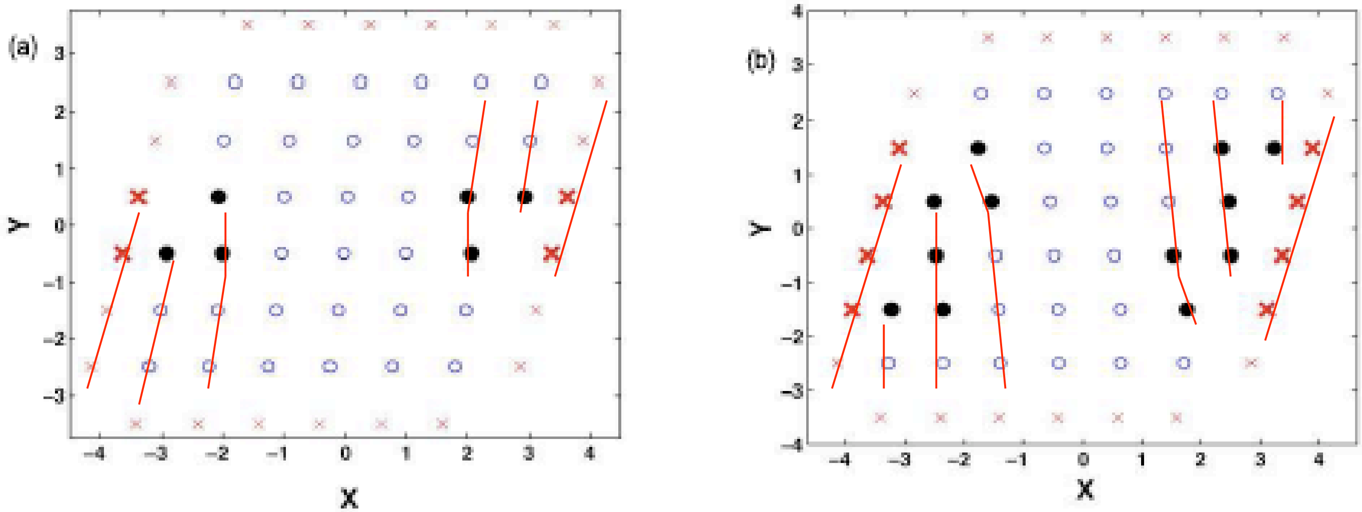


Figure 2: Configurations of the stationary solutions (a) BR1, (b) BR2, at $F_f = 0.259$. The crosses represents the positions of the boundary atoms which are fixed by the shear boundary condition.

One or two dipoles are observed depending on the way final stress F_f is reached (t_r= ramping time selects the final configuration):

$$c\, t_r = F_f\, ,\; F(t) = c\, t\, H(t_r - t) + F_f\, H(t - t_r).$$

More possibilities? Bifurcation diagram.

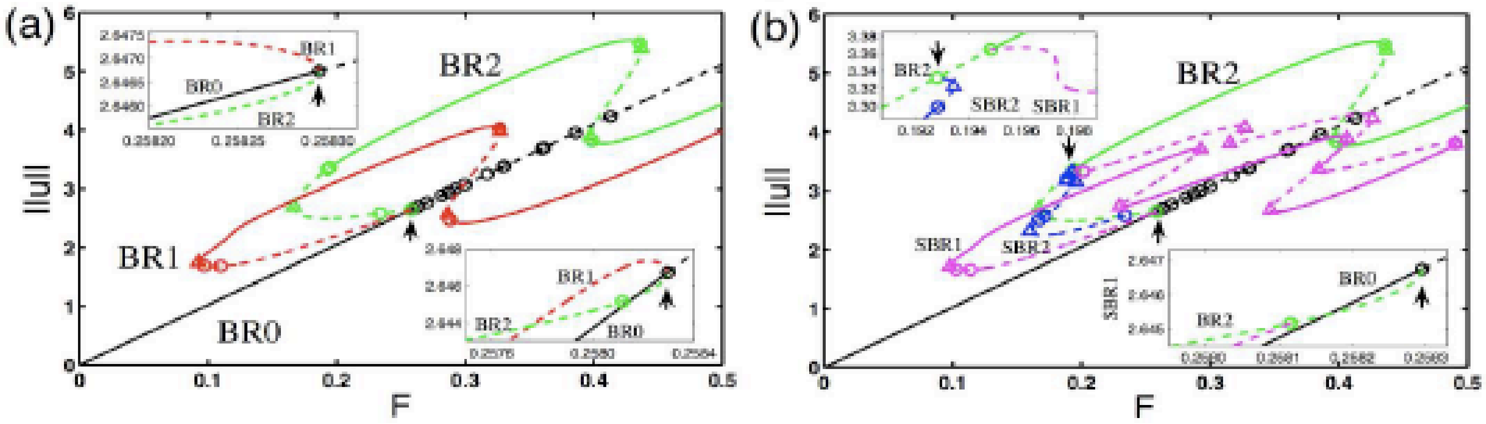


Figure 1: (a) Bifurcation diagram showing only the primary stationary branches issuing from the homogeneous solution BR0. At F_c, branches BR1 and BR2 appear as a subcritical pitchfork bifurcation from BR0 (see the insets). (b) Bifurcation diagram in which BR1 has been omitted and secondary bifurcation branches SBR1 and SBR2 issuing from BR2 are shown. Zooms near the bifurcation points are shown in the insets. In all cases, solid lines correspond to stable solutions, dashed lines to unstable solutions, limit points are marked as triangles and bifurcation points as circles. Parameter values are: $A = 1$, $a = 0.25$.

The branch of stationary stable solutions originating at the perfect lattice for F=0 dies at $F=F_n$. A subcritical pitchfork bifurcation takes place. Two initially unstable branches which later become stable are created.

• **At $F=F_n$ an eigenvalue vanishes. Defects nucleate in the region where the corresponding eigenfunction φ attains its largest values.**

• **Why do dipoles split? Because the threshold for nucleation is larger than the threshold for dislocation motion.**

• **Why one or two dipoles?**

Branch 1: $s(F_n) + \alpha\,\varphi$, $\alpha \sim (F-F_n)^{1/2}$
Branch 2: $s(F_n) - \alpha\,\varphi$

The stable stationary sheared lattice near F_n is perturbed by either adding or subtracting the eigenfunction. Two different perturbations give rise to two different patterns

• **Hysteresis: Stable solutions corresponding to a sheared lattice with and without defects coexist for F close to F_n.**

• **Nucleation may be observed before reaching F_n.**

Nucleation criterion

• Nucleation of dislocations happens for shear strengths F near (but not above) a threshold F_n.

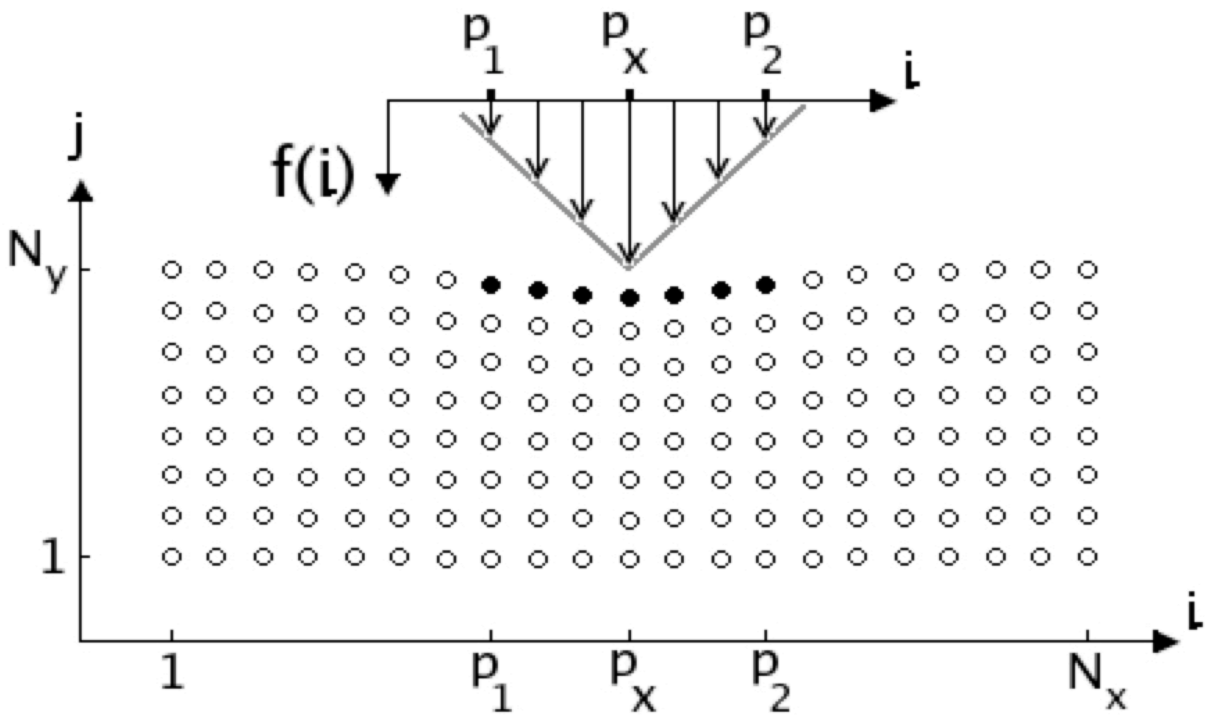
• Below the threshold, the linearized problems about the stationary configurations have negative eigenvalues. The sheared lattices without defects are stable.

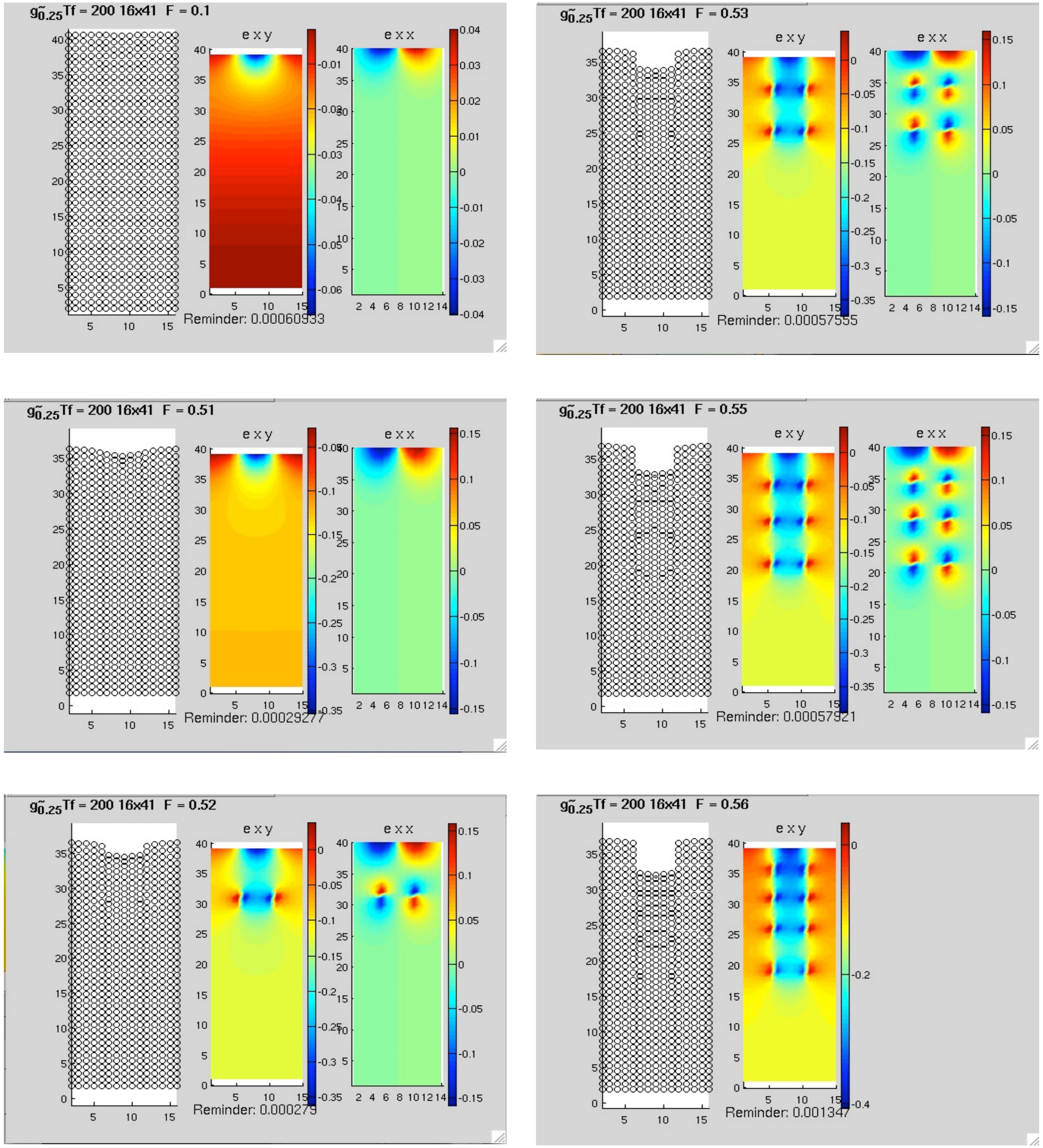
• At the threshold, a subcritical pitchfork bifurcation occurs, at least one eigenvalue vanishes and changes sign. The associated eigenvector locates the nucleation region (maximum values).

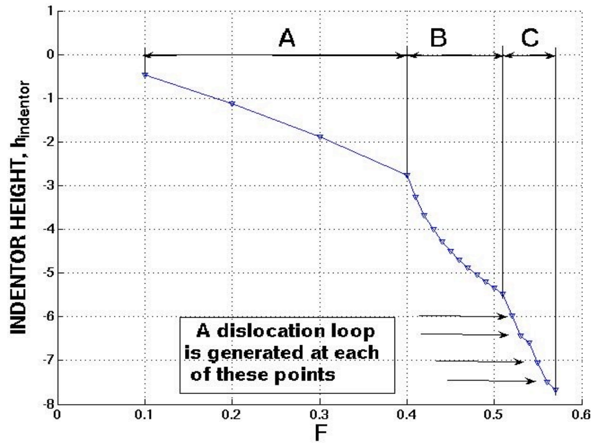
• The atraction basin of the sheared lattice without defects shrinks. A jump to a dislocated branch is likely before reaching F_n.

• The nucleated pattern is not unique. Different defect types can be nucleated depending on how the load is applied.

In more complex geometries, similar criteria may hold.
A simple indentation test:







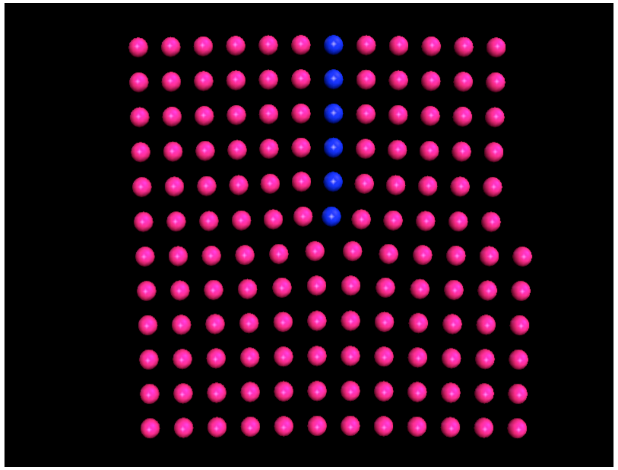
After the first loop is nucleated, other loops follow. The first discontinuity in the curve marks the change from elastic to plastic and should correspond to a bifurcation.
The rest?

6. Bifurcation theory for depinning

Why do static defects start moving?

- **Static edge dislocations are generated from the singular solution $b\theta(x,y/\sqrt{A})/2\pi$ (the angle function $\theta \in [0,2\pi)$)**

- **We apply a shear stress of strength F in the x direction in a lattice with a static dislocation.**

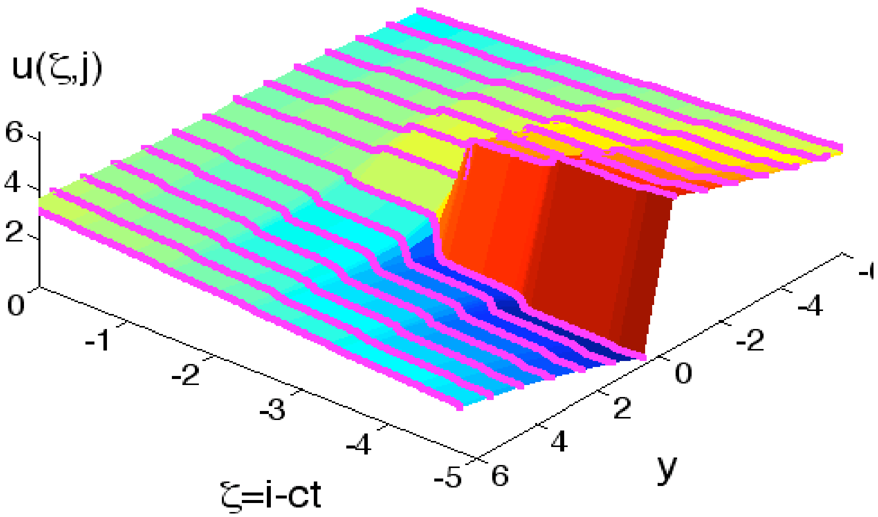


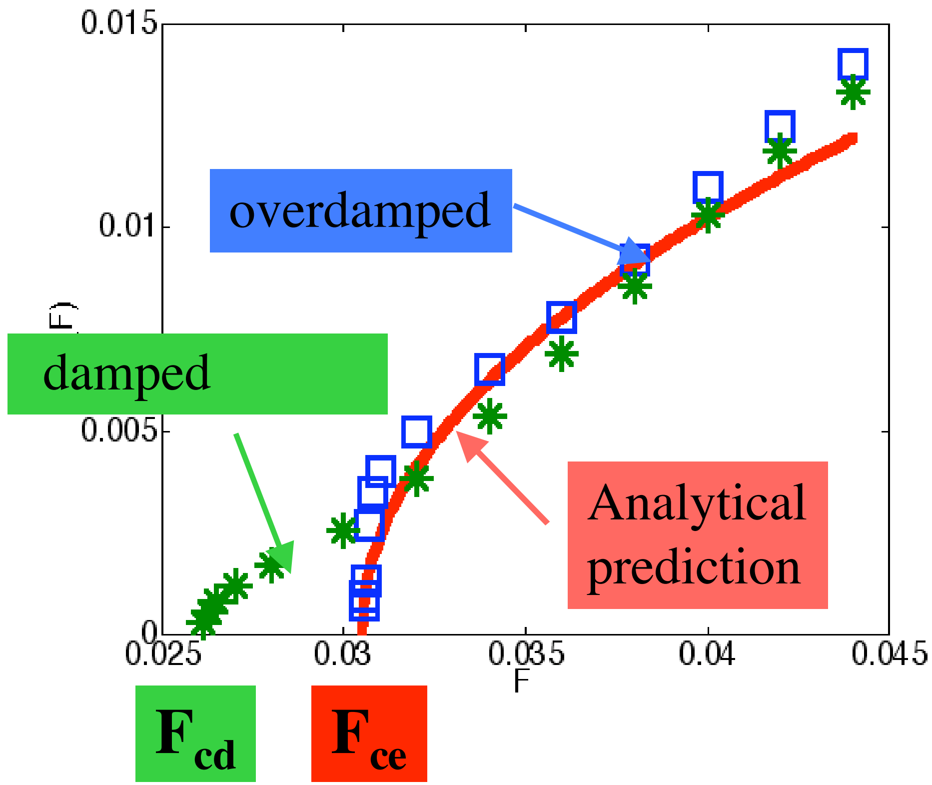
- **Two thresholds for motion:**
  dynamic threshold $F_{cd} \leq$ static threshold F_{cs}

  Below F_{cs}, pinned dislocations (static Peierls stress).
  Above F_{cd}, moving dislocations (dynamical Peierls stress).
  $F_{cd}=F_{cs}$, in the overdamped limit $m=0$.

(Carpio AML 2002, Carpio-Bonilla PRL 2003)

- **Moving dislocations identified with traveling wave fronts,** $u_{ij} = u(i\text{-}ct,j)$. **Their far field moves uniformly at the same speed** $\theta(x\text{-}ct,y/\sqrt{A}) + F\,y$





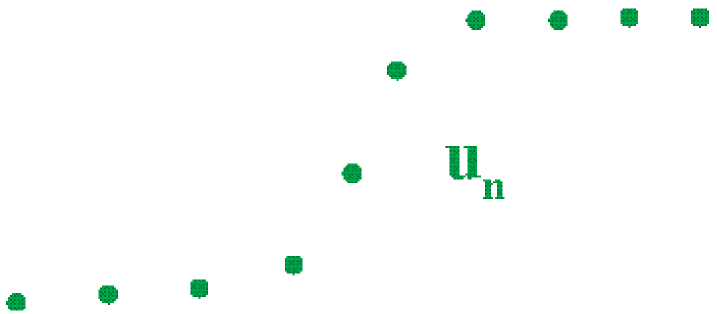
In the overdamped limit (m=0) the static critical stress F_{cs} and the velocity are predicted by a bifurcation analysis:

- **Linear stability of the stationary solutions for $|F| \le F_{cs} \Rightarrow$ negative eigenvalues, one vanishes at $F=F_{cs}$.**
- **Normal form near F_{cs}: $\varphi' = \alpha\,(F-F_{cs})+\beta\,\varphi^2 \quad \Rightarrow$ solutions blow up in finite time**
- **Wave front profiles exhibiting steps above F_{cs} $\Rightarrow$ at F_{cs} profiles become discontinuous.**
- **Near F_{cs}, wave velocity is the reciprocal of the width of blow up time interval : $|c(F)|=\sqrt{\alpha\beta(F-F_{cs})}/\pi$.**

In the general case (m≠0) a new threshold appears. This is easier to understand in 1D models.

7. One dimensional waves

Pinned wave fronts

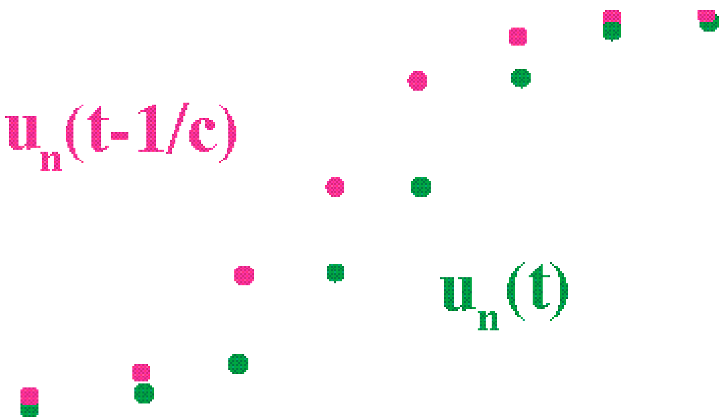


Frenkel-Kontorova (1938)

1D defect$\rightarrow$ kink in a chain

Moving wave fronts

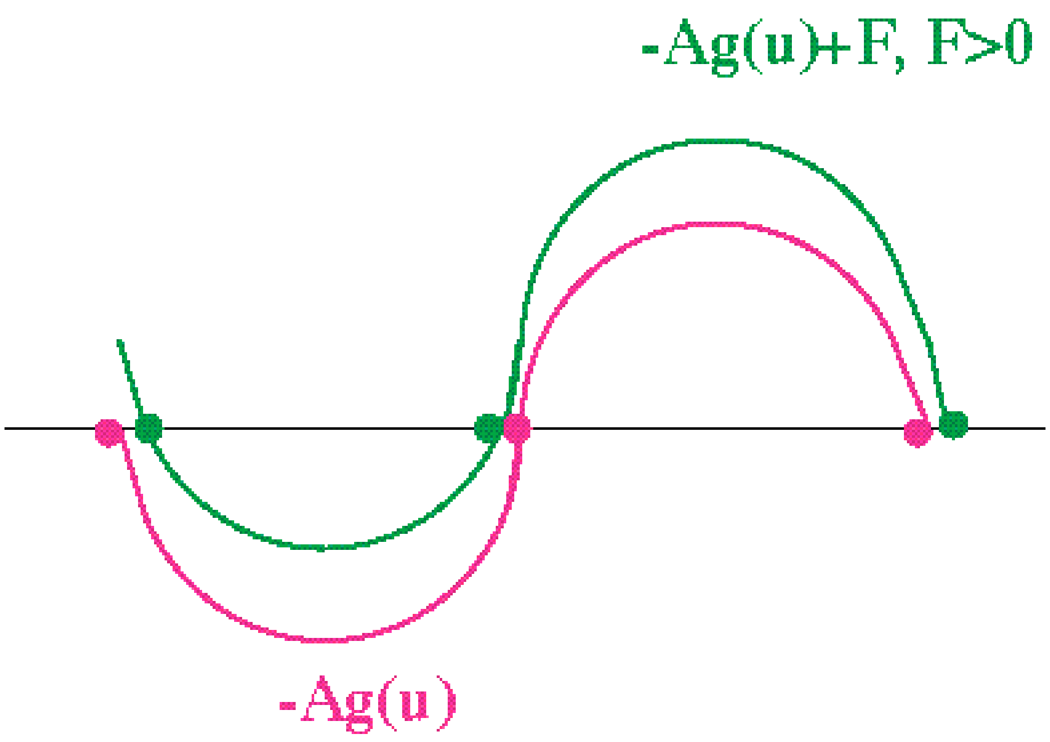
$$u_n'' + \alpha\, u_n' = u_{n+1} - 2u_n + u_{n-1} - A\sin(u_n) + F$$



$$u_{n+1}(t) = u_n(t-1/c),$$

$$u_n(t) = w(n-ct)$$

$$u_n'' + u_n' = u_{n+1} - 2u_n + u_{n-1} - A\,g(u_n) + F, \quad g(s) \text{ bistable}$$



3 zeros, two of them stable.

Fronts: Solutions connecting the two stable zeros.

Speeds?
Thresholds?

Typical choices:

$g(s) = \sin(s)$

$$g(s) = \begin{cases} s, & 0<s<1/2 \\ s+1, & 1/2<s<1 \end{cases} \text{ extended periodically}$$

$$\varepsilon u_n'' + \alpha\, u_n' = u_{n+1} - 2u_n + u_{n-1} - Ag(u_n) + F, \quad g \text{ piecewise linear}$$

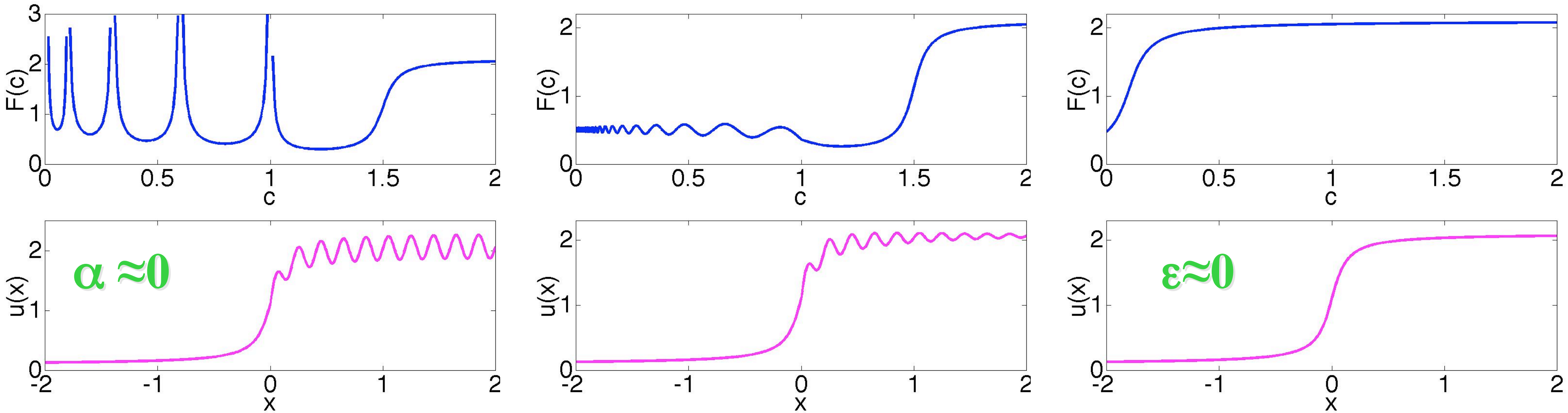
- $u_n(t) = u(n-ct) \Rightarrow$ differential-difference equation for $u(x)$, c, $x=n-ct$

$$c^2\, \varepsilon\, u''(x) - c\, \alpha u'(x) = u(x+1) - 2u(x) + u(x-1) - Au(x) + H(-x) + F(c)$$
$$u(-\infty) \approx U_1(F(c)/A),\ u(\infty) \approx U_3(F(c)/A),$$
$$u<1/2 \text{ for } x<0,\ u>1/2 \text{ for } x>0$$

- profile $u(x)$ and relationship between F and c are given by contour integrals, that can be calculated by residues
- infinitely many complex poles, plus zero, plus a finite set of real poles if $\alpha=0$

$$u(x) = \frac{F}{A} - \frac{A}{\pi i} \int_\Omega \frac{e^{ikx}}{kL(k)}\, dk, \quad L(k) = A + 4\sin(k/2)^2 - k^2 \varepsilon c^2 - k\alpha c\, i$$
$$u(1/2) = 0 \Rightarrow F(c)$$

Atkinson-Cabrera PRB 1965, Carpio-Bonilla PRE 2003, Carpio PRE 2004



• $\alpha = 0$ finite number of real poles $\Rightarrow$ contour indented according to a radiation condition, profiles exhibit uniformly oscillating tails

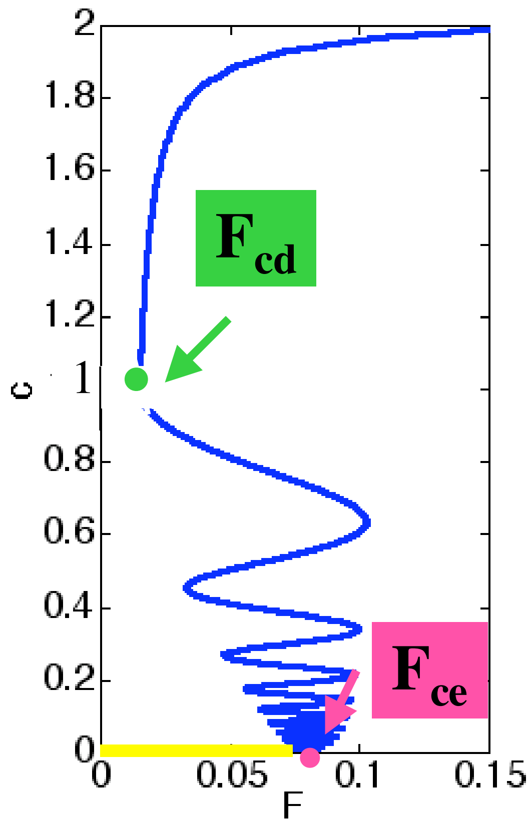
• $\alpha = 0$ resonance in double poles $\Rightarrow$ fronts with different profile and velocity coexist for a given F, only one branch of stable solutions

• there exist a minimal velocity and a minimal force needed to sustain wave front propagation $\Rightarrow$ dynamic critical $\neq$ static critical F

• $\varepsilon = 0$ infinitely many imaginary poles with large imaginary part $\Rightarrow$ monotone F(c) and u(x), no coexistence

- Two thresholds: $F_{cd}(A) \leq F_{ce}(A)$
  $|F| \geq F_{cd}(A)$ $\exists$ smooth traveling wavefronts
  $|F| \leq F_{cs}(A)$ $\exists$ static discrete fronts
  Static and dynamic Peierls stresses, friction
- If $\alpha << 0$, F fixed, coexistence:
  - Stable traveling and pinned fronts coexist
  - Traveling fronts with different profiles and speeds coexist, only one stable
- Fronts start to propagate with positive speed above a minimun force
- Saddle-node bifurcation in the branch of traveling waves, $|c(F)-c_m| = k\sqrt{(F-F_{cd})}$, oscillatory front profiles
- Same conclusions seem to hold when g is smooth
- Deep contrast when compared to

$$u_{tt} - u_{xx} = -\sin(u) + F$$



Bifurcation diagram

$$u_n' = u_{n+1} - 2u_n + u_{n-1} - A\sin(u_n) + F$$

Overdamped limit: $F_{cd}(A) = F_{ce}(A)$

- $|F| \le F_{ce}(A)$, stationary discrete wave fronts .
- $|F| > F_{ce}(A)$, $u(n-ct)$: smooth traveling wave fronts .
- $c \to 0$ as $F \to F(A)^+$.
- $F_{ce}(A)>0$ for large enough A (strongly discrete limit).
- $F_{ce}(A) \to 0$ as $A \to 0$ (continuum limit).
- Stationary solutions are continuous only if F=0.
- Stationary and moving wave fronts do not coexist.

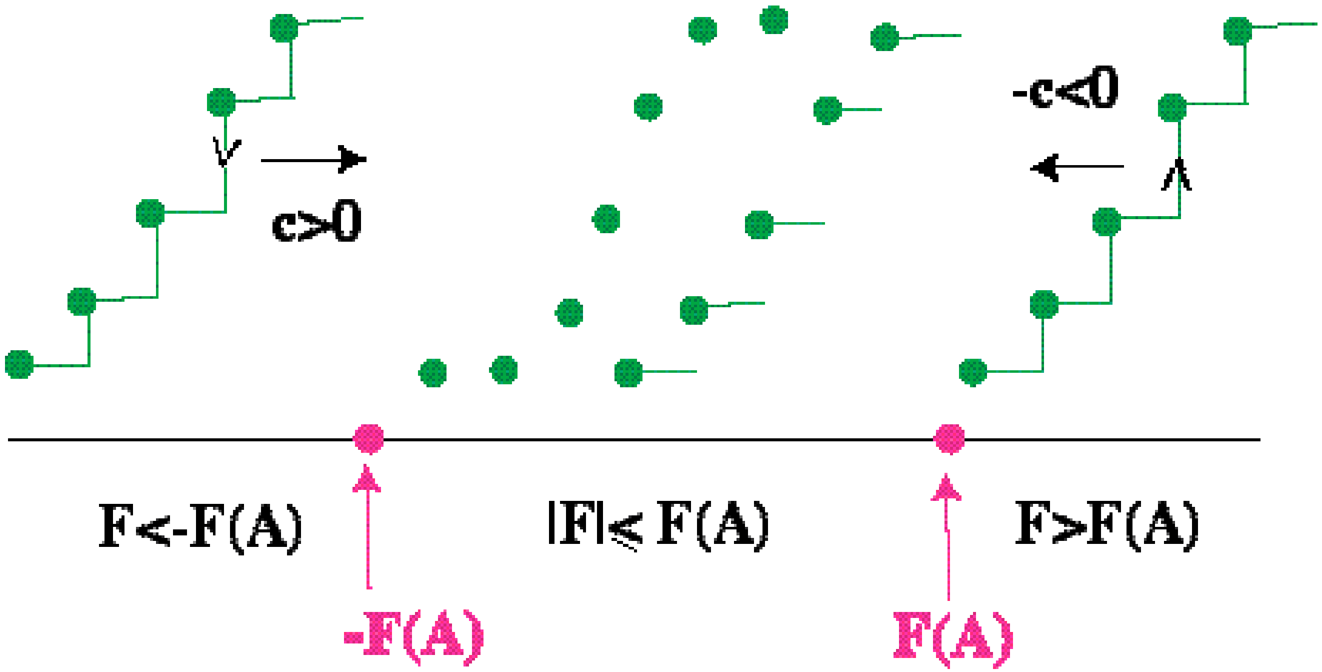
$$-c\,u'(x) = u(x+1) - 2u(x) + u(x+1) - A\sin(u(x)) + F$$
$$u(-\infty)=U_1(F/A),\ u(\infty)=U_2(F/A),\quad x=n-ct$$

Carpio,Chapman,Hastings,Mcleod, EJAM (2000)

Discrete transition: $F(A)>0$, $c(F) \approx k\sqrt{(F-F(A))}$.

(Generic) **Wave front profiles become discontinuous.**

Saddle-node bifurcation $\lambda=0$ in $F(A)$.



Continuous transition: $F(A)=0$, $c(F) \approx k\,(F-F(A))$.

(Anomalous)

Carpio-Bonilla, PRL (2001), SIAP (2003), Fath, Physica D (1998)

5. Conclusions and open problems

- Simple discrete models: dislocations are stationary or traveling wave solutions.

- Open existence problems in simple math setting.

- Analytical criterion to predict the critical stress for homogeneous nucleation of dislocations in a perfect crystal and the location of nucleation sites. Similar criteria for nucleation in indentation or fracture tests?

- Analytical theory for depinning transitions as global bifurcations explaining role of static and dynamic Peierls stresses.

- Qualitative agreement with experiments. Quantitative? Do these analytical theories survive in MD models?