Bulk and atomic dislocations in crystallographic structures

Outline:

1. Definition - what do we mean by “dislocation”
2. Motivation - why would we study such a thing
3. Brief theory of dislocations - and cool things they do (climb, creep, pin, etc)
4. Brief history of experiments - neutron, TEM, x-ray
5. XPCS experiment - design, goals, issues
    - 5.1 How would we induce them?
    - 5.2 How would we measure them?
    - 5.3 What would we learn?
    - 5.4 What issues might there be?

What is a “dislocation”?

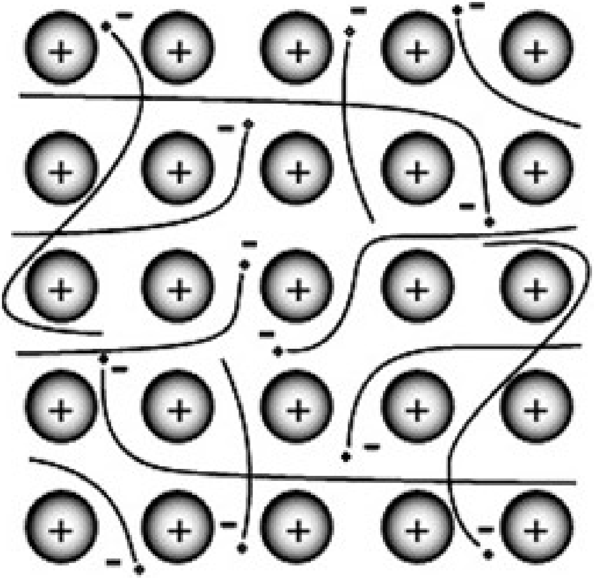
A dislocation is a crystallographic defect (irregularity) within a crystal (ordered) structure

More specifically, a topological defect that is sometimes called a soliton (particle-like stable solution to the equations of motion)

Motivation

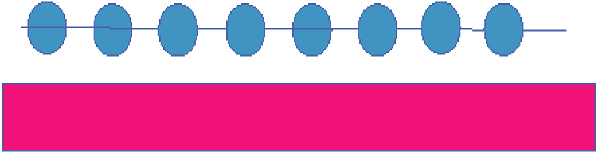
Material properties depend on how dislocations form, move, and interact. For example, plasticity (permanent deformation under load)

Electronic conductivity



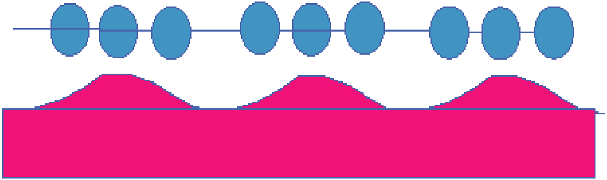
Drift velocity of charge density waves

Ions uniformly spaced



uniform electron density

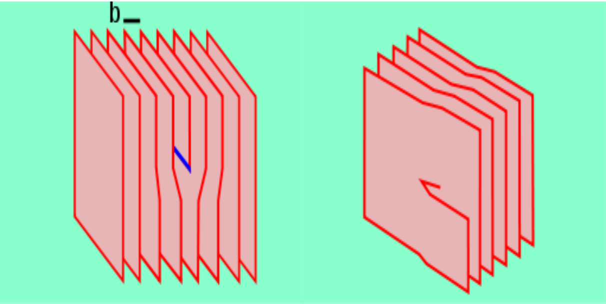
Ions develop static periodic distortion



electron density modulated (charge density wave)

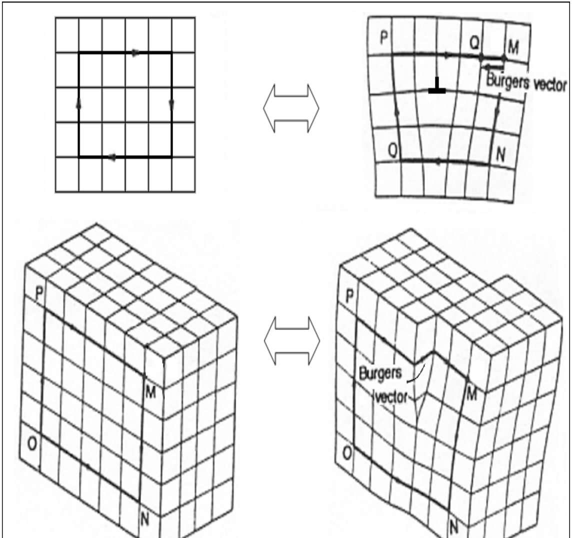
Classifying dislocations

Atomic (single atom diffusion) vs. Bulk (atomic planes, etc). Two main types are edge (left) and screw (right)



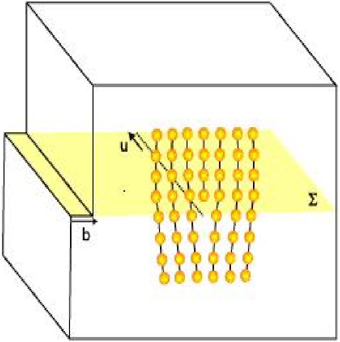
Classifying dislocations cont.

Visualize a perfect crystal and introduce a square around future place of dislocation. Burgers vector is what is needed to complete the loop after the dislocation is introduced (which breaks the loop).



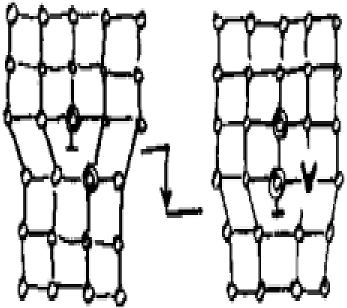
Weird things dislocations do

- Creep - movement of dislocations throughout the crystal lattice. Causes plastic deformation of crystals and, ultimately, the material. Proceeds along glide plane:



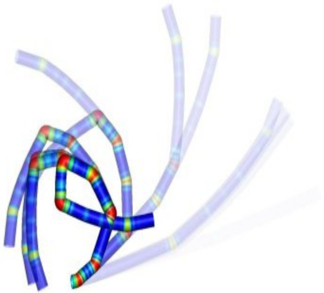
Weird things dislocations do

- Climb - just like creep, but moves perpendicular to creep direction



Weird things dislocations do

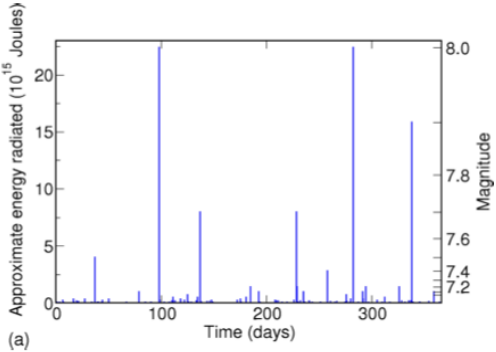
- Microavalanche - multiple dislocations results in jammed configuration, then long range interaction allow destruction of jammed regions in avalanche like process



These can be characterized by material independent power law size distribution

Crackling noise

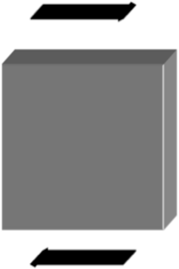
What is the sound of a paper crumpling? Time series the same as earthquakes occurring in 1995



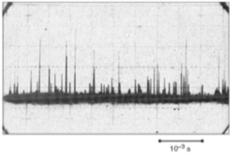
In general, a system responds to external conditions in a series of jumps spanning a broad range of sizes. Popcorn does not crackle (lots of similar sized small events) nor does chalk (snaps once when stressed beyond certain point).

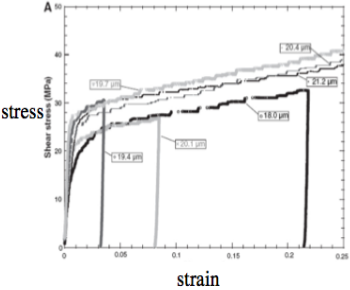
Crackling noise - materials

Universality. Slowly sheared metals show discrete jumps!

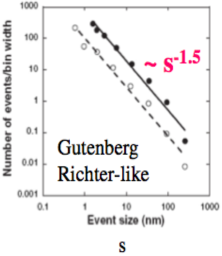


Acoustic emission



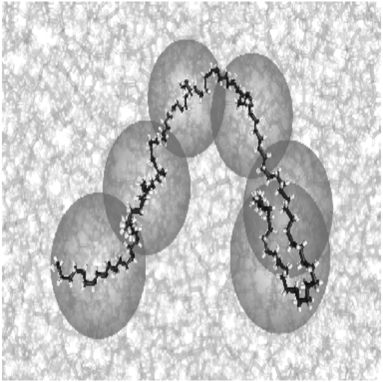


jump size distribution



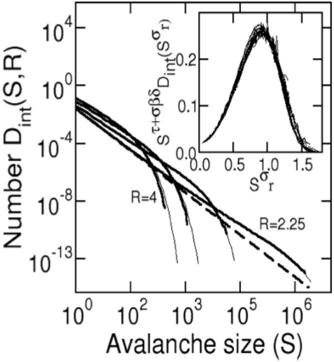
Crackling noise - theory

Two approaches: calculate behavior on long length/time scales by course graining microscopic fluctuations (renormalization group)



Crackling noise - theory

Other approach is to invoke universality. Since the microscopic details don't matter, make up a simple model with same behavior (same universality class) and solve it



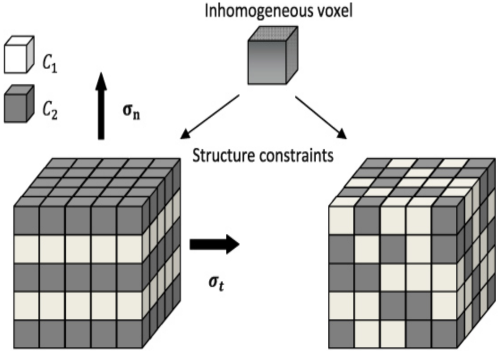
Above: Magnets respond to slowly varying external field by changing magnetization in series of avalanches. Thin line = model prediction, straight-dashed = power-law distro at the critical point.

Crackling noise - model

Simple model of a magnetic material.

- Cubic grid of magnetic domains S_i that have ± 1 north pole orientation
- External field represented by $H(t)$
- Randomness in domain shapes and other disorder by h_j

Net force on domain $= H(t) + \Sigma_{n.n} J S_j + h_i$

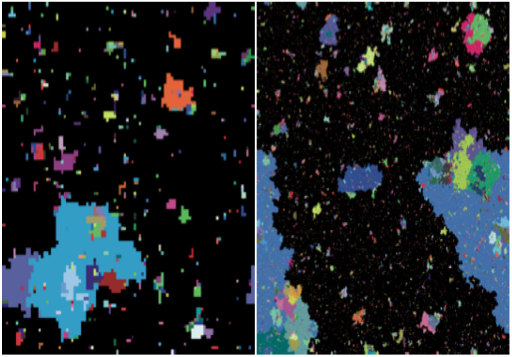


(a). Anisotropic layered structure

(b). Isotropic uniform structure

Crackling noise - model

Results (cross section slices) from the model run at the critical point where avalanches barely continue.



Each avalanche drawn in different color. Left is 100^3 domains, right is 1000^3 domains. Simple models do a decent job predicting the scaling.

Previous work

- Atomic diffusion in oriented single crystal $Cu_{90}Au_{10}$ at 540 K with XPCS
- Microstructure of avalanches during the Cobalt phase transition with XPCS
- Stacking faults in silicon (annealed in oxygen) with CXRD
- Charge density wave dislocation in $K_{0.3}MoO_3$ with CXRD

Focus: XPCS in $Cu_{90}Au_{10}$

What do they do?

- Monitor spatial/temporal variations of scattered xray along several directions in reciprocal space
- probe decay times as function of crystal orientation, tells you about motion of atoms on the lattice (diffusion direction)
- look at autocorrelation function $g^{(2)}$ because it's related to van Hove's pair correlation function G(dx,dt) (under certain assumptions), which tells you about the probability for a site to be occupied given where it was at the previous time step
- assume a model (dilute substitutional alloy on a bravais lattice) so you can calculate decay law and compare with experiment

In the end, you calculate autocorrelation functions and fit exponentials to them

Focus: XPCS in $Cu_{90}Au_{10}$

Scales?

- Mean time between exchanges at 543 K is 37±1 min
- Bulk diffusivity of $10^{-24} m^2/s$, smallest ever measured
- time series collected for 2 hours, 10s exposure per frame

What do they learn?

- model with nearest neighbor exchange reproduces measurements better than second nearest neighbor jumps
- dynamical behavior depends on the neighborhood!
- in some sense they setup the experiment this way. One could increase short range order, by lowering T or increasing Au, and approximations would break down

Designing an experiment

Desirable properties

- Strong scatterer
- Easy to induce dislocations mechanically
- Few complicating factors

Ideas

- Elemental (or ball milled powder?) iron/lead with a screw
- Nanoislands perhaps as function of temperature
- slowly compressed nickel micro crystals (avalanche)

What would we learn?

- Hopefully something about creep, climb, micro avalanche, pinning
- Are local or non local effects important, compare with a model
- Characteristic time and length scales

In the end we just want to see changes as we change the parameters of the experiment (turn the screw, increase the T, etc)