Lecture 17 - Dislocation Theory

Dr. Nicholas Smith

Wichita State University, Department of Aerospace Engineering

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schedule

- 14 Apr - Project Work Day
- (19 Apr) - Class Canceled
- Project Work Days

outline

- dislocation theory
- dislocations in elasticity
- peach koehler force
- discrete dislocation dynamics

dislocation theory

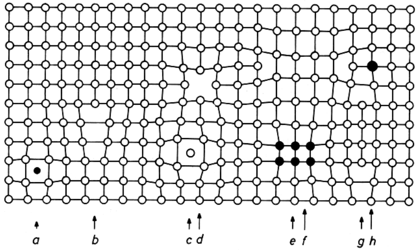
damage vs. dislocation

- We previously discussed a couple of damage models for materials
- Void growth for ductile materials and micro-crack coalescence for brittle materials
- Sometimes initial defects are neither voids nor micro-cracks
- Dislocation theory attempts to model the effects of material discontinuities that are not cracks

material defects

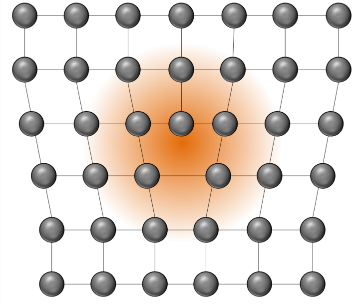
- There are many different types of material defects
- 0-dimensional defects
  - Point defects (vacancies, interstitials)
  - Impurity atoms
- 1-dimensional defects
  - Dislocations
- 2-dimensional defects
  - Stacking faults
  - Grain boundaries
- 3-dimensional defects
  - Voids
  - Precipitates
  - More complicated stacking faults

material defects

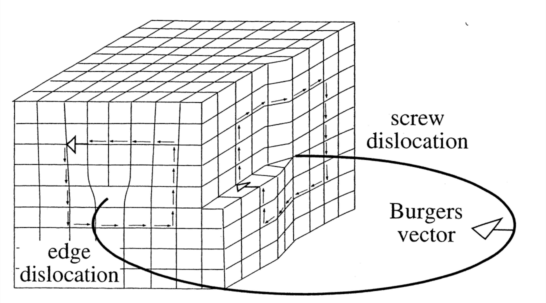


a) Interstitial impurity atom, b) Edge dislocation, c) Self interstitial atom, d) Vacancy, e) Precipitate of impurity atoms, f) Vacancy type dislocation loop, g) Interstitial type dislocation loop, h) Substitutional impurity atom

edge dislocations



screw disolcation



dislocation animations

- link[1]

[1] https://www.doitpoms.ac.uk/tlplib/dislocations/dislocation_motion.php

- There are multiple ways of modeling discontinuities
- Elasticity Theory - strong discontinuity in the displacement field
- Peach-Koehler force
- Discrete Dislocation Dynamics

dislocations in linear elasticity

screw dislocation

- A Volterra dislocation is defined as a discontinuity of the displacement field over a line segment or surface
- For screw dislocations, we consider the anti-plane problem with $u_1 = 0$, $u_2 = 0$, $u_3 = w(x, y)$
- For an isotropic material, the only non-zero stress and strain components are

$$\epsilon_{13} = \frac{1}{2}\frac{\partial w}{\partial x} \qquad \epsilon_{23} = \frac{1}{2}\frac{\partial w}{\partial y}$$

and

$$\sigma_{13} = \mu\frac{\partial w}{\partial x} \qquad \sigma_{23} = \mu\frac{\partial w}{\partial y}$$

screw dislocation

- There is only one non-trivial equilibrium equation in this case

$$\frac{\partial \sigma_{13}}{\partial x_1} + \frac{\partial \sigma_{23}}{\partial x_2} + \frac{\partial \sigma_{33}}{\partial x_3} = 0$$

- Which gives the governing equation

$$\frac{\partial^2 w}{\partial x_1^2} + \frac{\partial^2 w}{\partial x_2^2} = \nabla^2 w = 0$$

screw dislocation

- We can now convert the governing equation to polar coordinates

$$\nabla^2 w = \left(\frac{\partial^2}{\partial^2 r} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} \right) w = 0$$

- Solving by the separation of variables with $w(r, \theta) = f(r)g(\theta)$ we find two ODE's

$$\frac{d^2 f}{dr^2} + \frac{1}{r}\frac{df}{dr} - \frac{n^2 f}{r^2} = 0$$
$$\frac{d^2 g}{d\theta^2} + n^2 g(\theta) = 0$$

screw dislocation

- The only admissible solution (with finite displacement at $r = 0$) to this is

$$g(\theta) = A + B\theta$$
$$f(r) = C \ln r + D$$

- We require $C = 0$ since our solution must be valid at $r = 0$, and the jump condition means $A = 0$

- Further, since θ is a "constant" in r, we can combine the remaining constants, B and D to find

$$w(r, \theta) = B\theta$$

screw dislocation

- The jump condition requires that

$$w(r, 2\pi) - w(r, \theta) = b$$

- Hence

$$w(r, \theta) = \frac{\theta b}{2\pi}$$

$$w(x, y) = \frac{b}{2\pi} \arctan\left(\frac{y}{x}\right)$$

edge dislocation

- We can use an Airy stress function in plane strain to solve the edge dislocation problem
- See derivation in text pp. 303-305
- Elasticity solutions are not often able to model dislocations very well
- Some simple estimates (energy per unit length) are generally useful when applied within appropriate limits of the solution

peach koehler force

peach koehler force

- If we consider a dislocation loop that undergoes some virtual displacement
- We can find the virtual work done by this virtual displacement
- The decrease in potential energy due to the virtual displacement is the external virtual work done along the dislocation loop

$$\delta E = -F \cdot \delta\eta = -\int_L F_l dl \cdot \delta\eta$$

- This is the Peach-Koehler equation, and it can be used to predict the direction a dislocation will move under external stresses

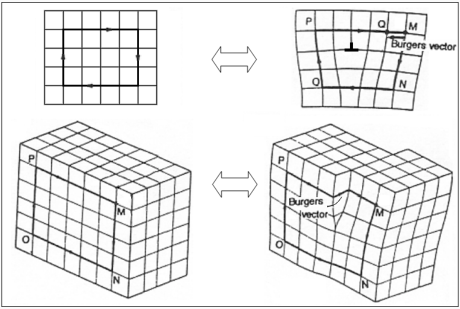
peach koehler force

- The Peach-Koehler force can be expressed in a simplified form as

$$F_l = g \times t$$

- Where t is the unit vector of the dislocation line and $g = \sigma \cdot b$ where b is the Burger vector

burger vector



examples

- straight screw dislocation
- straight edge dislocation

discrete dislocation dynamics

discrete dislocation dynamics

- There are many different forms of discrete dislocation dynamics analyses
- One form is based on the Galerkin weak formulation, used in finite elements
- The virtual work principle is used to build the formulation

discrete dislocation dynamics

- In addition to the usual virtual displacements, there are other internal work components to be considered
- These are often lumped together with friction, but also can included chemical forces (Osmotic force)
- Multiple dislocation loops can be discretized to transform the integral for virtual work into a summation