MSE160 Notes: Materials NTK

Eli Scott and Aman Bhargava

April 29, 2019

Contents

0.1 Basic Properties

- **Resilience**: Ability to absorb energy and recover it upon unloading (elastic energy)
- **Tensile Strength**: Absolute peak stress on stress-strain curve.

- **Fracture Toughness**: K_c, Fracture toughness (amount of energy absorbed before rupture)
- **Polymorphism**: Ability to have more than one molecular structure.
- **Amorphous**: Non-crystalline solid w/o long-range order.
- **Yield Stress**: Stress that causes 0.2% elastic deformation.
- **Cathodic Protection**: When you use an anodic material to protect a cathodic material from corrosion.

0.2 Material Design

1. Choose what to min/max
2. Decide on functionality (supporting, min deflection)
3. Decide objectives
4. Decide constraints
5. Figure out free var
6. Derive function for objective and constraints
7. Eliminate free variable using constraints
8. Solve for geometric/functional/material parameters
9. Always maximize
10. Cost parameter = material index/cost per kg

0.3 Crystal Structures

Theoretical Density:

$$\rho = \frac{n * A/N_a}{V_c}$$

Where n is the number of atoms per unit cell, A is the atomic mass, N_a is avogadro's number, and V_c is the volume of the unit cell.

0.3.1 Simple Cubic

- Packing efficiency: 52.4%
- Coordination number: 6
- One atom at each corner.

0.3.2 Body Centered Cubic

- Packing efficiency: 68%
- Coordination number: 8
- One atom in the middle and one atom at each corner.
- Slip system: plane = $(0, 1, 1)$, direction = $< 1, 1, 1 >$

0.3.3 Face Centered Cubic

- Packing efficiency: 74%
- Coordination number: 12
- Eigth of atom at corners. Half atoms on each face.
- Slip system: plane = $(1, 1, 1)$, direction = $< 1, 1, 1 >$

Trend for coordination number in ionic crystal $\frac{r_{cation}}{r_{anion}}$

0.3.4 Ductile-Brittle Transition

BCC and polymers experience transition from brittle to ductile from low to high temperatures.

0.4 Strength of Crystalline Materials (Metals)

0.4.1 4 Strengthening Mechanisms:

1. Alloying (larger and smaller atoms)
2. Precipitation/"particle" strengthening (relies on the fact that distortions can't easily pass through graini boundaries)

3. Cold work/work hardening
4. Grain size reduction

Equation to fit work hardening stress-strain response

$$\sigma_t = K(\epsilon_t)^n$$

Where t indicates 'true' as opposed to engineering values, K is a constant and n is the hardening exponent.

0.4.2 Conditions for Substitutional Solid Solutions

- $\Delta r < 15\%$
- Similar electronegativities
- Same crystal structures
- Similar valences

Empiric relationship between σ_y and concentration of alloy C: $sigma_y \sqrt{C}$

0.4.3 Resolved Shear Stress:

$$\tau_r = \sigma_o * cos(\lambda) * cos(\phi)$$

λ is the angle between the σ_o and the plane, ϕ is the angle between the normal of the plane and σ_o

$\tau_{crss} = \frac{\sigma_y}{2}$ is the critical resolved shear stress.

0.4.4 Defects

Types of Defects:

1. Point defects (vacancy, self-interstitial, substitutions)
2. Linear defects (dislocations)
3. Area defects (grain bounds)

Conditions for dislocation motion: $\tau_r > \tau_{crss}$

0.4.5 Equilibrium Concentration of Point Defects

$$\frac{N_v}{N} = exp(\frac{-Q_v}{kT}$$

Where $\frac{N_v}{N}$ is the ratio of vacancies to potential vacancies (i.e. number of atoms), Q_v is activiatioin energy, k is Boltzmann's constant, and T is temperature.

0.4.6 Fatigue

Fatigue is cyclic stressing. Here are the main parameters:

1. S: amplitude of cyclic stress
2. σ_0: mean stress
3. Frequency of stressing

$$\frac{da}{dN} = \Delta K^m$$

Where a = half crack length, N = number of cycles, ΔK $\Delta\sigma * \sqrt{(a)}$, m is a constant

S_{fat} **is the minimum** S **for fatigue behavior.**

0.4.7 Hall-Petch Equation

Gives you σ_y from grain size.

$$\sigma_y = sigma_0 + k_y * d^{-1/2}$$

Where σ_0 and k_y are constants and d is the diameter of the grain size.

0.5 C R A C K

0.5.1 Griffith's Formula: σ_m

Crack tip stress.

$$\sigma_m = 2 * \sigma_o * \sqrt{a/p_t}$$

Where p_t is the radius of curvature, a is half crack length, and σ_o is the applied stress.

Propagation criterion: When $\sigma_m > \sigma_c$

0.5.2 σ_c

Critical stress,

$$\sigma_c = \sqrt{2E\gamma_s}\pi * a$$

Where E is modulus of elasticity, γ_s is the specific surface energy (add γ_p = plastic deformation energy if ductile), a is half crack length.

Basically just the stress that cracks can withstand before propagating.

0.5.3 K

At crack failure,

$$K_c = Y * \sigma * sqrt\pi * a$$

Where K_c is fracture toughness of material, Y is a constant, and a is the half crack width.

Two failure cases here: either cracks are too large or σ is too large.

0.6 Electrical Properties

0.6.1 4 Ways to Increase Resistivity?

1. Increase temperaturre
2. Increase grain boundaries, dislocations
3. Add impurities
4. Add vacancies

Calculating resistance of a sample: $R = \frac{L}{A*\sigma}$

0.6.2 P vs. N-Type Doping

P-type brings the acceptor band down significantly. N-type brings the donor band up. P-type results in more free holes, N-type results in more free electrons.

Current Density $= J = I/A =$ current/cross sectional area.

Electric Field Potential $= E = V/L$

0.6.3 New Ohm's Law

$$J = \sigma * E$$

0.6.4 Calculating σ

$$\sigma = n|e|\mu_e + p|e|\mu_h$$

Where n is the number of mobile electrons, p is the number of holes, μ_e is electron mobility and μ_h is the hole mobility.

Voltage threshold for semiconductors: $2eV$