MSE160 Notes: Materials NTK

Eli Scott and Aman Bhargava

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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.

0.3.3 Face Centered Cubic

- \bullet Packing efficiency: 74%
- Coordination number: 12
- $\bullet\,$ Eighh of atom at corners. Half atoms on each face.
- Slip system: plane = (1, 1, 1), direction = $\langle 1, 1, 1 \rangle$

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 activiation 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, $\Delta K \ \Delta \sigma * \sqrt(a)$, 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 CRACK

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 $\sigma_m > \sigma_c$

$0.5.2 \quad \sigma_c$

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