Materials selection

CES Software

Engineering Materials

Metal & Alloys

steel-cored tyres — Composites 复合材料 — wire-reinforced cemet 刚丝加劲混凝土

cermets 金属陶瓷

CFRP 碳纤维增强复合材料

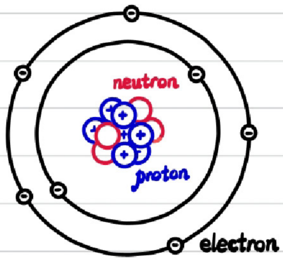
GFRP 玻璃纤维增强塑料（玻璃钢）

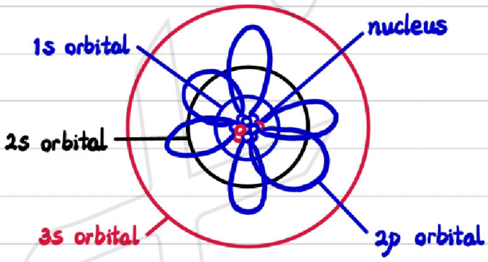
filled polymers 填充聚合物

Polymers 聚合物 — Ceramics 无机非金属

Bonding between atoms

The atom



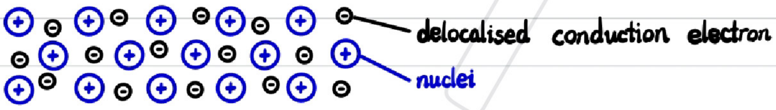


- orbital have shapes
- orbital have directionality

→ affect atom arrangement in soild

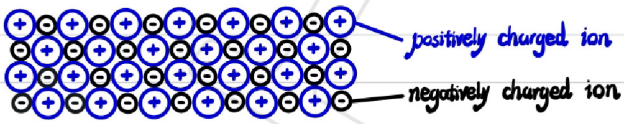
Primary bonds relatively strong

Metallic bond Al、Cu、Ag、Mg、Ti ...



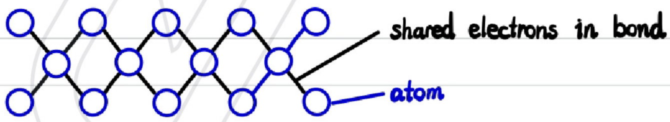
- strong bond
- non-directional
- electrons are very mobile → strong thermal and electrical conductivity
- free electrons reflects photons → shiny

Ionic bond NaCl、SiC ...



- strong bond
- non-directional
- don't conduct electricity → good insulator (in soild state)

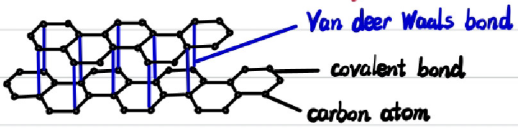
Covalent bond Diamond ...



- very strong bond
- highly directional
- no conductivity → good insulator

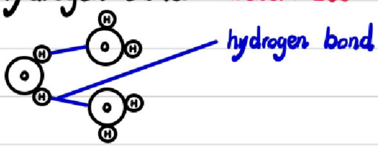
Secondary bonds relatively weak bonding by electrostatic attraction between electrically neutral molecules

Van deer Waals bond Graphite between layers, Argon gas ...



· weak bond · non-directional

Hydrogen bond Water, Ice ...



· weak bond · directional

Mixed bonds

Metals metallic (mainly) + covalent bond stiff and strong + high melting point + conductive materials

Ceramics covalent (mainly) bond very stiff and strong + very high melting point + very good insulator

Polymers long chains of macromolecules 高分子 covalent bonds + chains interact by secondary bonds
chain is very strong but adhere 粘附 weakly to other chains + very low stiffness and strength
+ very low melting point + no conductivity

Fundamental Mechanical Properties of Metals

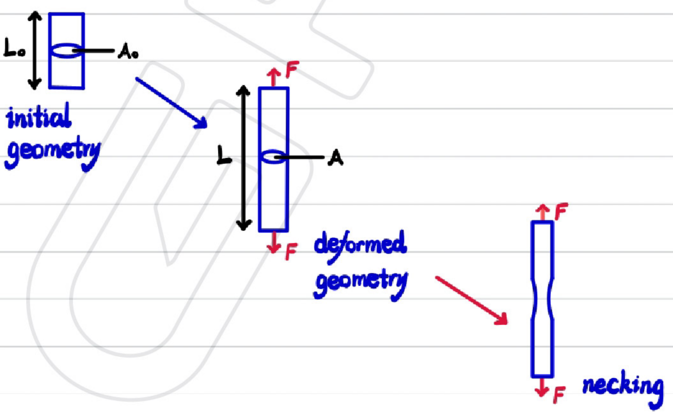
Structure insensitive Density $\rho = \frac{dm}{dV}$ kg/m³ Young's Modulus $E = \frac{\partial \sigma}{\partial \varepsilon}$ N/mm²

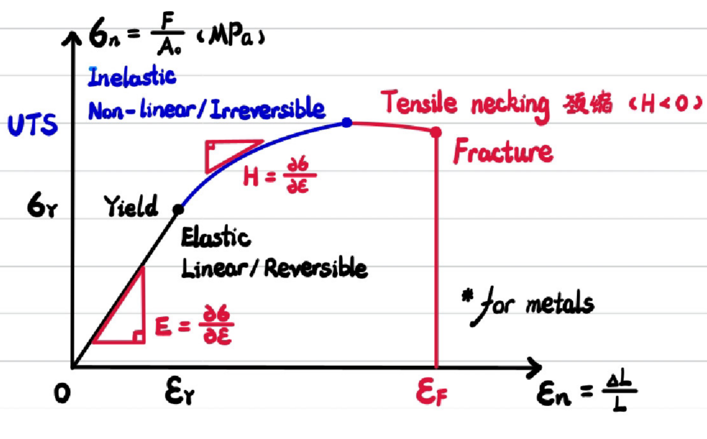
Structure sensitive Yield stress σ_Y N/mm² Yield strain ε_Y Ductility ε_F

Hardening Modulus $H = \frac{\partial \sigma}{\partial \varepsilon}$ N/mm² Ultimate Tensile Stress UTS N/mm²

Fracture toughness resistance to crack propagation 传播 K_{Ic} $N\sqrt{mm}/mm^2$

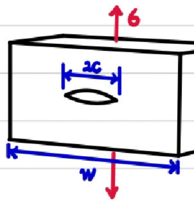
Uniaxial 单轴的 Tensile Test





Fracture Toughness

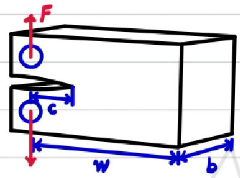
Central-cracked plate



failure stress

$K_{1c} = \sigma^* \sqrt{\pi c}$ ($c \ll W$)

Compact tension



failure load

$K_{1c} = 1.64 \frac{F^*}{bW}\sqrt{\pi c}$ ($c \ll W$)

Procedure for Selection

① Translate design requirements · function · constraints · objectives · free variables

⟶ solution material choice that meet all the constraints

② Screening using constraints eliminate materials that can not do the job

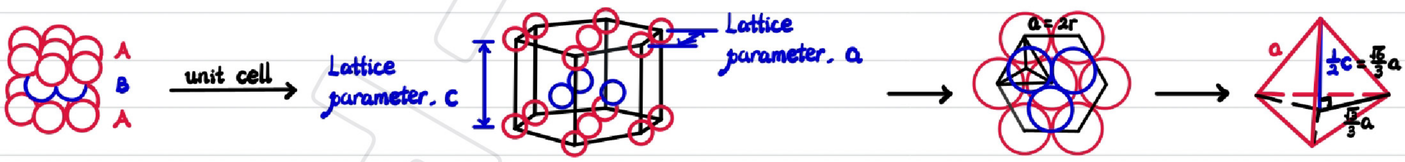
③ Rank using objective ⟶ performance metric / 'material indices' ⟶ gradients on Ashby Graphs

Metals

Polymorphism 同质多晶

Crystal structures

HCP (Hexagonal Closed Packed) Crystals Mg, Ti at room temperature, Co at room temperature

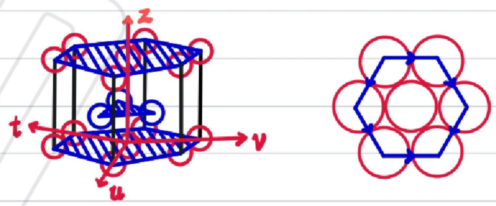


Z coordination number number of atoms in direct contact with a certain atom $= 6 + 2 \times 3 = 12$

N number of spheres in unit cell $= 3 + 12 \times \frac{1}{6} + 2 \times \frac{1}{2} = 6$

$\frac{V_{atom}}{V_{cell}}$ packing density $= \frac{6(\frac{4}{3}\pi r^3)}{[6(\frac{1}{2}\cdot a \cdot \frac{\sqrt{3}}{2}a)]\cdot c} = \frac{6(\frac{4}{3}\pi r^3)}{[6(\frac{1}{2}\cdot 2r \cdot \sqrt{3}r)]\cdot \frac{4}{3}\sqrt{6}r} = \frac{8\pi r^3}{24\sqrt{2}r^3} = \frac{\sqrt{2}}{6}\pi = 0.74$

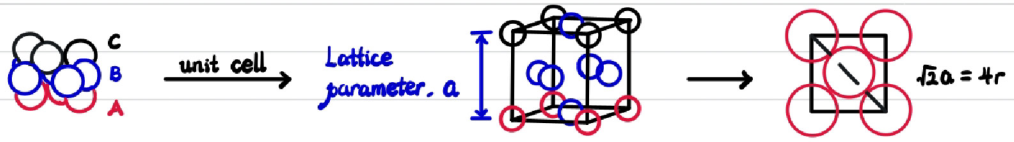
slip system



Closed packed planes $\{0001\}$

Closed packed directions $\langle 11\bar{2}0 \rangle$

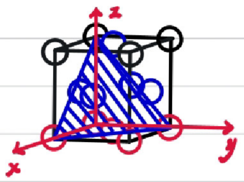
FCC (Face Central) Crystals   Al, Ni, Fe at high temperature, Co at high temperature

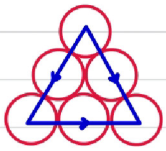


Z coordination number $= 4 + 2\times 4 = 12$ N number of spheres in unit cell $= 8\times\frac{1}{8} + 6\times\frac{1}{2} = 4$

$\frac{V_{atom}}{V_{cell}}$ packing density $= \frac{4(\frac{4}{3}\pi r^3)}{a^3} = \frac{4(\frac{4}{3}\pi r^3)}{(2\sqrt{2}r)^3} = \frac{\frac{16}{3}\pi r^3}{16\sqrt{2}r^3} = \frac{\sqrt{2}}{6}\pi = 0.74$

slip system

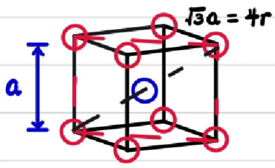




Closed packed planes {1 1 1}

Closed packed directions < 1 1 0 >

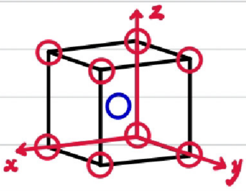
BCC (Body Central) Crystals   Ti at high temperature, Fe at room / very high temperature

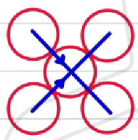


Z coordination number $= 2\times 4 = 8$ N number of spheres $= \frac{1}{8}\times 8 + 1 = 2$

$\frac{V_{atom}}{V_{cell}}$ packing density $= \frac{2(\frac{4}{3}\pi r^3)}{a^3} = \frac{\frac{8}{3}\pi r^3}{(\frac{4\sqrt{3}}{3}r)^3} = \frac{\sqrt{3}}{8}\pi = 0.68$

slip system





Closed packed planes   No

Closed packed directions < 1 1 1 >

Polymorphism   pure metals can have more than one crystal structure at different temperature

Basics Strengthening Mechanisms

Soild solution strengthening

· strength ↑   · ductility ↓ more brittle

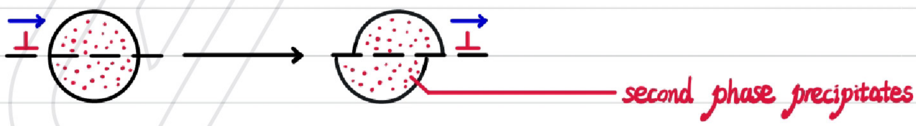
 substitutional replace host atom    interstitial fit into gap between host atom

distortion by the solute atoms ⟶ dislocation hindered by the interaction of the stress - strain field

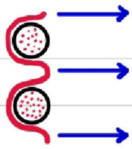
Precipitation strengthening

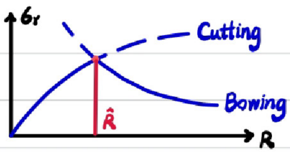
· strength ↑   · ductility ↓ more brittle

Cutting ⟶ numerious + close - spaced + small particles cut by dislocations ⟶ larger shear force required



Bowing ⟶ fewer + wide - spread + large particles bowed - around by dislocations ⟶ larger shear force required



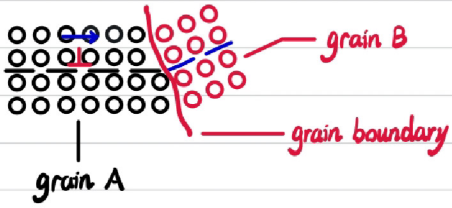


Grain refinement strengthening

· strength ↑ · ductility ↑ more ductile

reduce grain size ⟶ increase grain boundary area ⟶ increase material strength

* grain boundary is barrier to slip ⟶ dislocation change direction ⟶ discontinuity in slip planes

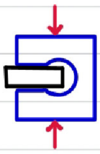


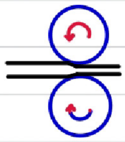
Hall-petch equation $\sigma_y = \sigma_0 + k_y d^{-\frac{1}{2}}$

Work hardening

· strength ↑ · ductility ↓ more brittle

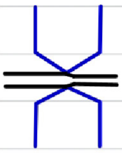
cold work increase dislocation density interacting each other ⟶ stress ⟶ hiders other dislocations

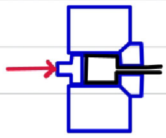

forging


rolling

changing cross-sectional area

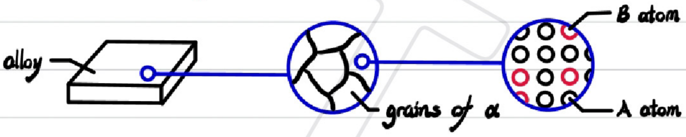
$$CW\% = \frac{A_0 - A_d}{A_0} \times 100\%$$


drawing


extrusion

Basics

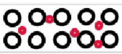
Alloys mixed of elements — dominate material must be metal



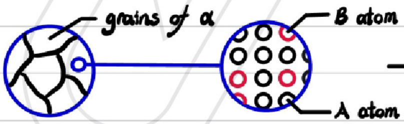
* grains growth by soildification

Soild solutions form by mixed of elements

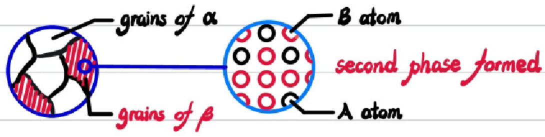

substitutional


interstitial

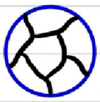
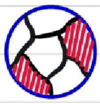
Solubility limit



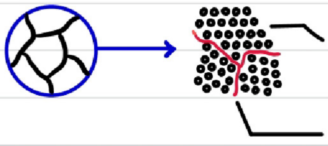
$\xrightarrow{\text{adding B atoms}}$ exceed solubility limit



Phase a region of material with uniform physical and chemical properties

 single-phase  two-phase

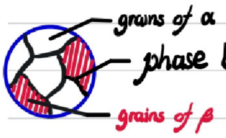
Grain boundaries

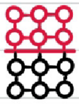
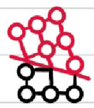


grain a region with same crystal orientation

grain boundary $\gamma_{gb} \sim 0.5\,J/m^2$ * faster diffusion * 'outsized' impurity atoms diffuse to gb

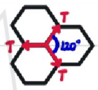
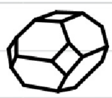
Phase boundaries

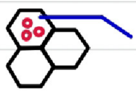
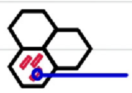


 coherent 连贯地 → coherency strain → semi-coherent →  incoherent

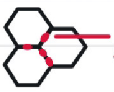
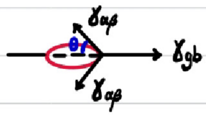
$\gamma_{\alpha\beta} \sim 0.05\,J/m^2$ $\gamma_{\alpha\beta} = \gamma_{gb} \sim 0.5\,J/m^2$

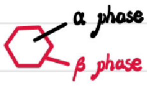
Shapes of grain shapes that minimises the total interfacial 界面的 energy $E = \gamma_{gb} \cdot A$

1-phase $\xrightarrow{\gamma_{gb} \text{ is isotrophic}}$ A_{max} with E_{min} $\xrightarrow{2\text{-}D}$  $\xrightarrow{3\text{-}D}$  tetrakaidecahedron 十四面体

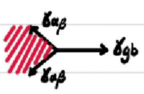
2-phase $\xrightarrow{\gamma_{\alpha\beta} \text{ is isotrophic}}$  spherical crystals $\xrightarrow[\gamma_{\alpha\beta} \text{ depends on orientation between } \alpha \text{ and } \beta]{\gamma_{\alpha\beta} \text{ is non-isotrophic}}$  a plate

Interphase 相于相间 boundaries meet

 β forms at α grain boundaries → balance of surface tensions  $\gamma_{gb} = 2\gamma_{\alpha\beta}\cos\theta$



$\xrightarrow{\gamma_{\alpha\beta} \le \frac{1}{2}\gamma_{gb}}$ $\theta = 0$ β phase spread along α grain boundaries

 $\xrightarrow{\gamma_{\alpha\beta} = \gamma_{gb}}$ $\theta = 60°$ tetrakaidecahedral * $\xrightarrow{\gamma_{\alpha\beta} \ne \gamma_{gb}}$ complex β grain shapes to achieve E_{min}

Alloy system all the alloy can be made from the components

Components the elements that makes up an alloy

Composition 构成 usually measured in weight (mass) %

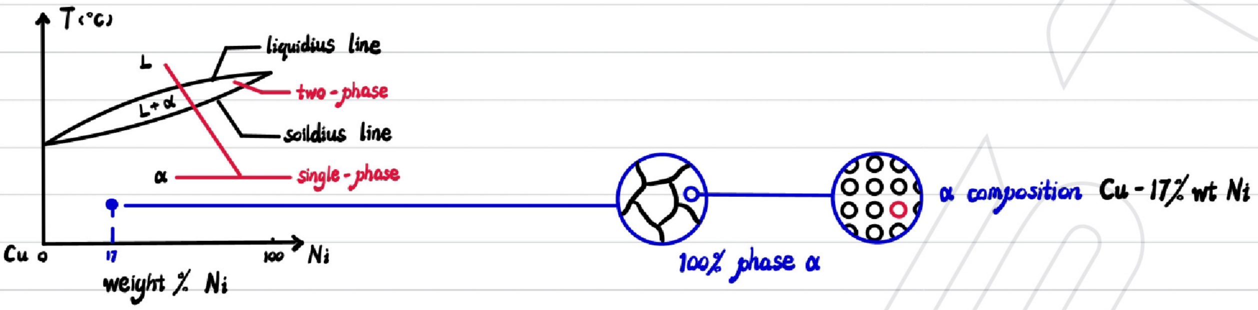
Consititution 组成 overall composition + number of phases + composition of each phase + volume % of each phase

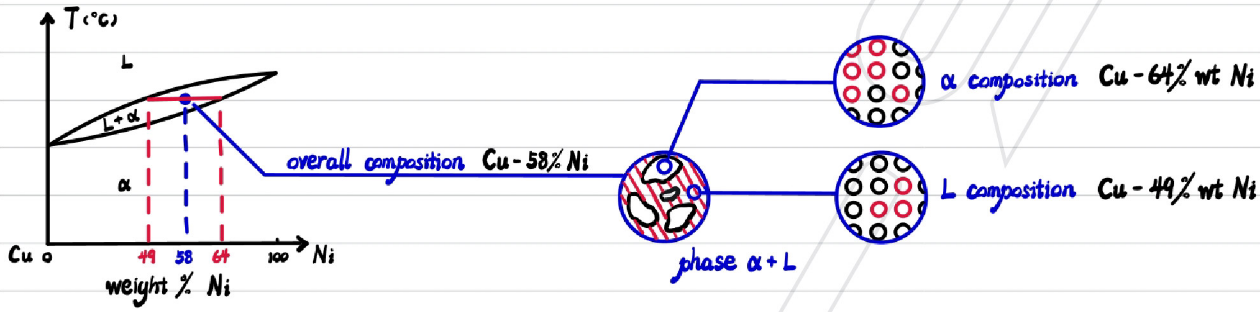
Alloy consititution = overall composition + temperature

Geometry of the microstructure = (size + spacing + shape) of the grain + processing route

Phase Diagrams

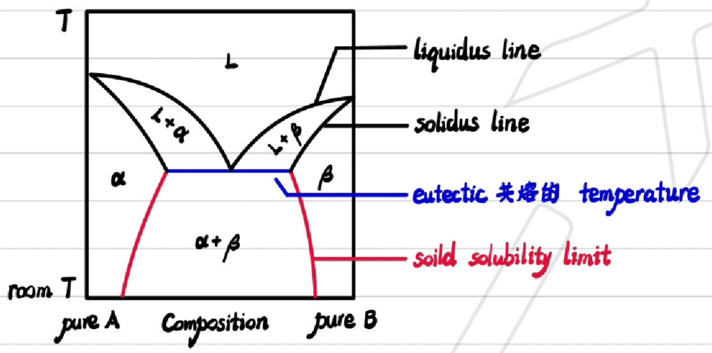
Binary phase diagram   no solubility limit

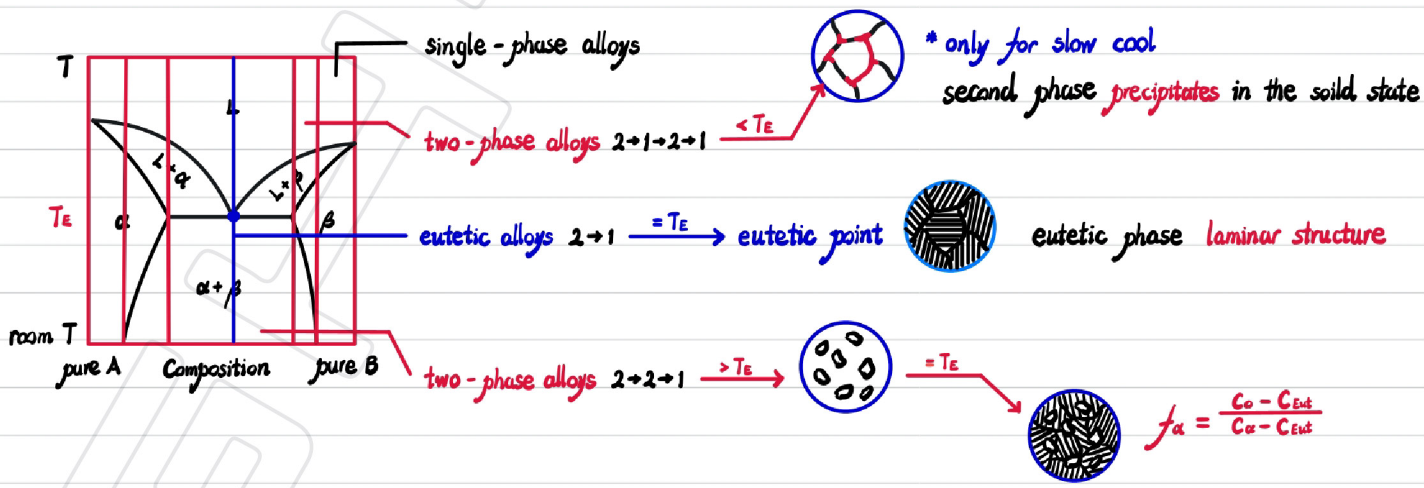




$\longrightarrow f_\alpha + f_L = 1$ and $64\%\,wt\, f_\alpha + 49\%\,wt\, f_L = 58\%\,wt \longrightarrow f_\alpha = 60\%$ and $f_L = 40\% \longrightarrow f_\alpha = \frac{C_0 - C_L}{C_\alpha - C_L}$

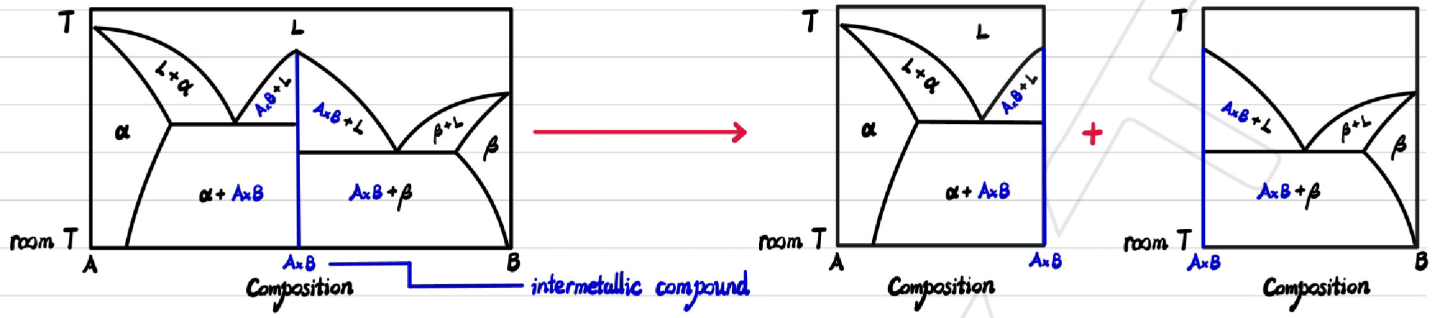
Eutectic phase diagram   with solubility limit





Eutectic system

Eutetic $L \rightarrow$ 2 soilds   Peritectic 包晶的 L + soild $\longrightarrow$ new soild   Eutectoid 共析的 1 soild $\longrightarrow$ 2 soilds



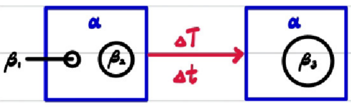
Phase Transformation

Driving force W_f free work available $\doteq -\Delta U$ change in internal energy

Gibbs energy $G = H - TS$

ΔG Gibbs free energy $= \Delta H - T\Delta S \xrightarrow{\Delta G < 0}$ driving force to change $\longrightarrow$ phase transformation

Coarsening 晶粒粗大化



* $V_{\beta_3} = \frac{4}{3}\pi r_3^3 = V_{\beta_1} + V_{\beta_2} = \frac{4}{3}\pi r_1^3 + \frac{4}{3}\pi r_2^3$

$\Delta G = (A\gamma)_{final} - (A\gamma)_{initial} = 4\pi\gamma\left[(r_1^3 + r_2^3)^{\frac{2}{3}} - (r_1^2 + r_2^2)\right] \xrightarrow{\text{very low } \gamma}$ minimises precipitate growth

Undercooling 过冷

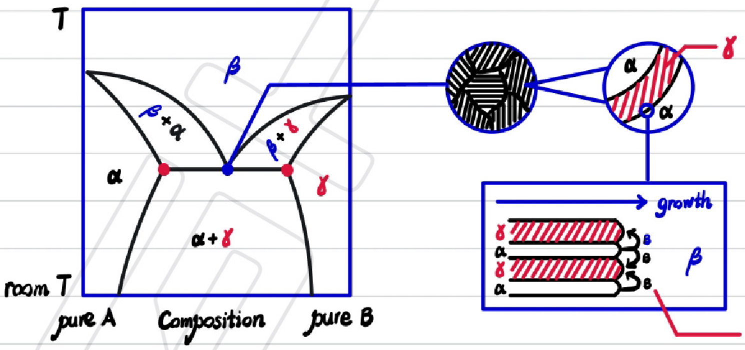
$0 = \Delta H - T_m$ melting temperature $\Delta S \xrightarrow{\text{near } T_m}$ for $T < T_m$, $\Delta G = \Delta H - T\frac{\Delta H}{T_m} = \Delta H\left(\frac{T_m - T}{T_m}\right)$

opposites

* from kinetic side $T\downarrow \longrightarrow$ probability the atom jump from liquid to soild $\downarrow$

Diffusion mass transport by atomic motion

Eutectoid growth $\beta \xrightarrow[\text{very short time}]{\text{simultanious growth}} \alpha$ small amount of B + γ exceed solubility limit large amount of B



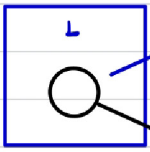
eutectoid phase laminar structure

eutectoid transformation

B find fastest path leave α join γ going to neighbouring phases

Nucleation form grains

Nucleating soild in a liquid



S-L interface is formed $\Delta G_{interface} = A\gamma_{SL}$

spherical soild nucleus

$\Delta G = -V\Delta G_V + \Delta G_{interface} = -\frac{4}{3}\pi r^3 G_V + 4\pi r^2 \gamma_{SL}$

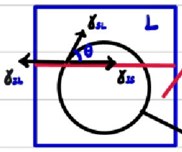
gained (first term), required (second term)

phase transformation $(-\Delta G)$ when $\frac{d\Delta G}{dr} < 0$ $\xrightarrow{\frac{d\Delta G}{dr}=0}$ $r_{crit} = \frac{2\gamma_{SL}}{\Delta G_V}$

$\xrightarrow{\text{near } T_m}$ for $T < T_m$, $\Delta G = \Delta H\left(\frac{T_m - T}{T_m}\right)$ $\longrightarrow$ $r_{crit} = \frac{2\gamma_{SL} T_m}{\Delta T \Delta H} \propto \frac{1}{\Delta T} = \frac{1}{\text{rate of undercooling}}$

Heterogeneous 异质 nucleation

nucleation occurs on the surface of crucible / inclusions 包裹体



inclusion

spherical soild nucleus

* nucleants 成核剂 TiB_2 or Al_3Ti

** also happened on defect in soild phase

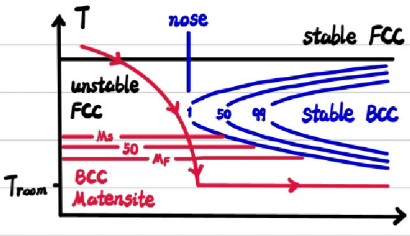
Homogeneous no defects very rare $V_{crit} = \frac{4}{3}\pi r_{crit}^3$ > Heterogeneous $V_{crit} = \frac{\pi}{3}(2 - 3\cos\theta + \cos^3\theta) r_{crit}^3$

$\xrightarrow{r_{crit}\downarrow \text{ for same } V}$ grain refinement strengthening

TTT (time - temperature - transformation) curves

Displacive (Martensitic) transformation

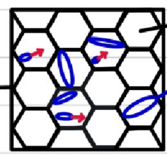
only for polymorphism



large driving force $\longrightarrow$ displacive transformation

$\Delta G \longrightarrow$ strain energy $\longrightarrow$ very hard

metastable BCC 优先级 < stable BCC



Steel

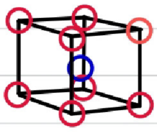
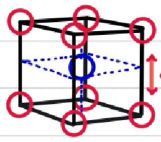
Phase in steel Ferrite δ-phase BCC Fe $\xrightarrow{T\downarrow}$ Austenite γ-phase FCC Fe $\xrightarrow{T\downarrow}$ Ferrite α-phase BCC Fe

Carbon steel Eutectic $L \rightarrow \gamma\text{-}Fe + Fe_3C$ Cementite Eutectoid = Pearlite * this case $\gamma\text{-}Fe \rightarrow \alpha\text{-}Fe + Fe_3C$

Mechnical properties of carbon steels

slow cooled $C\uparrow \xrightarrow{\%\text{ eutectoid}\uparrow} \%\,Fe_3C\uparrow \xrightarrow[Fe_3C \text{ is brittle}]{Fe_3C \text{ is a hard phase}}$ yield strengh↑ + UTS↑ + $\varepsilon_F\downarrow$ nucleate cracks

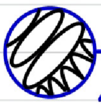
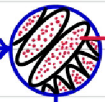
Martensite $C\uparrow \longrightarrow T_{Eutectoid}\downarrow + T_{Nose}\downarrow + t_{Nose}\uparrow \longrightarrow$ cooling rate ↓ for Martensitic transformation

 BCC Fe $\xrightarrow{C\uparrow}$  $\updownarrow \Delta L$ BCT (body centred tetragonal 四方) Fe stability ↑

└ more carbon distorted BCT lattice hardness ↑ + ductility ↓

Improve quenched 淬火 properties

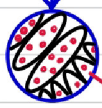
Tempering 退火 reheat after Matensitic transformation $\xrightarrow{E_{thermal}\uparrow}$ C diffuse out BCT-Matensite $\xrightarrow{\text{react with Fe}}$ $\alpha + Fe_3C$

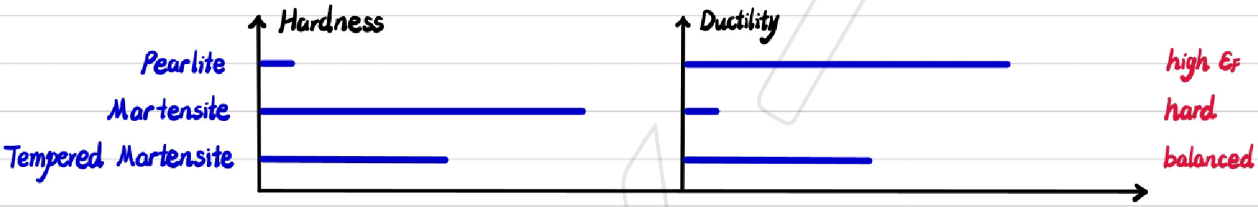
 Martinsite $\xrightarrow[\text{BCT} \rightarrow \text{BCC}]{T\uparrow \text{ in small } \Delta t}$  $\alpha + Fe_3C$

↓ $\varepsilon_F \uparrow$

small closely spaced Fe_3C ⟶ precipitation strengthening ↓ strength ↑ + hardness ↑

$\Delta t \uparrow$ — no ideal

 after coarsening ⟶ strength ↓ + hardness ↓



Engineering Steel 0.25 - 0.45 wt% C medium carbon steels

Alloying strategies

① improve hardenability adding Mo, Mn, Cr, Ni —— the ability of steel to form Matensite on quenching

② give soild solution strengthening Alloy and precipitation strengthening tempering by form carbides 碳化物

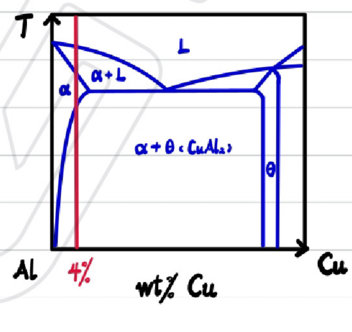
③ give corrosion resistance adding Cr

④ stabilise Austenite γ-phase at T_{room} adding Mn, Cr

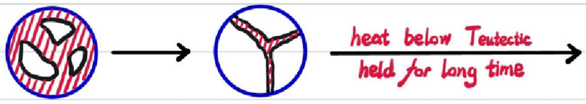
Alluminium Alloys

Lightweight material with $\rho < 4.5 g/cm^3$ at T_{room} $\xrightarrow{\times \text{ too reactive} \quad \times \text{ too expensive} \quad \times \text{ toxic}}$ Al, Mg, Ti

Al - 4Cu

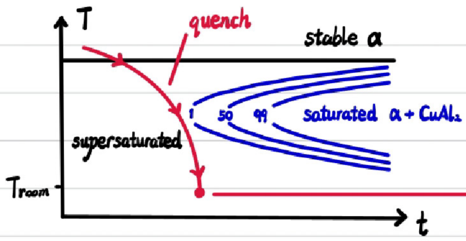


Homogenising 均质化 solution heat treatment



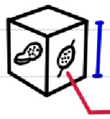
remove eutectic + homogenise solute content

SSSS supersaturated 过饱和的 soild solution



large -ΔG ⟷ little thermal energy → nucleation is difficult

* equilibrium CuAl₂ (θ)

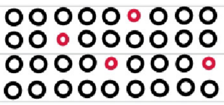


very different lattic parameter to α

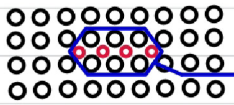
All interface incoherent

Precipitation sequence in Al-Cu

① initial quenched structure SSSS in α solid solution strengthening



② stage I Cu atom cluster 聚集 to form "Guinier-Preston zones" coherency stress strengthening

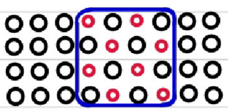


GP-zones disc-shaped

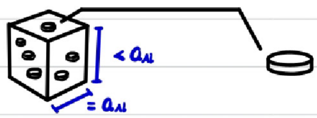
face coherent with α phase

edge coherent but with coherency strain

③ stage II GP-zones act as nucleation sites for metastable phase θ″ precipitation strengthening cut $\xrightarrow{\Delta t}$ bow-around

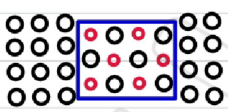


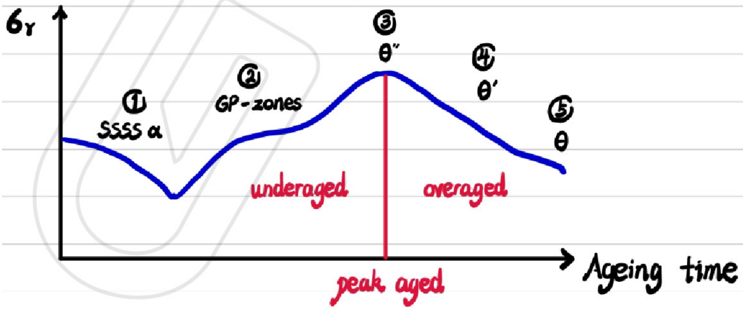
* tetragonal crystal for θ″



④ stage III another metastable phase θ′ form

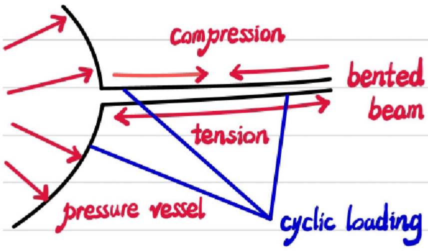
⑤ stage IV form equilibrium θ-CuAl₂ ⟶ all interface incoherent





Al naming system Cu 2xxx Mg and Si 6xxx Zn 7xxx Li 8xxx

Al alloy selection for aero-planes



upper wing · compressive strength · stiffness · fatigue resistance

lower wing · tensile strength · fatigue resistance · fracture toughness

fuselage · tensile strength · fatigue resistance · fracture toughness

Operating temperature at high speed $\xrightarrow{\text{friction}}$ elevated temperature *switch to Ti-alloys at M = 2

Magnesium Alloys

Advantages of Mg

· lightest structural material · precipitation hardenable like Al-alloys · good creep resistance 抗蠕变性

Disadvantages of Mg

· low melting point · low stiffness · low ductility HCP — only 1 slip plane · corrosion properties only OK

· very flammable banned in civil aircraft and F1 for a long time

Specific stiffness $\frac{E^n}{\rho}$

AZ31 Mg-3Al-1Zn satellite panels $\xrightarrow{\text{quenching + tempering}}$ $Mg_{17}Al_{12}$

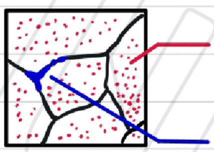
WE43 Mg-4Y-3Nd-Zr aero-transmission housings 变速箱体 at elevated temperature $\xrightarrow{\sim 250°C}$ $\frac{T}{T_m} > 0.3$

Advantages · best properties · high service temperature 200-300°C · superior strength to Al alloys at 250-300°C

Disadvantages · expensive than Al alloys · Y is difficult to handle

* 4% Y and 3% Nd $\xrightarrow{\text{high T}}$ completely dissolved $\xrightarrow{\text{quenched}}$ SSSS precipitation strengthening

** Zr act as nucleation sites to form fine grains grain refinement strengthening



small β'/β ppts against dislocation creep

retarding crack growth against diffusion creep * $\xrightarrow{\frac{T\uparrow}{\Delta t}}$ coarsening reduce strengthening

Titanium Alloys

Advantages of Ti

· lightweight $\rho \approx 4.5 g/cm^3$ · high melting point · excellent corrosion resistance

· high specific strength · excellent properties at elevated temperatures · good compatibility with CFRP

Disadvantages of Ti

· expensive to machine · low wear resistance 耐磨性 · difficult to form

· pick up oxygen and nitrogen above 500°C —— cannot recycling

Polymorphism Liquid Ti $\xrightarrow{T\downarrow}$ β-Ti BCC $\xrightarrow{T\downarrow}$ α-Ti CPH

α or β stabiliser α stabilisers O, Al, N, C β stabilisers V, Mo, Nb, Fe Neutral Sn, Zr

α alloys single phase at T_{room} —— no precipitation strengthening

Near-α alloys aeroengine compressor blade * α diffuse much slower ⟶ good creep resistance

α-β alloys aeroengine fan blade *

"basket weave" 编织篮子
structure of α plates between β
good fatigue resistance + good creep resistance

Near-β alloys landing gear

good strength at low T * do not consider creep performance

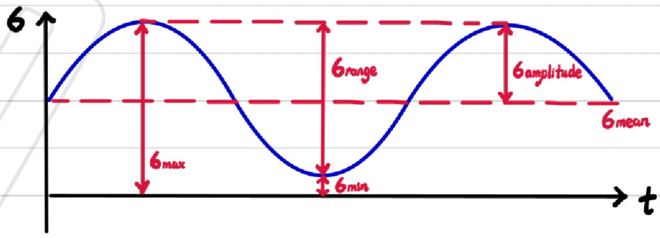
β alloys β-Ti with a few % α-Ti at T_{room}

very good strength at low T * β-Ti diffuse much faster than α-Ti poor properties at elevated T

Fatigue 疲劳

Fatigue of materials cyclic loading ⟶ fail at stress below tensile stress

Definitions



stress ratio $R = \frac{\sigma_{min}}{\sigma_{max}}$

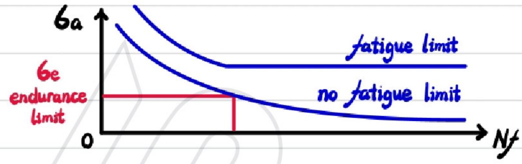
* $R = -1$ for load around $\sigma_{mean} = 0$

LCF (low cycle fatigue) $< 10^4$ cycles under relatively high $\sigma_{amplitude}$ $\sigma > \sigma_Y$

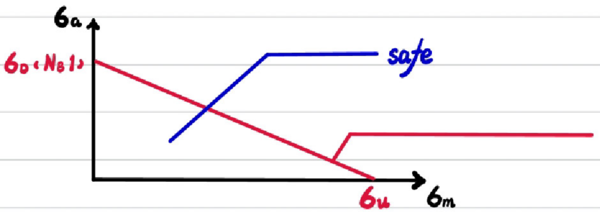
HCF (high cycle fatigue) $> 10^4$ cycles under relatively low $\sigma_{amplitude}$ $\sigma < \sigma_Y$

S-N curve stress amplitude $\sigma_a = \frac{\sigma_{max} - \sigma_{min}}{2}$ vs number of cycles N_f when $\sigma_{mean} = 0$

- tensile stresses lead to shortened life times crack opening
- compression to an extension in fatigue life crack closure

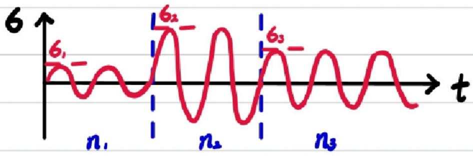


Goodman Law if $\sigma_{mean} \neq 0$



$\frac{\sigma_a}{\sigma_0} + \frac{\sigma_m}{\sigma_u} = 1$ empirical formula

Palmgren - Miner - Rule linear - damage accumulation 积累

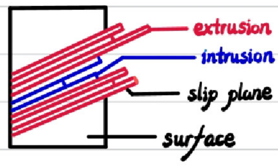


$\sum_i \frac{n_i}{N_i(\sigma_i)}$ < 1 survive; > 1 fail due to fatigue failure

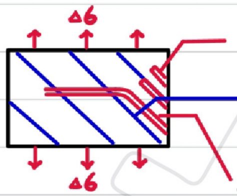
Fatigue crack initiation

LCF plastic deformation roughens the surface within small number of cycles

slip planes ⟶ sub-micrometre extrusions / intrusions ⟶ crack



* sources



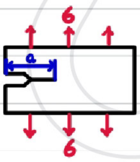
stage 1 crack initiate along the slip path

slip path

stage 2 crack grow perpendicular to tensile stress

HCF local plastic region notch 凹口 / scratch / change in section $\xrightarrow[\text{almost all the life}]{\text{concentrate the stress}}$ crack initiate

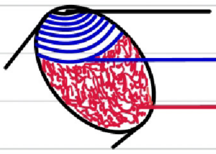
Fatigue crack growth



cyclic stress intensity factor $\Delta K = K_{max} - K_{min} = Y \Delta\sigma \sqrt{\pi a}$ * no crack growth when compression

critical crack size $K_c = Y \sigma_{max} \sqrt{\pi a_f} \longrightarrow a_f = \frac{1}{\pi} \left(\frac{K_c}{Y \sigma_{max}} \right)^2$ fatigue crack growth rate $\frac{da}{dN}$

Paris Law $\frac{da}{dN_f} = A(\Delta K)^m = A(Y\Delta\sigma\sqrt{\pi a})^m \longrightarrow N_f = \int_0^{N_f} dN = \frac{1}{AY^m\Delta\sigma^m\sqrt{\pi}^m}\int_{a_0}^{a_f}\frac{1}{\sqrt{a}^m}da$



initiation

crack propagation like beach marks

fracture each striation produced by single stress cycle

Predict fatigue lifetime

fail safe design compare σ_e fatigue limit to $\Delta K_{th} \longrightarrow$ threshold 门槛 ΔK crack no advancing below ΔK

* not sufficient as required large $A = \frac{F}{\sigma} \longrightarrow$ limited lifetime design Paris Law material insepection intervals

Creep 蠕变

Creep slow and continuous deformation with time at elevated T * $\varepsilon = f(\sigma, t, T)$

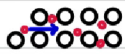
homologous temperature $\frac{T}{T_m}$ in K $\xrightarrow{>0.3}$ creep in metals

Diffusion net movement from a region of higher concentration to a region with lower concentration

Fick's Law J Flux $= -D$ diffusion coefficient $\frac{dc}{dx}$ concentration of molecules

Arrhenius equation $\dot{\varepsilon}_{ss}$ rate of reaction $= Ce^{-\frac{Q}{RT}}$ Q activation energy for thermally activated process

Diffusion mechanisms

solid solution interstitial diffuse much faster  substitutional  interstitial

grain boundary can act as fast diffusion paths * for small grain size, more grain boundaries

dislocation core can act as fast diffusion wires * for high dislocation density

Dislocation creep $\dot{\varepsilon} = A\sigma^n e^{-\frac{q}{kT}}$ temperature + applied stress relatively high

caterpilar modal

'unlocked' from obstacles e.g. precipitates

dislocation glide + dislocation climb = dislocation creep

$\longrightarrow$ Power Law creep

from dislocation creep at steady state + high stress level

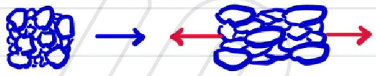
Diffusion creep $\dot{\varepsilon} = \frac{C6e^{-\frac{Q}{kT}}}{d^2}$ temperature + applied stress relatively low + grain size

at low stress level ⟶ Power Law falls quickly

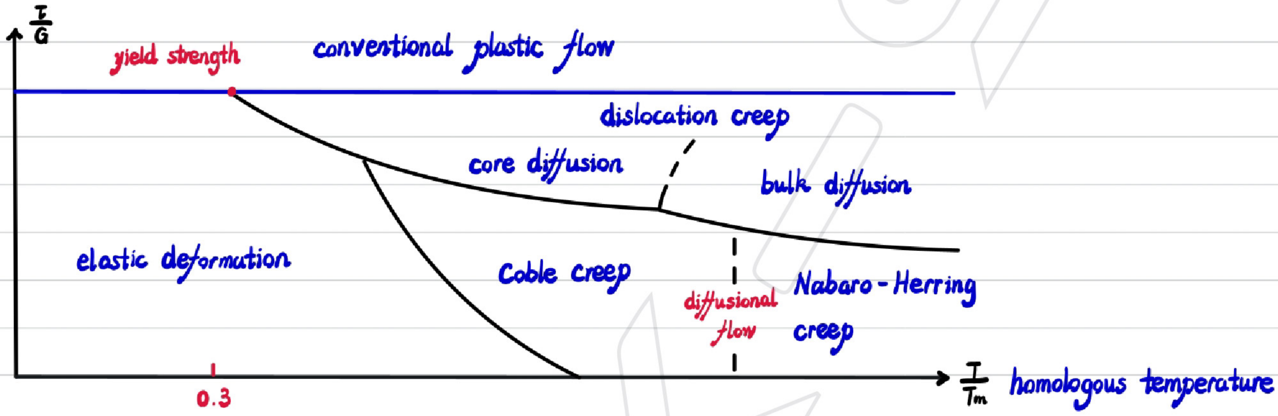
Coble creep diffuse along grain boundaries low T

Nabarro-Herring creep diffuse through the bulk 主体 of the material high T

* grain boundary sliding to maintain continuity in material



Ashby map



Designing against dislocation creep

1 ① high melting point $\frac{T}{T_m \uparrow}$

1 ② max obstacles to dislocation which stable at operation T

1 ③ choose an alloy where the majority phase has a high lattice resistance

Designing against diffusion creep

2 ① high melting point $\frac{T}{T_m \uparrow}$

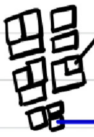
2 ② max grain size to give long diffusion distances and little gb diffusion

2 ③ choose an alloy with precipitates at gb's which stable at operation T ⟶ prevent gb sliding

High Temperature Alloy

Ni-Al system

dissolve all Ni into Al $\xrightarrow{\text{quenched}}$ SSSS $\xrightarrow{\text{tempering + aged}}$ precipitation strengthening uniform + fine Ni_3Al

good strength  — coherent interface → still hard to move

— very ordered → dislocation pass in pairs → still hard to move

good thermostability minimize coarsening

Ni superalloy compositions

60% Ni + precipitate formers Al, Ti + soild solution strengtheners Cr + oxidation protection Cr

Ni superalloy turbine blades

1st gen equiaxed → polycrystalline 多晶的 blade → 1② + 2③ against creep

* diffusion creep still a problem at high temperature

2nd gen columnar → long columar grains in loading direction → 1② + 2② + 2③ against creep

3rd gen single crystal → no grain boundaries → 1② + 2② against creep

* remove precipitate former → higher soildus temperature + lighter

Achieve higher operation T for Al superalloys $T_{operation} > T_m$

2nd gen columar → turbine blade film by cool air from compressor

3rd gen single crystal → film by cool air

→ coating by ceramic → oxidation protection + thermal shield

Corrosion and Oxidation

Oxidation removal of electrons to create positive ions $Al \rightarrow Al^{3+} + 3e^-$

Dry corrosion chemical reaction of a dry metal surface with an oxidising gas

Driving force of oxidation $-\Delta G$ oxide stable ΔG metal stable

* There is no correlation between driving force and oxidation rate

Measure time for oxidation by measure change of mass vs time * Δm increase exponentially with T

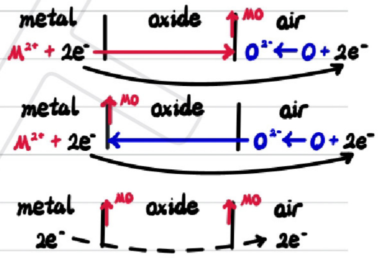
· Parabolic growth $\Delta m^2 = k_p t = A_p e^{-\frac{Q_p}{RT}} t$ · Linear growth $\Delta m = k_L t = A_L e^{-\frac{Q_L}{RT}} t$ · Linear loss $\Delta m = -k_L t$

Micromechanism of Parabolic Corrosion $(M^{2+} + 2e^-) + O^{2-} \longrightarrow MO + 2e^-$

① O^{2-} diffuses very slowly Fe M^{2+} and $2e^-$ diffuse outward to meet O^{2-}

② M^{2+} diffuses very slowly Ti O^{2-} diffuse inward to meet the M^{2+}

③ e^- more slowly in oxide Al slow growth at either interface



Parabolic Corrosion kinetic x^2 layer thickness $= k_p t$ where $k_p \propto -2D_0 e^{-\frac{Q}{RT}} \Delta C$

Protection against Parabolic Corrosion

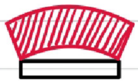
protective oxide forms stable oxide grow very slowly with electrical resistivity Al_2O_3

Micromechanism of Linear Corrosion

Linear growth when porosity 有孔性 in oxide — air react with metal through oxide

$\rho_{oxide} > \rho_{metal}$ oxide breaks-up

$\rho_{oxide} < \rho_{metal}$ oxide spalls 剥落



Linear loss when oxide is volatile 易挥发的 W, Mo * oxide evaporate at high T

Ni-based turbine blades parrabolic corrosion

① extend corrosion (oxidation) resistance by adding Cr against Ni

· $-\Delta G_{Cr} < -\Delta G_{Ni}$ high affinity 喜好 to oxygen · time for corrosion to same thickness rise

② extend corrosion (oxidation) resistance by couting with Al $\longrightarrow$ heat blade in furnance

Disadvantages of oxide films 膜

brittle $\xrightarrow{\Delta T}$ different thermal expansion coefficient between alloy and oxide $\longrightarrow$ 6 $\longrightarrow$ crack

$\longrightarrow$ initiate crack on alloys

Ceramics

Introduction

Key features · brittle · high T_m · hardness · low/medium density usually

Classification · glasses · viterous ceramics · engineering ceramics · cement concrete

Microstructure · ionic ceramics · covalent ceramics · silicate based ceramics

$\longrightarrow$ dislocation is very hard $\longrightarrow$ large lattice resistance

Brittleness low fracture toughness

Origin of cracks

· production · thermal stresses · corrosion (water) or abrastion 磨损 (dust) · during loading

Fracture

Fracture strength assume longest microcrack has length $2a_m$

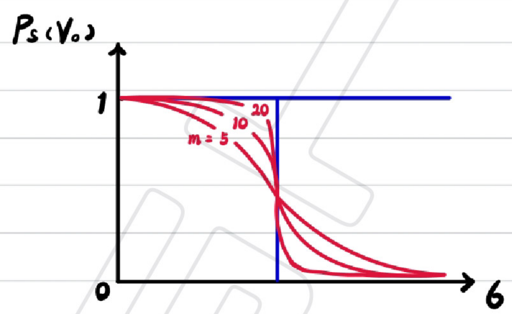
$\Delta K = Y \Delta \sigma \sqrt{\pi a} \longrightarrow \sigma_{crit} = \frac{K_c}{\sqrt{\pi a_m}}$

Thermal shock $\varepsilon_{TS} = \alpha \Delta T \longrightarrow \sigma_{TS} = E \alpha \Delta T \longrightarrow K$ thermal shock resistance $= \Delta T$ for σ_{TS}

Strength improvement · decreasing a_m quality control · increasing K_c alloying or composite

Weibull theory large sample $\longrightarrow$ more likely has larger flaws 缺陷 $\longrightarrow$ will fail at lower tensile stress

Survival probability $P_s(V_0) = e^{-(\frac{\sigma}{\sigma_0})^m}$ * σ_0 and m Weibull modulus are constant



lower $m \longrightarrow$ greater the variability of strength

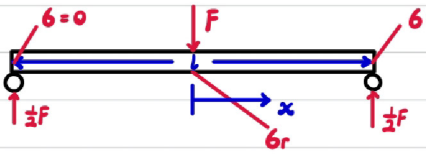
* for $m \approx 100 \longrightarrow$ treated as having single failure stress

** $P_s(V_0) = e^{-(\frac{\sigma}{\sigma_0})^m} \longrightarrow \ln P_s(V_0) = -(\frac{\sigma}{\sigma_0})^m$

$\longrightarrow \ln[\ln P_s(V_0)] = -m \ln(\frac{\sigma}{\sigma_0})$

$P_s(V) = [P_s(V_0)]^{\frac{V}{V_0}} \longrightarrow P_s(V) = e^{-[\frac{V}{V_0}(\frac{\sigma}{\sigma_0})^m]} = e^{-\frac{1}{V_0 \sigma_0^m}\int_V \sigma^m dV}$

Stress in bending $\sigma_{max, TS} = \sigma_r$ modulus of rupture $= \frac{6M_r}{bd^2}$ * $\sigma_r > \sigma_{TS}$



$$\int_A \sigma^m \, dA = 2\int_0^{\frac{1}{2}l} \left(\sigma_r \frac{\frac{1}{2}l - x}{\frac{1}{2}l}\right)^m (w\,dx) = \frac{wl\sigma_r^m}{m+1}$$

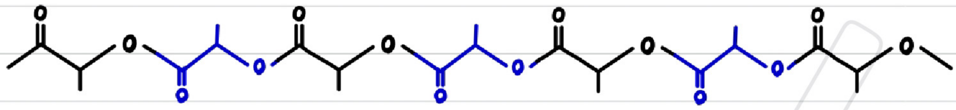
$$= \sigma_{TS} A = \sigma_{TS}(2wl)$$

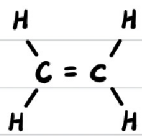
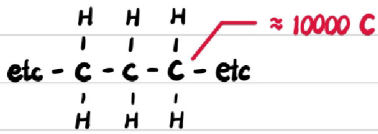
Polymers

Introduction

Macromolecular 高分子的 structure

a polymer chain is composed of repeating monomers linked head-to-tail by covalent bonds

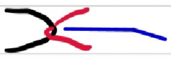


ethylene 乙烯 monomers  ⟶ polyethylene molecule 

Synthetic 人造的 polymers much shorter in length than natural polymers

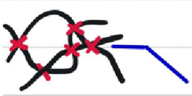
Structure

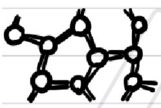
Single chain

 entanglement 缠绕物 ⟶ responsible for the mechanical properties e.g. viscosity and strength

⟶ Van deer Waals or hydrogen bonds between chains ⟶ low stiffness * covalent bond not loaded

Networks

 crosslink chemical links between chains ⟶ prevent molecule slipping past one another permanent

 supramolecular structure ⟶ thermosets

Classification

Thermoplastic 热塑性 entanglement

· proceed and shaped in liquid phase · rigid at T_{room}

Thermoset 热固性 supramolecular structure

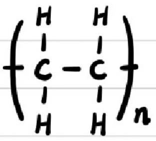
· shaping before curing 固化 · rigid at T_{room} · do not melt as T rise · degradation at very high T

Elastomers 弹性体 crosslink + entanglement

· elastic · very low modulus · properties are less temperature dependent

V.I.P (Very Important Polymers)

PE (Polyethylene) 聚乙烯 thermoplastic 牛奶桶 semi-crystalline

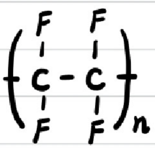


· extremely resistant to fresh water, salt water, food, ...

· cheap · easy to manufacturing · range of colours · range of transparency

· can be textured · can be metal coated · hard to print on

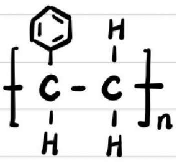
PTFE (Polytetrafluoroethylene) 聚四氟乙烯 thermoplastic 不粘锅涂层 semi-crystalline



· low friction · repel water · extremelly stable · expensive

* non-stick cooking utensils 厨具 ⟶ Teflon coated aluminium ⟶ Tefal

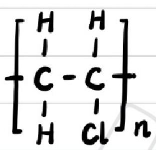
PS (Polystyrene) 聚苯乙烯 thermoplastic 透明 CD 盖 amorphus



· optically clear · cheap · easy to molded · brittle

* high impact PS is much stronger

PVC (Polyvinylchloride) 聚氯乙烯 thermoplastic 管道 amorphus



pure PVC ⟶ · rigid · brittle

flexible PVC ⟶ · rubber-like * extend properties by bending with other polymers

PMMA (Polymethacrylate) 聚甲基丙烯酸甲酯 thermoplastic 亚克力 amorphus

· transparent · close to glasses

PC (Polycarbonate) 聚碳酸酯 thermoplastic 车灯 amorphus

PET (Polyethylene terephalate) 聚对苯二甲酸乙二醇酯 thermoplastic 薯片包装袋 semi-crystalline

PEEK (Polyetheretherketone) 聚醚醚酮 thermoplastic L.E. crystalline

· high-performance · expensive

Epoxy 环氧树脂 thermoset 绝缘层 amorphus

· excellent mechanical + electrical + adhesive properties

· good resistance to heat and chemical attack · brittle · expensive

Unsaturated polyesters 不饱和聚酯树脂 thermoset 家具

· poorer mechanical properties than epoxy · poorer corrosion resistance than epoxy · cheaper

Nature rubber elastomer 轮胎 amorphus

· unique properties · tough · bouncy * widespread used

Nature polymers

Chain Length Distribution

Molar mass M (g/mol) * 1 mol = 6×10^{23} units

$\bar{M}_n$ (Number average molar mass) $M_n = \Sigma x_i M_i = \frac{\Sigma N_i M_i}{\Sigma N_i}$

number of entanglesments per chain ⟶ · strength · toughness · environmental stress cracking

$\bar{M}_w$ (Weight average molar mass) $M_w = \Sigma w_i M_i = \frac{\Sigma N_i M_i^2}{\Sigma N_i M_i}$

number of entanglesments per chain ⟶ · viscosity

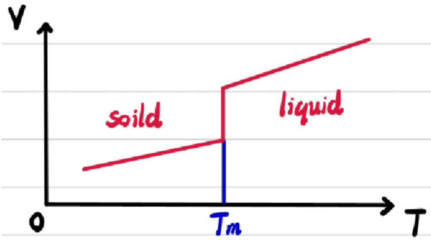
$\bar{M}_z$ (z-average molar mass) $M_z = \Sigma z_i M_i = \frac{\Sigma N_i M_i^3}{\Sigma N_i M_i^2}$

molecular weight fraction ⟶ · melt elasticity

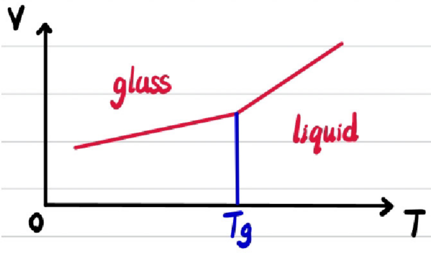
$\bar{M}_{z+1}$ (z+1-average molar mass) $M_{z+1} = \Sigma (z+1)_i M_i = \frac{\Sigma N_i M_i^4}{\Sigma N_i M_i^3}$

State Transitions

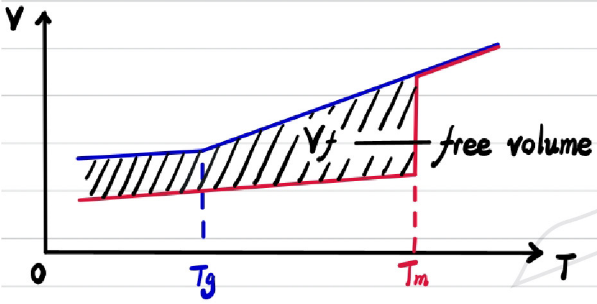
Crystalline materials melting



Amorphous 非晶形的 materials glass transition → only governed by kinetics



Physical state for polymers



Chain regularity (Tacticity 规度)

Isotactic all the side groups on the same side → easy crystallize

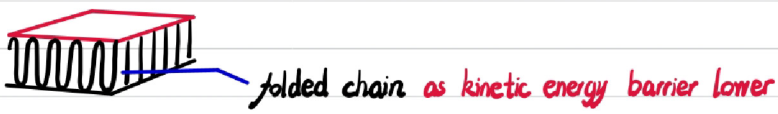
Sindiotactic alternate in a regular manner → can crystallize

Atactic random positions → cannot crystallize

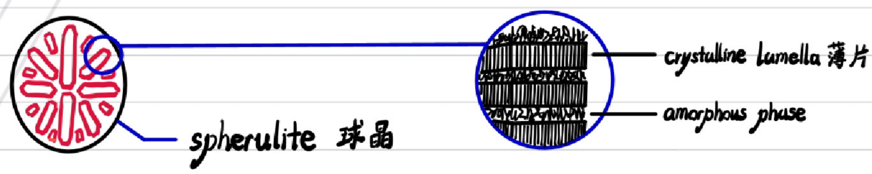
* transparent polymer is amorphus

Crystal Morphology 形态

Single crystal only if slow growth

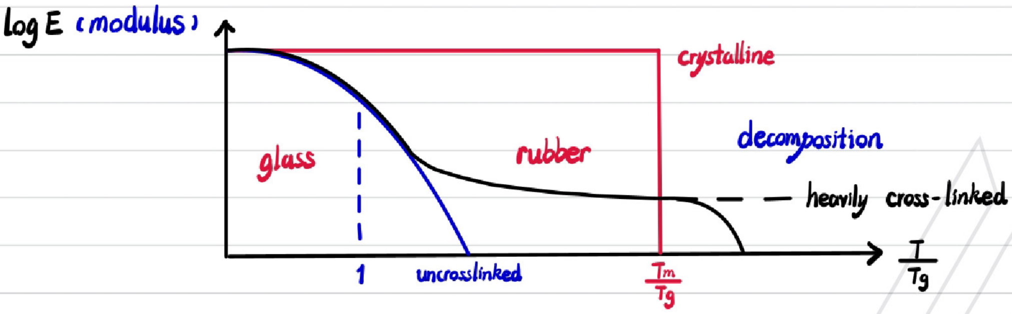


Polycrystalline



Rubber

State transitions



$T < T_g$ glassy state ⟶ energy - elasticity

$T > T_g$ rubbery state ⟶ material connected via entanglements + chemical crosslink ⟶ elastic

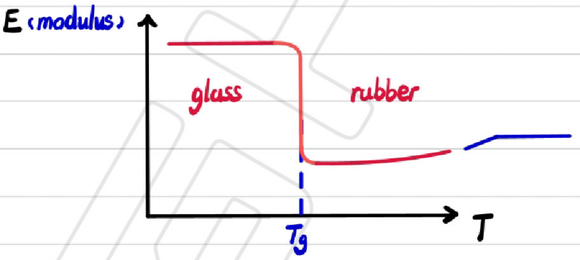
Stretched rubber contract when heated

Memory of state

Entropy Elasticity

Entropy spring

Entropy elasticity



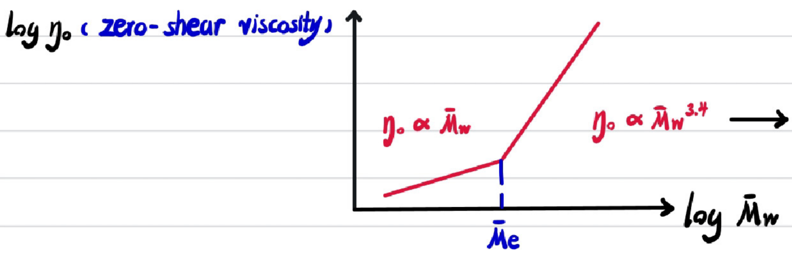
in elastic range ⟶ T↑ ⟶ E↑ slightly

Reptation 表面蠕动 theory

* creep

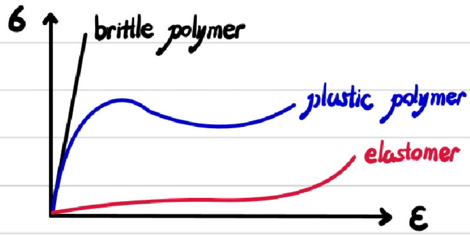
t_{tube} relaxation time $\propto$ M^3 length of macromolecule

Fluid state

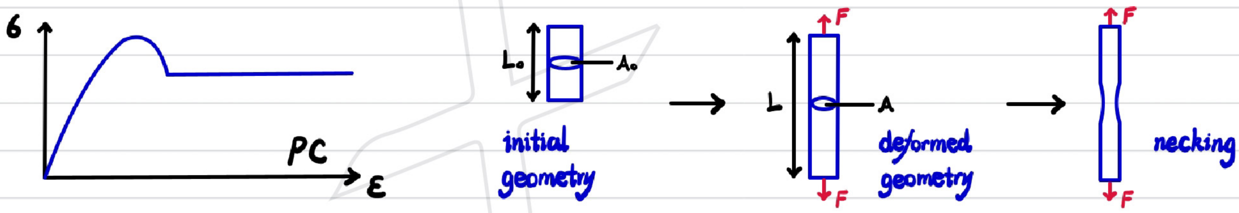


Mechanical Properties

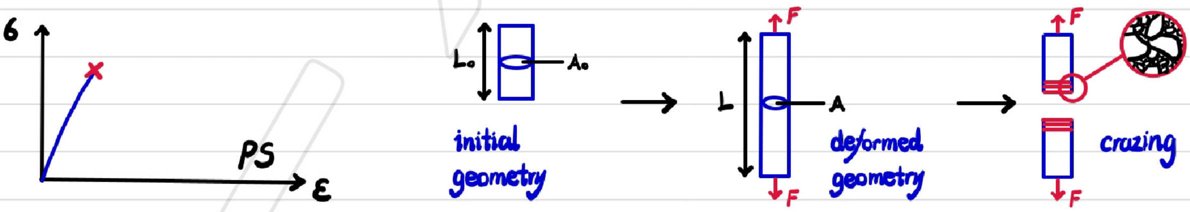
Stress - strain behaviour



Necking



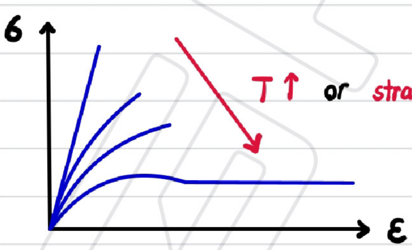
Crazing 龟裂

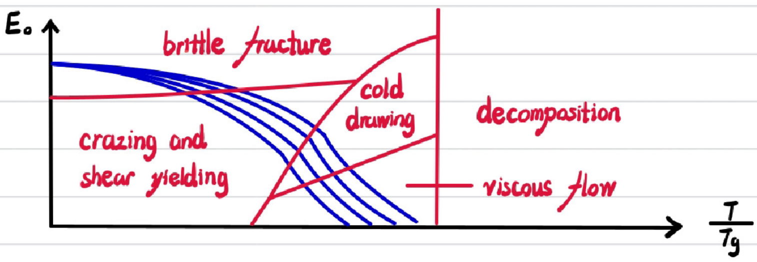


* for brittle thermoplastics and high cross-linked thermosets ⟶ brittle in tension but ductile in compression

** ductility of polymer depend on its resistance to yield and craze

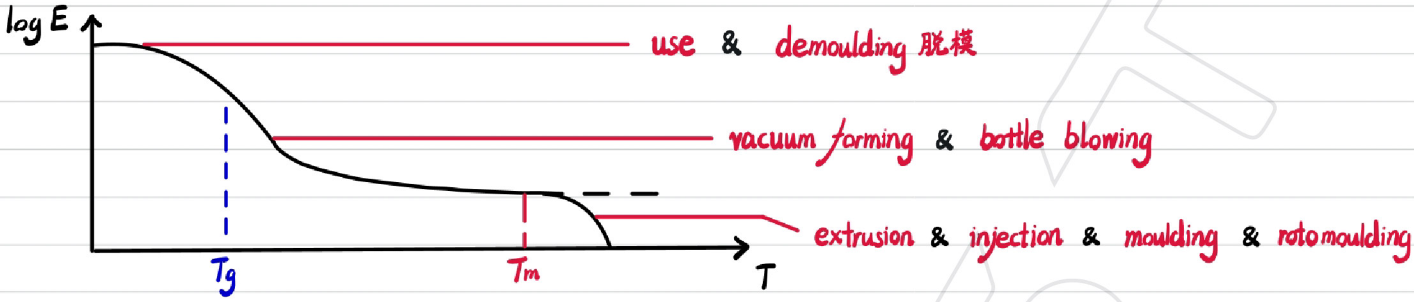
Temperature and strain rate





Processing

Summary



Rubber compounding

Extrusion by single & twin screwed extruder

· co-extrusion · sheet extrusion · film extrusion · blown film extrusion

* die-swell 口型膨胀 ** melt fracture

Fibre spinning

· melt spinning · solution spinning for UWHMPE · aramid fibre spinning

Moulding

· injection moulding · injection blow moulding · rotational moulding

Vacuum foarming (thermomoulded)

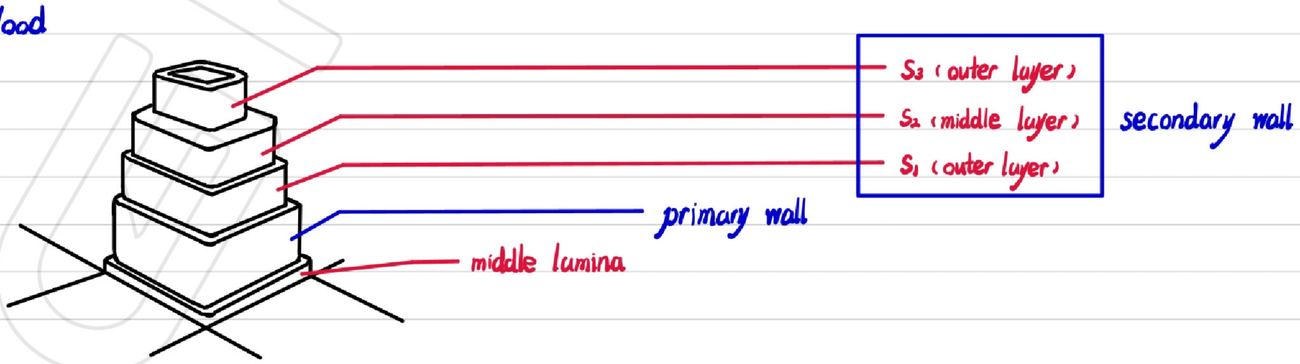
Composites

Introduction

Composite two or more physically or chemically distinct materials combined to improve properties

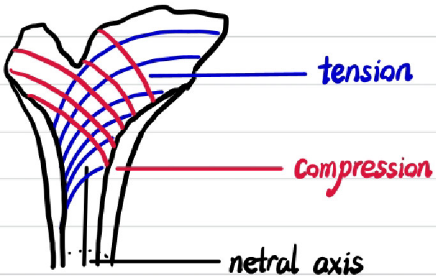
fibres + matrix $\xrightarrow{\text{process}}$ properties

Wood



Bamboo

Bone



Pros

· weight reduction for high specific stiffness and strength

· design flexibility & integrated parts

· environmental friendly low energy consumption to manufacturing

· safety crush structures

· low maintainance cost corrosion resistance

Cons

· expensive materials and processing

· lack of mass production technology for high-performance composites

· hard to recycle

· don't know how to design with anisotrophic 各向异性的 materials

· uncertainty to predict failure and life-time

Man-made composites

Polymer Matrix Composites (PMC's) * also known as Fibre Reinforced Polymers (FRP)

Metal Matrix Composites (MMC's) ⟶ automotive industry

Ceramic Matrix Composites (CMC's) ⟶ high temperature environments

Types of reinforcements

particulate 微粒　　flake 碎片　　fibre reinforced　　laminated　　composite

processibility ← 3D　2D　1D　cross-ply　angle-ply　uniaxial → mechanical property

Constitution

Most important sythetic fibres

glass　· strong　· stiff as Al　· cheap

carbon　elite fibre

· stiff　· strong　· bond well to polymetric adhesive (e.g. epoxies)

· good temperature resistance　· chemically inert 惰性的　· expensive

aramid 芳族聚洗酰　· very strong　· limit stiffness

Glass fibre

recall Weibull theory ⟶ fibre diameter ↓ ⟶ less likely have larger flaws ⟶ tensile stress ↑

Carbon fibre

* tailored 定做的 properties by change temperature ⟶ 1500°C $\xleftrightarrow[\quad]{\text{strength} \qquad \text{stiff (high E)}}$ 2500°C

Aramid fibre　kevlar

· good resistance to impact　· good resistance to abrasion 磨损　· poor compression strength

Other fibres

· boron　· silicon carbide　· natural (cellulose 纤维素)

Use fibres

good in tension + poor in compression $\xrightarrow[\text{prevent buckling}]{\text{bonding by adhesive}}$ composites

Thermosets matrices as adhesive

- polyestar
- vinylester
- epoxy

⟶ cost & properties

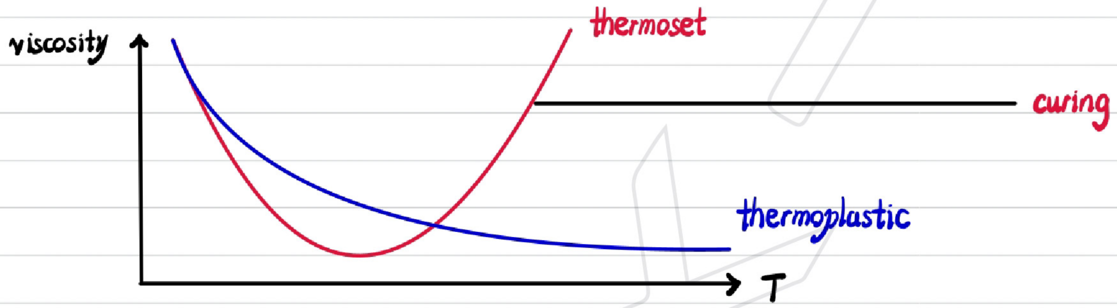
Thermoplastic matrices

- PES
- PEI
- PPS
- PEKK
- PEEK

pros · improve toughness · repairable · recyclable

cons · high viscosity · high processing temperature · poor strength · expensive for PEEK

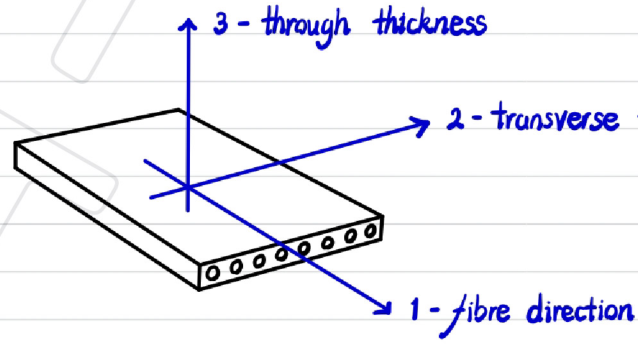
Viscosity



Mechanical Properties

Rule of mixture

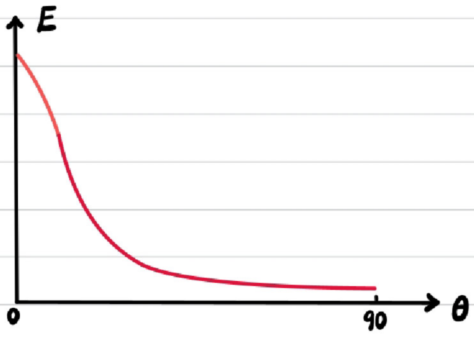
for undirectional lamina

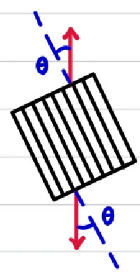


$\frac{1}{E_c} = \frac{V_f}{E_f} + \frac{V_m}{E_m}$

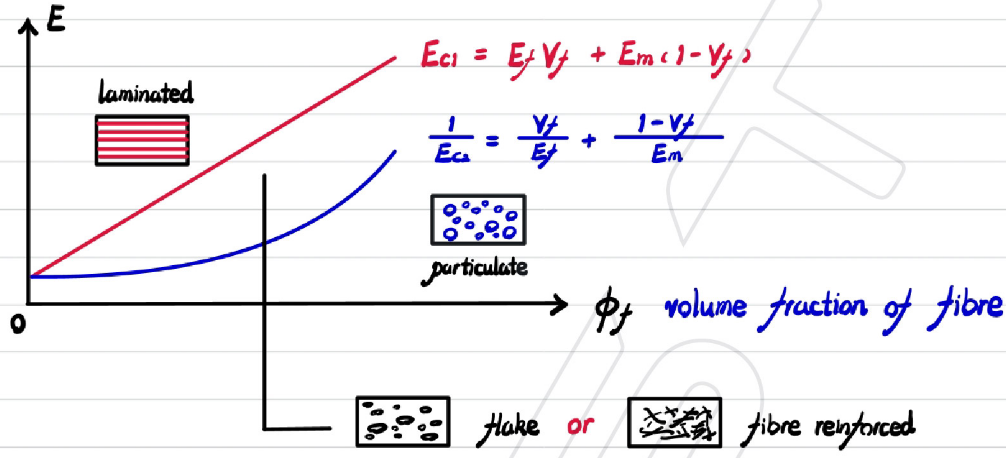
$E_c = E_f \cdot V_f + E_m \cdot V_m$

effect of angle tilt





θ angle between fibre and loading direction continuity of fibre



$E_{c1} = E_f V_f + E_m (1 - V_f)$

$\frac{1}{E_{c2}} = \frac{V_f}{E_f} + \frac{1-V_f}{E_m}$

Halpin - Tasi model

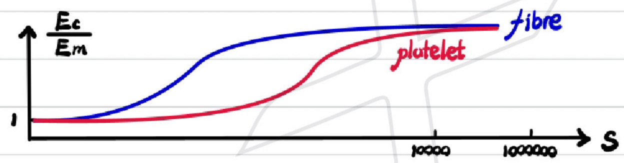
for discontinuous fibre composites $E = \frac{E_m (1 + \xi \eta f)}{1 - \eta f}$ where $f = V_f$

where $\eta = \frac{\frac{E_f}{E_m} - 1}{\frac{E_f}{E_m} + \xi}$ where ξ shape factor

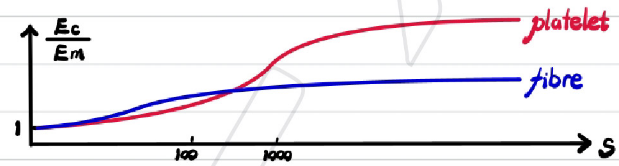
* aspect ratio $s = \frac{\text{largest dimension}}{\text{smallest dimension}}$

E_{c1} of (laminated) = E_{c1} of (fibre) when $s = \frac{L}{d} > 100 \sim 1000$

for isotrophic



for orientated

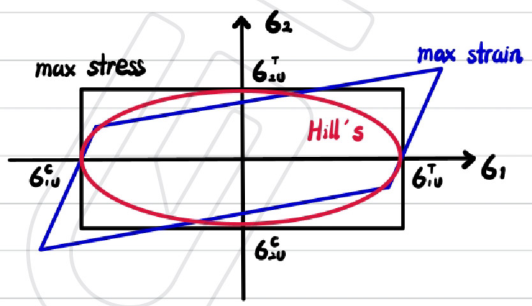


Longitudinal tensile strength

$\sigma_{1UT} \approx V_f \sigma_{UTf}$ and $\sigma_2 = \frac{\sigma_m}{SCF}$ —— stress concentration factor

Longitudinal compressive strength

Failure criteria

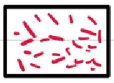
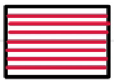
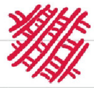


· not possible to have experimental one

· non-interactive failure criteria very approxiamate

· interactive failure criteria

Architecture

Fibre composites  short fibre  laminated  2D - weaves → 3D - weaves

Undirectional prepegs 预浸料 tapes · best performance · expensive · sensitive to defects

Non - crimp fabrics / uniwave 无卷曲织物 · cheap

Non - woven 编织 mat

Woven fabric · cheap · superior drape 覆盖

Textile 纺织 architectures

Braided 辫状的 fabric · very tough · tend to have void · better for triaxil load

Through - thickness reinforcement

Processing

Improtant factors · viscosity of matrix · softy · cost · surface finish · performance

Hand lay - up · cheap · simple · wide choice of material · high void content · turbine blade

Spray - up · cheap · fast · heavy (resin 树脂 - rich) · lightly load panels

Filament winding · fast · economy · good properties · chemical stroage tank

Pultrusion 拉挤成型 · very fast · economy · bridges

Resin 树脂 transfer moulding (RTM) · low void · safe · smooth surface · small complex aircraft

Vacuum infusion 灌注 · lower cost than RTM · complex · train body panel

Seamann composite resin injection moulding (SCRIMP) · boat

Bladder moulding

Autoclave moulding · high fibre contents · extremely safe · very expensive · F1 · wings

Metal matrix composites · foil diffusion bonding solid state · spray deposition liquid state