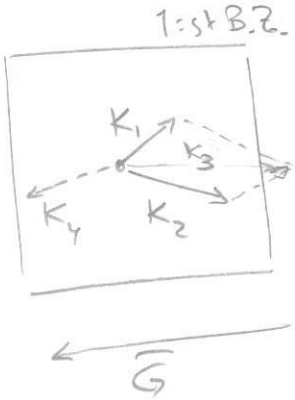
Umklapp process

Phonon collision

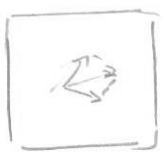


$$\bar{K}_1 + \bar{K}_2 = \bar{K}_3$$

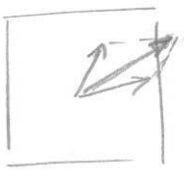
but $|\bar{K}_3| > |\bar{G}/2|$

$$\Rightarrow \bar{K}_4 = \bar{K}_3 - \bar{G}$$

$$|\bar{K}_4| < |\bar{G}/2|$$



N-process



U-process

Umklapp-processes needed to get thermal equilibrium

× Total phonon wave vector $\bar{K}_t = \sum_{\text{1stB.Z.}}^{\text{all phonons}} \bar{K}$

× Population changed through phonon-phonon interaction, but $\bar{K}_t$ does not change as long as no U-process.

* Thermal equilibrium: $\bar{K}_t = \bar{0}$

For U-process to occur, $\bar{K}$-vectors of size at least $\bar{G}/4$ need to be present.

Since $\omega = v_s \cdot K$ (Debye)

$\Rightarrow$ large ω, i.e, $\hbar\omega$ energies should be available

$$n(\omega) = f_{BE} = \frac{1}{e^{\hbar\omega/k_B T} - 1} \approx e^{-\hbar\omega/k_B T} \quad \text{at low } T$$

$$\bar{K} = \frac{\bar{G}}{4} \quad \Longleftrightarrow \quad \text{"}\omega \approx \frac{\omega_D}{4}\text{"}$$

$$\Rightarrow \quad n(\omega) \approx e^{-(\Theta_D/4T)}$$

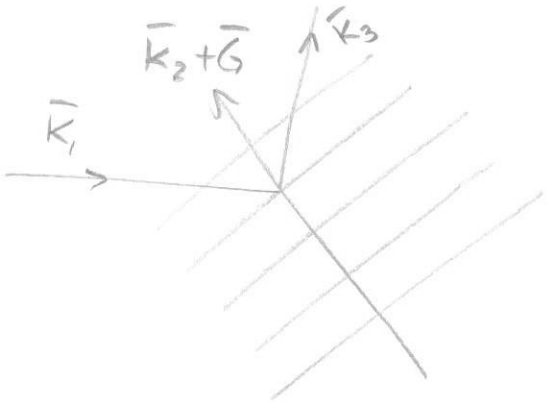
Collision of two phonons: $\sim n^2 \sim e^{-(\Theta_D/2T)}$

(probability for ω-process)

Phonon - phonon interaction

<u>Energy</u>: $\hbar\omega_1 + \hbar\omega_2 = \hbar\omega_3$

<u>Momentum</u>: $\hbar\bar{K}_1 + \hbar\bar{K}_2 + \hbar\bar{G} = \hbar\bar{K}_3$



"$\bar{K}_1$ is diffracted by $\bar{K}_2$"

(inelastic diffraction)

Electron - phonon interaction

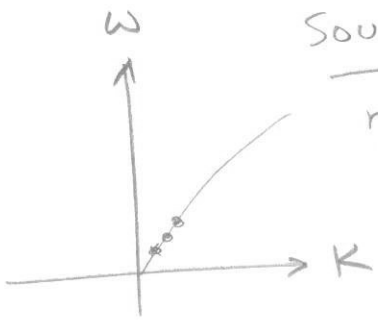
1) Temperature dependence of electrical resistance

2) Superconductivity

Comparing sound propagation and heat conductivity

Sound propagation

not diffusion-like



$K_1 + K_2 = K_3$

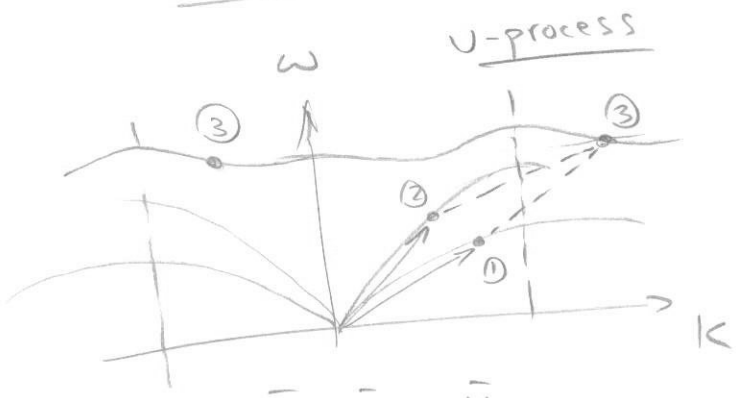
$\omega_1 + \omega_2 = \omega_3$

$v_g^{(1)} = v_g^{(2)} = v_g^{(3)}$

typical n-process

Heat conductivity

diffusion-like



$\bar{K}_1 + \bar{K}_2 = \bar{K}_3$

$\omega_1 + \omega_2 = \omega_3$

Phonon-interaction gives large changes of group velocity

$v_g = \frac{\partial \omega}{\partial k}$

Thermal current:

Before: $\hbar\omega_1 \cdot v_g^{(1)} + \hbar\omega_2 v_g^{(2)} > 0$

After: $(\hbar\omega_1 + \hbar\omega_2) \cdot v_g^{(3)} < 0$

(example)

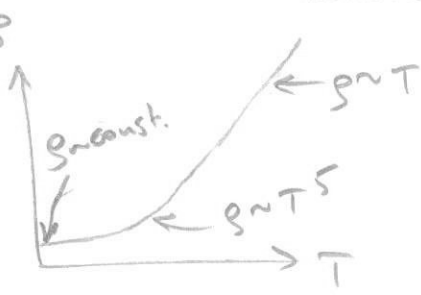
Electrical resistivity

Due to ⊗ imperfections

- Point defects (0D) — $\rho \sim$ const.
- Dislocations (1D)
- Grain boundaries (2D)

⊗ interaction with lattice vibrations

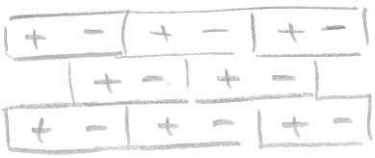
Resistivity



$\rho \sim T \quad T >> \Theta_D$

$\rho \sim T^5 \quad T << \Theta_D$

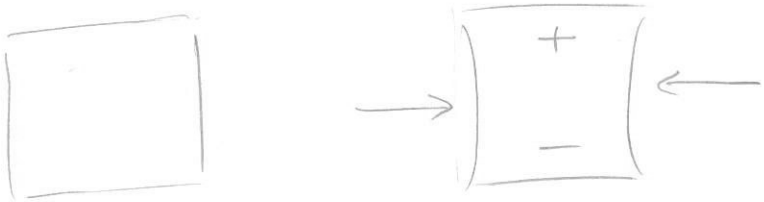
Pyroelectricity



Nonvanishing dipole-moment of primitive cell

Piezoelectricity

Strain



Ferroelectricity

typically

2nd order transition

Pyroelectric | "normal"

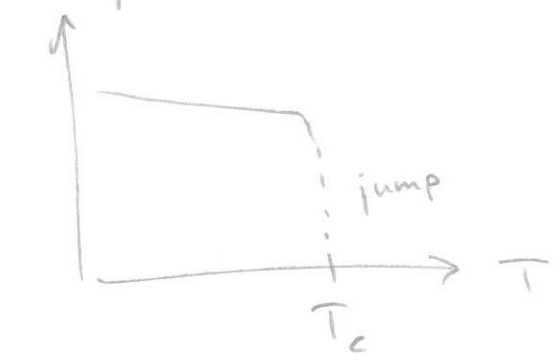
T

T_c

curie temperature

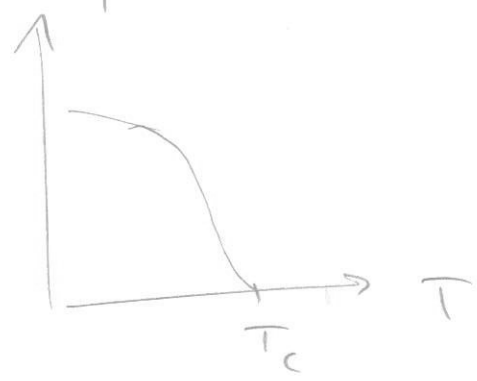
1:st order ex. $\bar{P}$

order param →



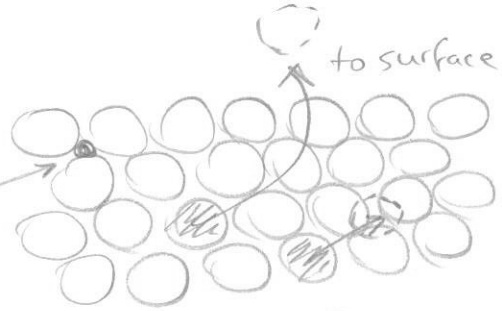
2nd order

order param.



Vacancies

Schottky defect



Frenkel defect

{ vacancy + intersitial

$$n_v = N_0 \, e^{+T\Delta S/k_B T} \cdot e^{-U_0/k_B T}$$

- N_0: # atoms
- $e^{+T\Delta S/k_B T}$: term ≈ 1 from entropy increase due to changes in lattice vibrations when vacancy is formed
- $e^{-U_0/k_B T}$: energy required to form vacancy

Thermally activated — equilibrium concentration

$U_0 \sim$ cohesive energy $\sim$ eV

Quick cooling of sample from high temp. = Quenching

$\Longrightarrow$ higher conc. of vacancies frozen-in.

Resistivity $\quad \rho = \underset{\text{phonon}}{\rho(T)} + \rho_{\text{vacancies}} + \rho_{\text{other defects}}$

$$\rho_{\text{vacancies}} = c \cdot n_v$$

Concentration of Frenkel defects

Energy to move atom from lattice site to interstitial pos.

$$\varepsilon_I = \varepsilon_v + \varepsilon_M$$

ε_v: vacancy

ε_M: migrate from surface to interstitial pos.

ε_v from $\quad \frac{n}{N-n} = e^{-\varepsilon_v / k_B T}$

N = number of possible vacancy positions ($\sim$ # of atoms)

ε_M from $\quad \frac{n}{N'-n} = e^{-\varepsilon_M / k_B T}$

N' = # of possible interstitial pos.

$$\Rightarrow \varepsilon_I = k_B T \cdot \ln\left(\frac{N-n}{n}\right) + k_B T \ln\left(\frac{N'-n}{n}\right) \qquad (N' > N \text{ typically})$$

$$\varepsilon_I = k_B T \cdot \ln\left[\frac{(N-n)(N'-n)}{n^2}\right]$$

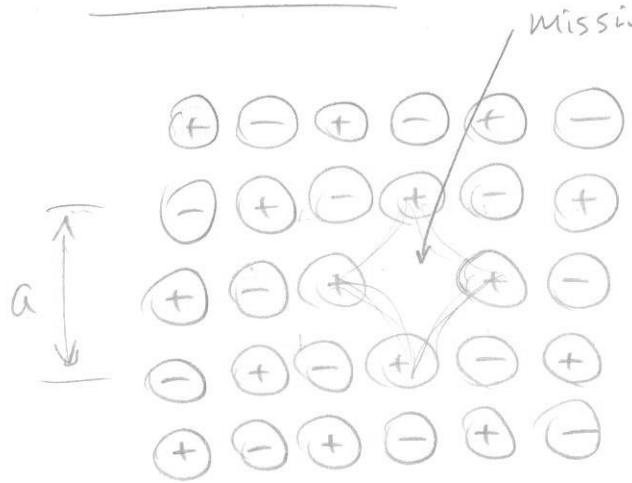
$$n = \sqrt{n^2} = \left\{ \begin{matrix} n \ll N \\ n \ll N' \end{matrix} \right\} = \sqrt{NN'}\, e^{-\varepsilon_I / 2k_B T}$$

Similarly: Formation of electrostatically neutral vacancy pair:

$$n \sim N \cdot e^{-\varepsilon_p / 2k_B T}$$

ε_p = energy to form a pair

Color centers



⇓

positively charged area

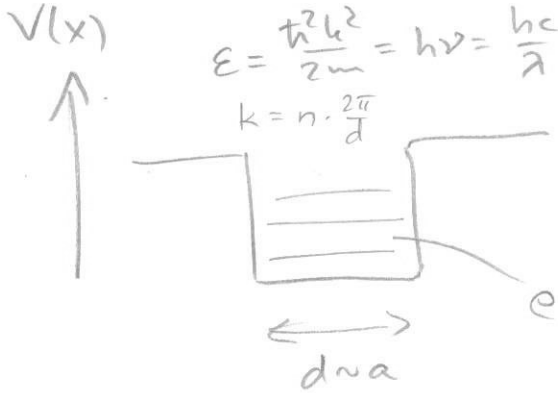
⇓

attracts electron

⇓

"potential well"

"artificial atom"



States in energy gap ⟹ optically active

Color of otherwise transparent crystals

Other possibility: Charged ions in otherwise charge-neutral crystals

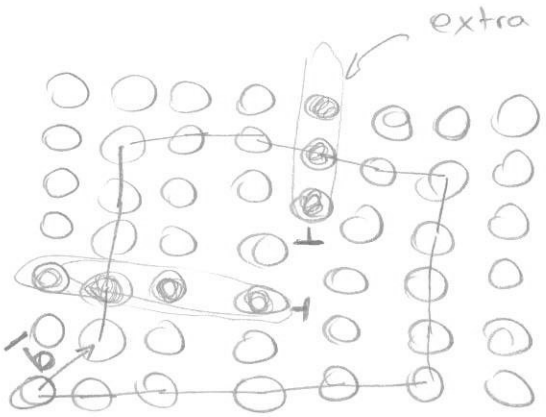
Irradiation of crystals with γ-radiation ⟹ color changes

Dislocations

Line defects

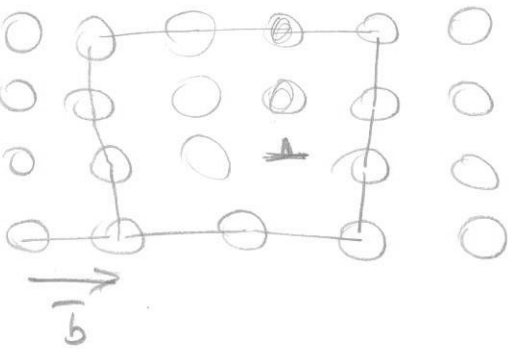
× Screw dislocation

× Edge — ⊥ — ⊥



$\bar{b}$: Burger vector

To find $\bar{b}$: Go around dislocations in defect-free material.



$\bar{b}$ ⊥ to edge dislocation (going into paper)

Work hardening
- Hammer on Cu-foil
- Bend wire a few times

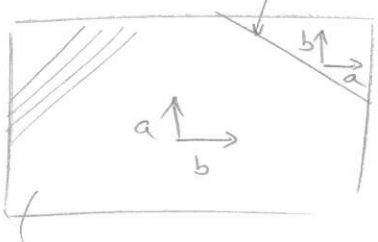
⇓ more dislocations

⇓ network of dislocations

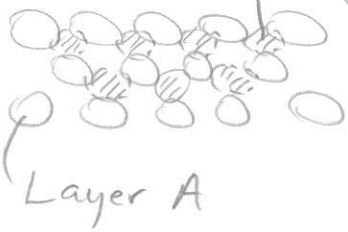
⇓ no motion of dislocations

⇓ harder mtrl. (but more fragile)

Surface defects



ex. orthorhombic crystal



Stacking faults

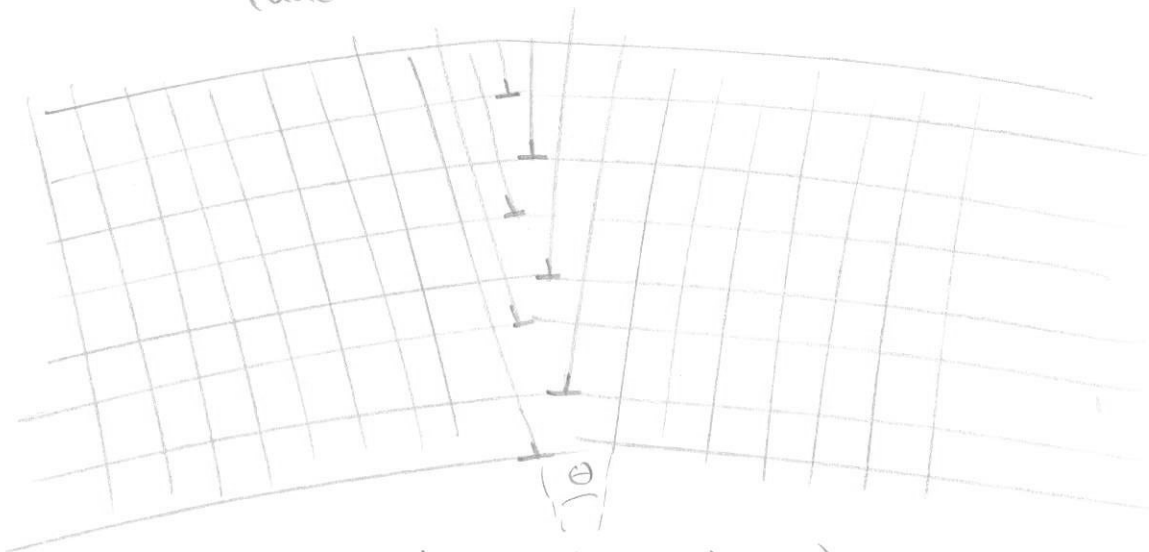
ABABABCBABAB

etc.

Grain boundary

Low-angle grain boundary

Distance between dislocations
function of grain misalignment angle



(not every atomic plane shown)

Show that the phonon momentum $\bar{p} \neq 0$ only for the mode $\bar{K} = 0$

Background The phonon is the quantized lattice vibration

A classical model gives displacements

$$U_s = U \cdot e^{isKa}$$

U — amplitude and time-dependence $\sim e^{-i\omega t}$

Proof

For $\bar{K} = 0$:

$$P = M \cdot \frac{dU}{dt} \cdot \sum_{s=0}^{N-1} 1 = M \cdot \frac{dU}{dt} \cdot N \neq 0$$

No spatial dependence. All atoms in the lattice move in the same way, i.e, all crystal is moving.

Translation — no phonon wave

For $\bar{K} \neq 0$

$$P = M \cdot \frac{d}{dt} \sum_{s=0}^{N-1} U_s = M \cdot \frac{dU}{dt} \sum_{s=0}^{N-1} e^{isKa} = \left\{ \text{geometrical series} \right\} =$$

$$= M \cdot \frac{dU}{dt} \cdot \left(\frac{1 - x^N}{1 - x} \right) \Bigg|_{x = e^{iKa}} =$$

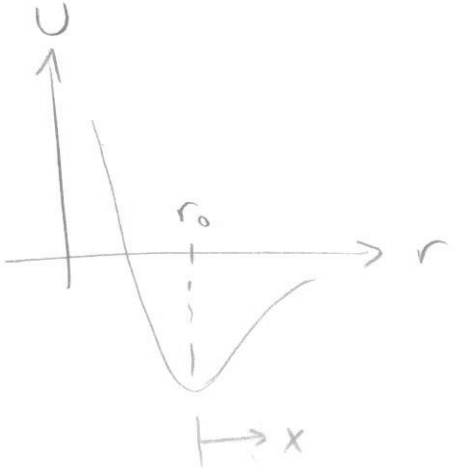
$$= M \cdot \frac{dU}{dt} \cdot \frac{1 - e^{iNKa}}{1 - e^{iKa}} = \left\{ \text{Periodic boundary cond. } K = \pm p \cdot \frac{2\pi}{Na} \right\} =$$

$$= M \cdot \frac{dU}{dt} \cdot \frac{1 - \underbrace{e^{i \cdot 2\pi p}}_{=1}}{1 - e^{iKa}} = 0$$

On the average there is no momentum for the whole chain.

Show That the thermal expansion is zero for a lattice with harmonic interactions.

Background



Harmonic:

$$U \sim (r - r_0)^2$$

Let x be the deviations from equilibrium pos. r_0

Set $U(x) = cx^2 - gx^3 - fx^4$

Use classical model - Boltzmann statistics

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x \cdot e^{-U(x)/k_BT}\,dx}{\int_{-\infty}^{\infty} e^{-U(x)/k_BT}\,dx} = \frac{\int_{-\infty}^{\infty} x \cdot e^{-\frac{cx^2+gx^3+fx^4}{k_BT}}\,dx}{\int_{-\infty}^{\infty} e^{-\frac{cx^2+gx^3+fx^4}{k_BT}}\,dx} \approx \left\{\begin{matrix}\text{series}\\ \text{exp.}\end{matrix}\right.$$

$$\approx \frac{\int_{-\infty}^{\infty} x \cdot e^{-cx^2/k_BT}\left(1 + \frac{gx^3}{k_BT} + \frac{fx^4}{k_BT}\right)dx}{\int_{-\infty}^{\infty} e^{-cx^2/k_BT}\,dx} = \frac{\int_{-\infty}^{\infty} \frac{gx^4}{k_BT} e^{-\frac{cx^2}{k_BT}}\,dx}{\int_{-\infty}^{\infty} e^{-cx^2/k_BT}\,dx} =$$

$$= [\ldots] = \frac{3g}{c^2} \cdot k_BT$$

$$g = 0 \implies \langle x \rangle = 0$$