Phonons

at low temperatures

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Phonons

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Outline

1. Microscopic description of crystal vibrations, phonon band structure, experimental probes

2. Phonon kinetics in insulators

3. Electron-phonon coupling and phonon kinetics in metals

4. Relaxation cascade in a detector

Born-Oppenheimer approximation

Solid = nuclei + electrons (valid up to several MeV)
or
Solid = atomic cores + valence electrons (valid up to several tens eV)

HEAVY $light$

$$\frac{M}{m} \sim 10^4 - 10^5$$

Born-Oppenheimer approximation

Step 1: Find the electron ground state at fixed positions of the nuclei $\{\mathbf{R}_n\}$

$$\hat{H}_{\mathrm{el}}(\{\mathbf{R}_n\}) = -\sum_i \frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}_i^2} + \sum_{i<j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{i,n}\frac{Z_n e^2}{|\mathbf{r}_i - \mathbf{R}_n|}$$

$$\hat{H}_{\mathrm{el}}(\{\mathbf{R}_n\})\,\Psi(\{\mathbf{r}_i\}|\{\mathbf{R}_n\}) = E_0(\{\mathbf{R}_n\})\,\Psi(\{\mathbf{r}_i\}|\{\mathbf{R}_n\})$$

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$$\hat{H}_{\mathrm{el}}(\{\mathbf{R}_n\})\,\Psi(\{\mathbf{r}_i\}|\{\mathbf{R}_n\}) = E_0(\{\mathbf{R}_n\})\,\Psi(\{\mathbf{r}_i\}|\{\mathbf{R}_n\})$$

Step 2: Use the obtained electron ground state energy $E_0(\{\mathbf{R}_n\})$ as an additional potential energy of the nuclei:

$$\hat{H}_{\mathrm{N}} = -\sum_n \frac{\hbar^2}{2M_n}\frac{\partial^2}{\partial \mathbf{R}_n^2} + \sum_{n<n'}\frac{Z_n Z_{n'} e^2}{|\mathbf{R}_n - \mathbf{R}_{n'}|} + E_0(\{\mathbf{R}_n\})$$

Born-Oppenheimer approximation

Step 1: Find the electron ground state at fixed positions of the nuclei $\{\mathbf{R}_n\}$

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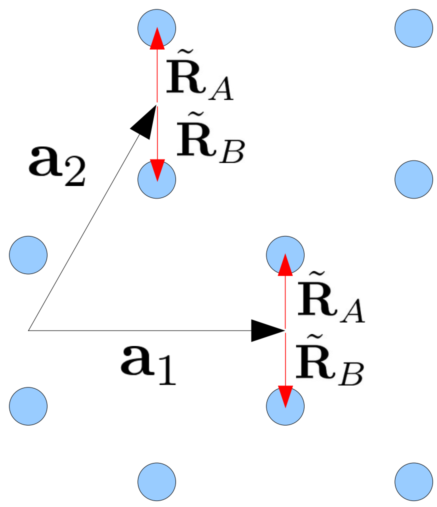
minimize with respect to $\{\mathbf{R}_n\}$

equilibrium atomic positions

Small vibrations: harmonic modes



Crystal: $N \to \infty$ unit cells, ν atoms per unit cell

Equilibrium atomic positions:

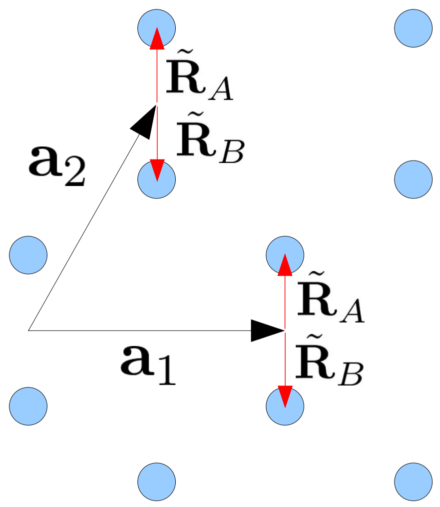
$$\mathbf{R}^{\mathrm{eq}}_{n_1,n_2,n_3,j} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 + \tilde{\mathbf{R}}_j$$

Indices: $j = 1, \ldots, \nu$ atoms in unit cell

$\alpha, \beta = x, y, z$ Cartesian components

$(n_1, n_2, n_3) \equiv \mathbf{n}$

Small vibrations: harmonic modes



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Potential energy @ small displacements: $\mathbf{R}_{\mathbf{n},j} = \mathbf{R}^{\mathrm{eq}}_{\mathbf{n},j} + \mathbf{u}_{\mathbf{n},j}$

$$W(\{\mathbf{R}\}) = W(\{\mathbf{R}^{\mathrm{eq}}\}) + \frac{1}{2}\sum_{\mathbf{n},\mathbf{n}'}\sum_{j,j',\alpha,\beta} K^{jj'}_{\alpha\beta}(\mathbf{n}-\mathbf{n}')\, u_{\mathbf{n}j\alpha}\, u_{\mathbf{n}'j'\beta} + O(u^3)$$

pairwise interactions: equivalent to springs between atoms $K = \dfrac{\partial^2 W}{\partial\mathbf{R}\,\partial\mathbf{R}}$

Small vibrations: harmonic modes

Equations of motion:

$$M_j \frac{d^2 u_{\mathbf{n}j\alpha}}{dt^2} = \sum_{\mathbf{n}'j'} K_{\alpha\beta}^{jj'}(\mathbf{n}-\mathbf{n}')\, u_{\mathbf{n}'j'\beta}$$

Plane wave solutions:

$$\mathbf{u}_{\mathbf{n}j} = \frac{\mathbf{Q}_j}{\sqrt{M_j}}\, e^{i\mathbf{q}\mathbf{R}_{\mathbf{n}j} - i\omega t}$$

Eigenvalue problem to find $\mathbf{Q}_j$:

$$\omega^2 Q_{j\alpha} = \sum_{j'\beta} D_{\alpha\beta}^{jj'}(\mathbf{q})\, Q_{j'\beta}$$

Dynamical matrix $(3\nu \times 3\nu)$

$$D_{\alpha\beta}^{jj'}(\mathbf{q}) \equiv \sum_{\mathbf{n}} \frac{K_{\alpha\beta}^{jj'}(\mathbf{n})}{\sqrt{M_j M_{j'}}}\, e^{-i\mathbf{q}\mathbf{R}_{\mathbf{n}j}}$$

Small vibrations: harmonic modes

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Distinct solutions only for **q** in the 1st Brillouin zone

For each **q**, 3ν eigenvectors $\mathbf{Q}_j^\lambda(\mathbf{q})$

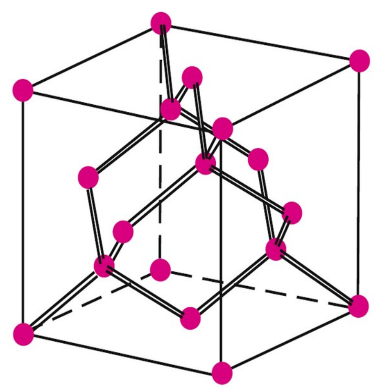
3ν eigenvalues $\omega^2_{\lambda,\mathbf{q}}$ $\qquad \lambda = 1, \ldots, 3\nu$

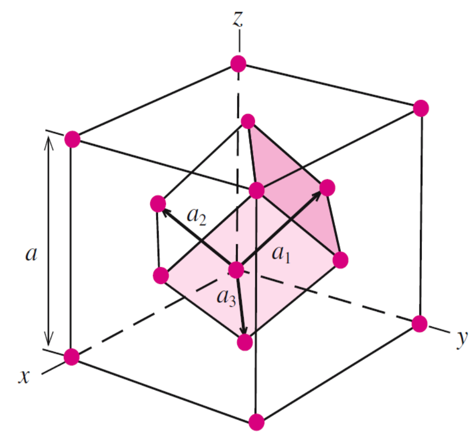
Estimate: $\hbar\omega_{\mathrm{ph}} \sim \hbar\sqrt{\frac{K}{M}}, \quad K \sim \frac{E_{\mathrm{el}}}{a^2}, \quad E_{\mathrm{el}} \sim \frac{\hbar^2}{ma^2} \sim 10\,\mathrm{eV}$

$$\boxed{\hbar\omega_{\mathrm{ph}} \sim \sqrt{\frac{m}{M}}\, E_{\mathrm{el}} \sim 30\,\mathrm{meV} = 350\,\mathrm{K}}$$

(1 eV = 11605 K)

Example: diamond crystal structure

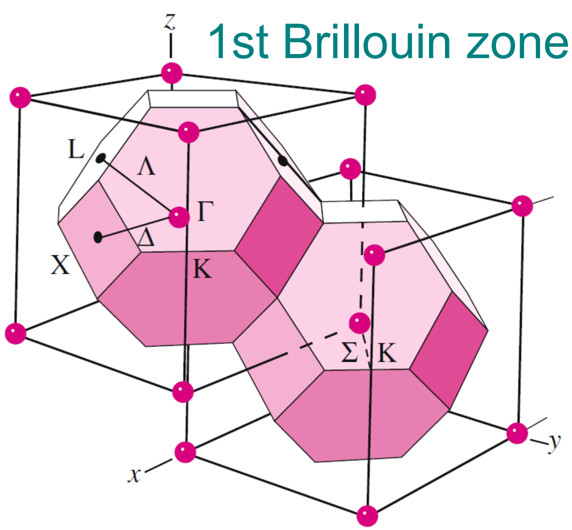




elementary translations
face-centered cubic lattice

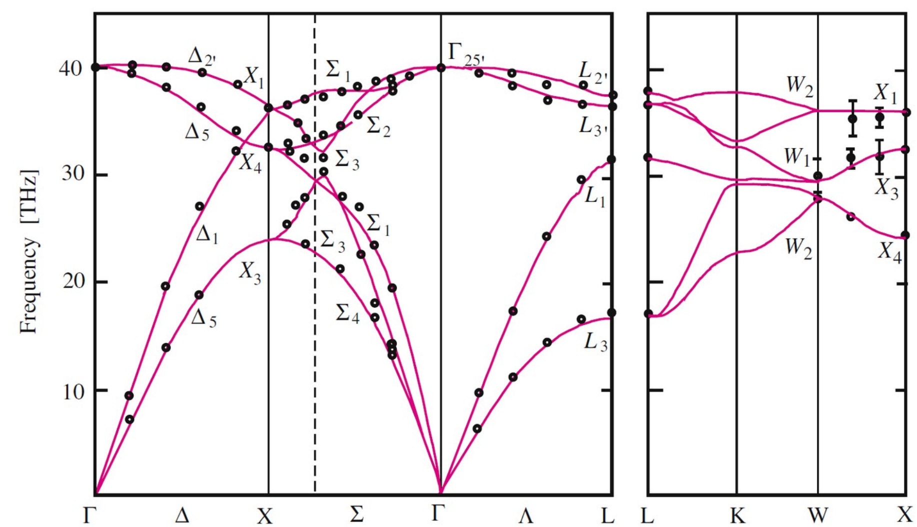
2 atoms in a unit cell
diamond, silicon,
germanium

1st Brillouin zone



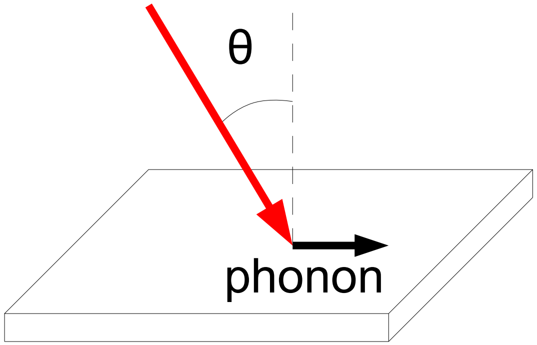
Phonon dispersion of diamond

$$2\pi\hbar \times 40\ \mathrm{THz} = 165\,\mathrm{meV}$$



P. Yu and M. Cardona, “Fundamentals of semiconductors”

Optical probe: infrared spectroscopy



Photon absorption:

momentum conservation $q = \frac{\omega}{c} \sin\theta$ very small

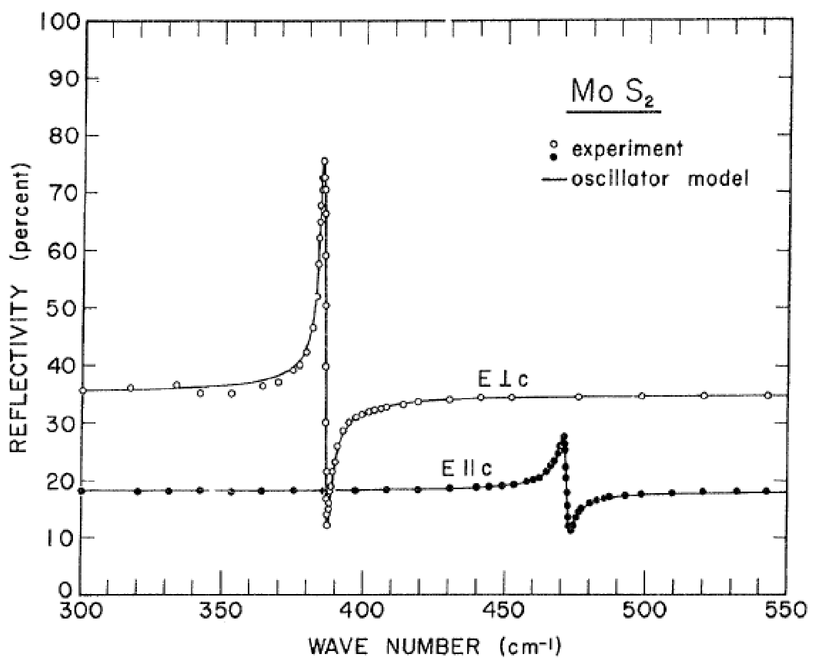
energy conservation $\omega = \omega_{q,\lambda}$

Polarizability

$$\alpha(\omega) = \mathrm{const} + \frac{A}{\omega - \omega_\lambda + i\Gamma_\lambda/2}$$

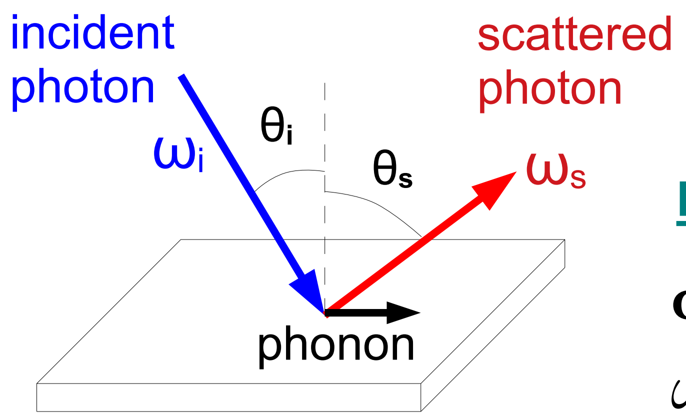
- measure absorption or reflectivity

Bulk MoS_2 from PRB **3**, 4286 (1971)



$$2\pi\hbar c \times 400\ \mathrm{cm}^{-1} = 50\ \mathrm{meV}$$

Optical probe: Raman spectroscopy

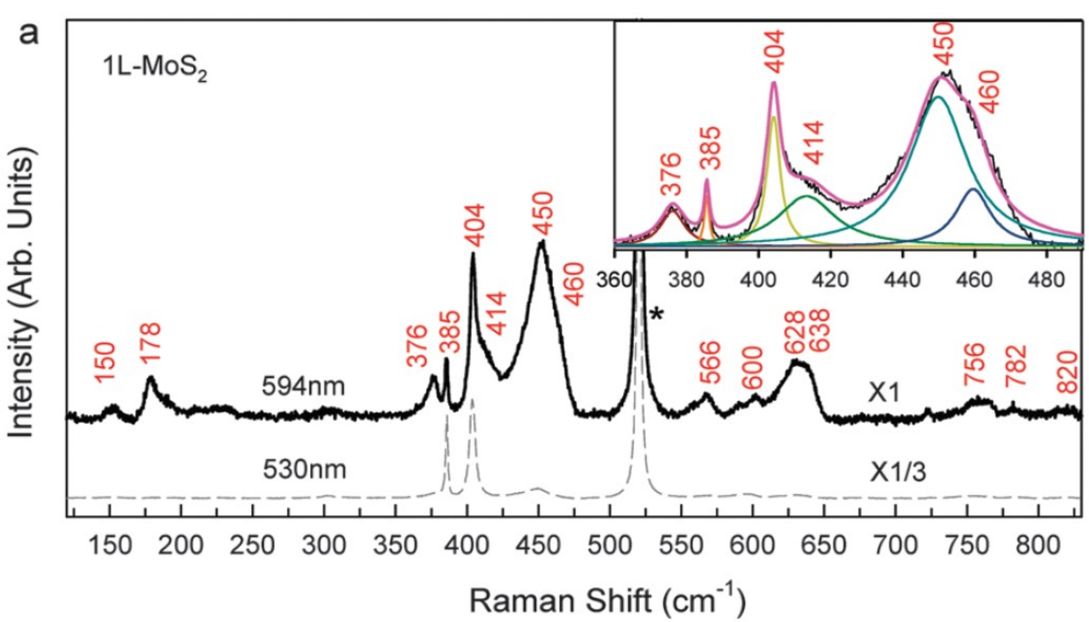


$\omega_s < \omega_i$ – Stokes ($T = 0$)
$\omega_s > \omega_i$ – anti-Stokes (thermal phonon population)

Energy-momentum conservation for *n*-phonon Stokes:

$$\mathbf{q}_1 + \ldots + \mathbf{q}_n = \text{"}0\text{"}$$

$$\omega_{\mathbf{q}_1\lambda_1} + \ldots + \omega_{\mathbf{q}_n\lambda_n} = \omega_\mathrm{i} - \omega_\mathrm{s}$$



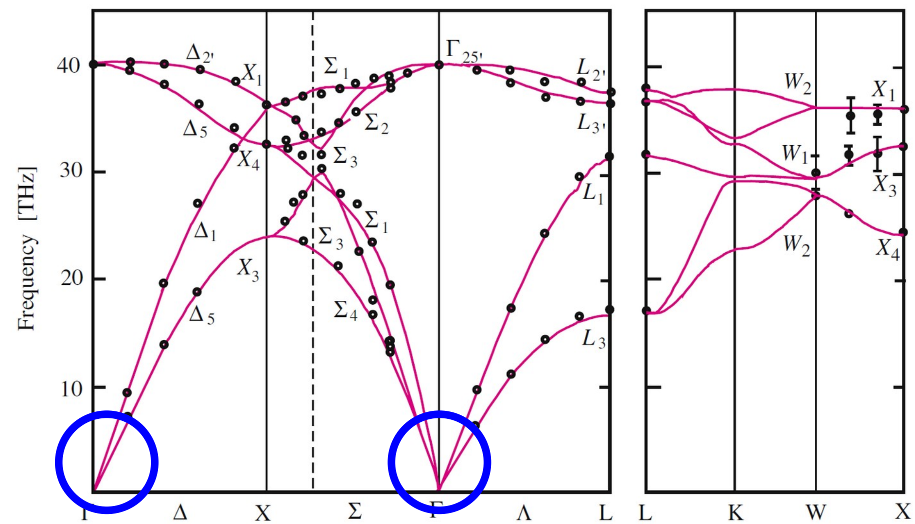
Raman spectrum of monolayer MoS_2

Zhang *et al*, Chem Soc. Rev. **44**, 2757 (2015)

Acoustic phonons

Crystal: continuous translation symmetry
spontaneously broken

soft Goldstone modes



$W(\{\mathbf{R}\})$ invariant under a constant shift

$$\mathbf{R}_{\mathbf{n}j} \mapsto \mathbf{R}_{\mathbf{n}j} + \mathbf{u} \quad \Rightarrow \quad \sum_{j,j'} D^{jj'}_{\alpha\beta}(\mathbf{q}\to 0) = \mathcal{D}_{\alpha\beta\alpha'\beta'}\, q_{\alpha'} q_{\beta'} + O(q^4)$$

symmetric 4-rank tensor

Sufficiently high crystal symmetry (tetrahedral, cubic) $\Rightarrow$

$$\mathcal{D}_{\alpha\beta\alpha'\beta'} = \mathcal{A}\,\delta_{\alpha\beta}\delta_{\alpha'\beta'} + \mathcal{B}\,(\delta_{\alpha\alpha'}\delta_{\beta\beta'} + \delta_{\alpha\beta'}\delta_{\alpha'\beta})$$

$$\begin{aligned}\sum_{j,j'} D^{jj'}_{\alpha\beta}(\mathbf{q}) &= \mathcal{A}\,\delta_{\alpha\beta}q^2 + 2\mathcal{B}\,q_\alpha q_\beta \\ &= \mathcal{A}\left(\delta_{\alpha\beta}q^2 - q_\alpha q_\beta\right) + (\mathcal{A} + 2\mathcal{B})\,q_\alpha q_\beta \\ &\equiv v_{\mathrm{T}}^2\left(\delta_{\alpha\beta}q^2 - q_\alpha q_\beta\right) + v_{\mathrm{L}}^2\,q_\alpha q_\beta\end{aligned}$$

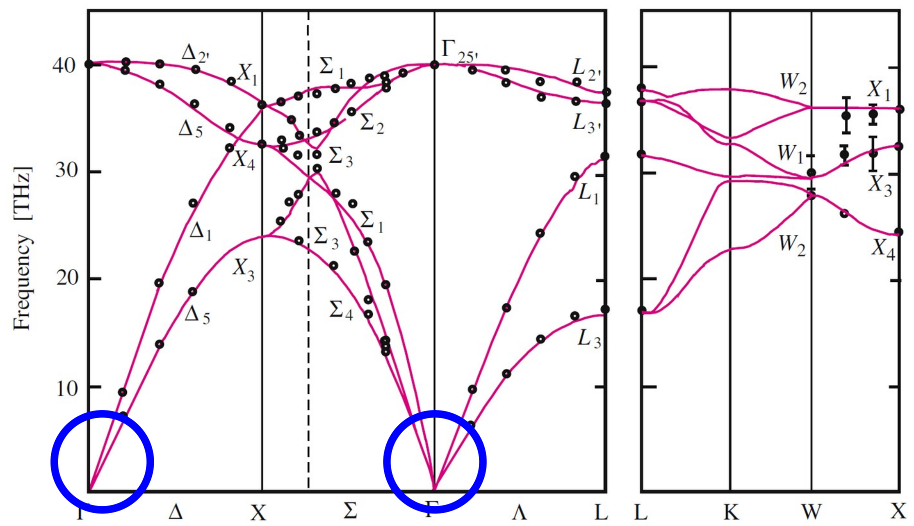
Transverse and longitudinal

sound velocity $v_{\mathrm{L}} > v_{\mathrm{T}}\sqrt{2}$

Acoustic phonons

Crystal: continuous translation symmetry
spontaneously broken

soft Goldstone modes



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symmetric 4-rank tensor

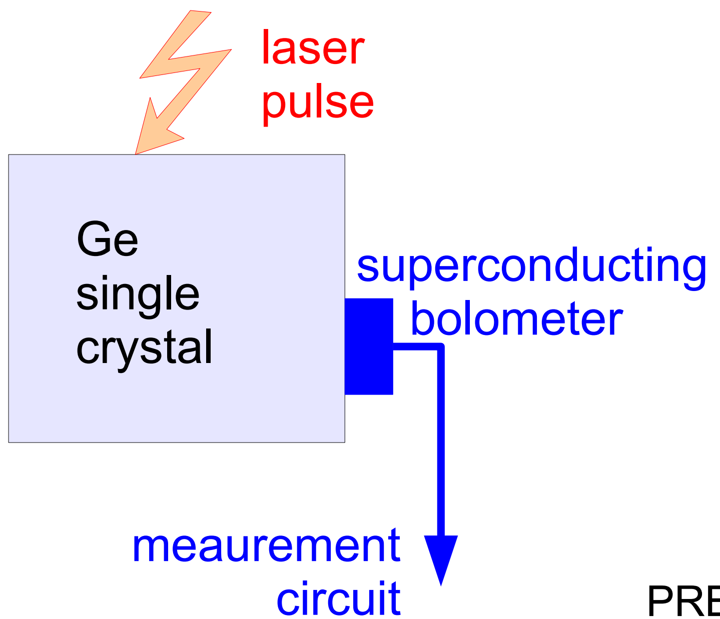
Sufficiently high crystal symmetry
(tetrahedral, cubic)

$$30\,\mathrm{meV} \times 1\,\text{Å}/\hbar \sim 5\,\mathrm{km/s}$$

Transverse and longitudinal
sound velocity $v_\mathrm{L} > v_\mathrm{T}\sqrt{2}$

aluminium:	6.4, 3.0 km/s
copper:	4.8, 2.3 km/s
silicon:	8.4, 5.8 km/s

Phonon imaging



Northrop & Wolfe
PRB **22**, 6196 (1980)

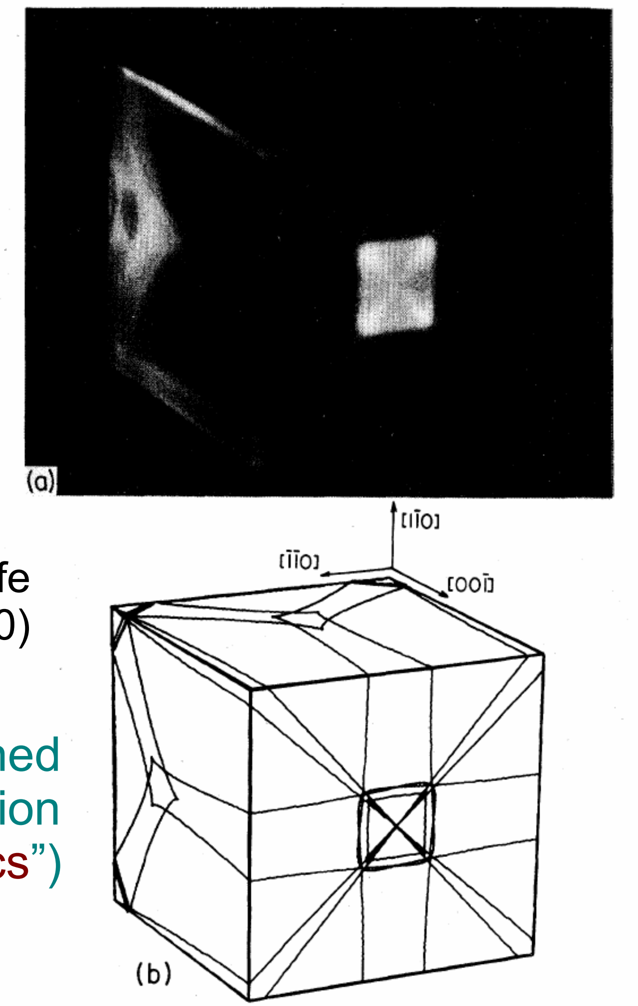


FIG. 11. (a) Ballistic phonon image with laser beam obliquely incident on three sample faces. The bolometer is in the center of the back left (001) face. (b) Calculated $J=0$ singularities projected onto an equivalent cube.

Ballistic phonon propagation is determined by the caustics in the phonon dispersion (“geometric acoustics”)

Phonon kinetics in insulators

Phonon specific heat

Energy density (per volume)

$$\mathcal{E}(T) = \sum_{\lambda} \int_{1\mathrm{BZ}} \frac{d^3\mathbf{q}}{(2\pi)^3} \frac{\hbar\omega_{\mathbf{q}\lambda}}{\exp(\hbar\omega_{\mathbf{q}\lambda}/T) - 1}$$

$T \gg \Theta_D$: $\dfrac{3\nu T}{V_{\mathrm{u.c.}}}$ — ν atoms per unit cell, volume $V_{\mathrm{u.c.}} \sim a^3$

$T \ll \Theta_D$: $\dfrac{\pi^2}{30}\left(\dfrac{T^4}{(\hbar v_{\mathrm{L}})^3} + \dfrac{2T^4}{(\hbar v_{\mathrm{T}})^3}\right)$

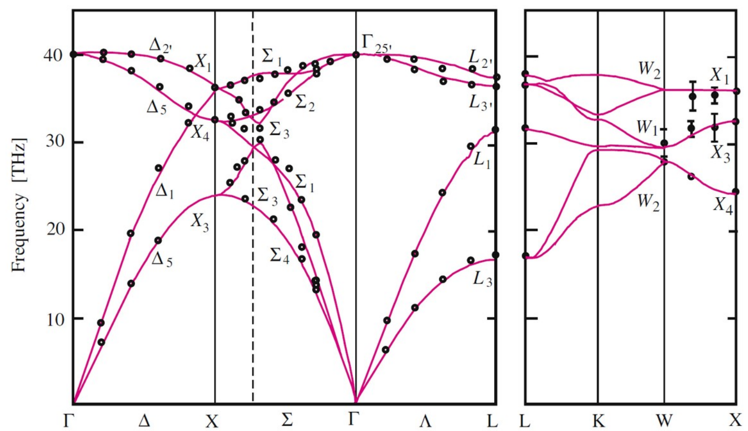
Debye temperature

$\Theta_D \sim \hbar\omega_{\mathrm{ph}}$ @ $q \sim \pi/a$

hundreds of Kelvins

Debye frequency

$\omega_D \equiv \Theta_D/\hbar$



$$C_v(T) = \frac{\partial \mathcal{E}(T)}{\partial T}$$

$T \gg \Theta_D$: $\dfrac{3\nu}{V_{\mathrm{u.c.}}}$ — classical harmonic oscillators (3 per atom)

$T \ll \Theta_D$: $\dfrac{2\pi^2}{15}\left(\dfrac{T^3}{(\hbar v_{\mathrm{L}})^3} + \dfrac{2T^3}{(\hbar v_{\mathrm{T}})^3}\right) \sim \dfrac{1}{\lambda_T^3}$ — thermal phonon wavelegth

Anharmonicity and phonon decay

Potential energy expanded in small displacements:

$$W(\{\mathbf{R}\}) = W(\{\mathbf{R}^{\mathrm{eq}}\}) + \frac{1}{2}\sum_{\mathbf{n},\mathbf{n}'}\sum_{j,j',\alpha,\beta} K_{\alpha\beta}^{jj'}(\mathbf{n}-\mathbf{n}')\,u_{\mathbf{n}j\alpha}\,u_{\mathbf{n}'j'\beta} + O(u^3)$$

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$$+ \frac{1}{6}\sum \Lambda_{\alpha_1\alpha_2\alpha_3}^{j_1j_2j_3}(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)\, u_{\mathbf{n}_1j_1\alpha_1}\, u_{\mathbf{n}_2j_2\alpha_2}\, u_{\mathbf{n}_3j_3\alpha_3} + O(u^4)$$

$$\Lambda \sim \frac{E_{\mathrm{el}}}{a^3} \sim 10\,\mathrm{eV}/\mathrm{\AA}^3$$

Anharmonicity and phonon decay

Potential energy expanded in small displacements:

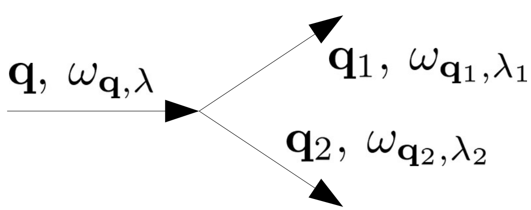
$$W(\{\mathbf{R}\}) = W(\{\mathbf{R}^{\mathrm{eq}}\}) + \frac{1}{2}\sum_{\mathbf{n},\mathbf{n}'}\sum_{j,j',\alpha,\beta} K_{\alpha\beta}^{jj'}(\mathbf{n}-\mathbf{n}')\,u_{\mathbf{n}j\alpha}\,u_{\mathbf{n}'j'\beta} +$$

$$+\frac{1}{6}\sum \Lambda_{\alpha_1\alpha_2\alpha_3}^{j_1j_2j_3}(\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3)\,u_{\mathbf{n}_1j_1\alpha_1}\,u_{\mathbf{n}_2j_2\alpha_2}\,u_{\mathbf{n}_3j_3\alpha_3} + O(u^4)$$

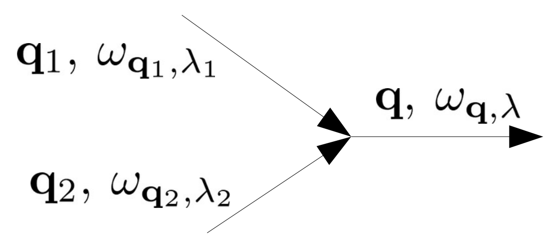
$$\Lambda \sim \frac{E_{\mathrm{el}}}{a^3} \sim 10\,\mathrm{eV}/\mathring{\mathrm{A}}^3$$

<u>Third-order processes:</u>

phonon decay



phonon fusion



energy conservation: $\omega_{\mathbf{q},\lambda} = \omega_{\mathbf{q}_1,\lambda_1} + \omega_{\mathbf{q}_2,\lambda_2}$

momentum conservation: $\mathbf{q} = \mathbf{q}_1 + \mathbf{q}_2 + \mathbf{b}$ reciprocal lattice vector (umklapp scattering)

Anharmonicity and phonon decay

High-energy phonon decay rate:

$$\frac{1}{\tau} \sim \frac{\hbar\Lambda^2}{M^3\omega_D^4}\left(\frac{T}{\hbar\omega_D}\right) \sim \omega_D \times \frac{1}{a^2}\boxed{\frac{\hbar\omega_D}{K}\left(\frac{T}{\hbar\omega_D}\right)}$$

if $T \gg \hbar\omega_D$

lattice constant

quantum fluctuations of the displacement

classical thermal fluctuations of the displacement

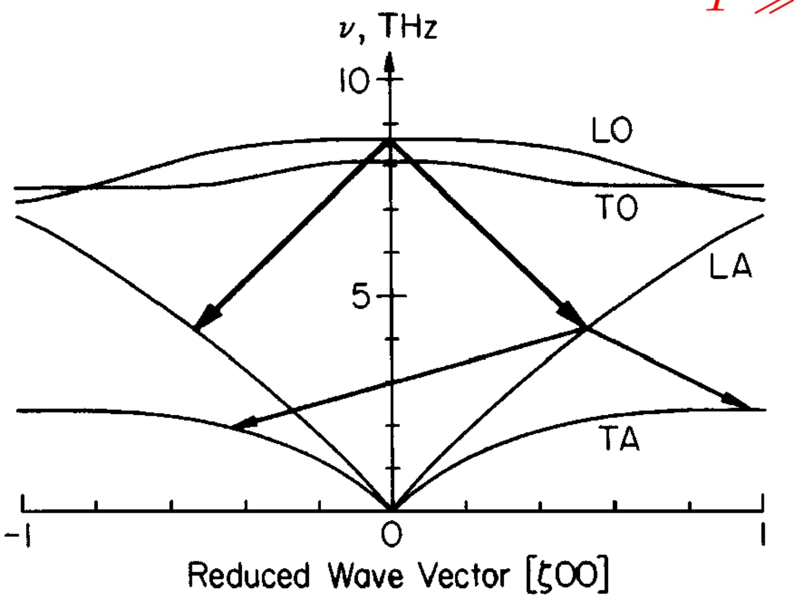


Figure 1 The splitting of an LO phonon into two acoustic phonons and subsequent decay into lower-frequency phonons. The dispersion curves are for GaAs. (from J. P. Wolfe, “Imaging Phonons”)

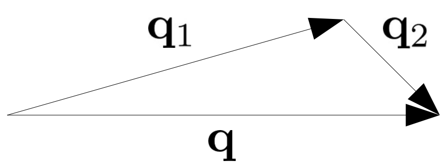
$$\boxed{\frac{1}{\tau} \ll \omega_D}$$

uncertainty principle **ok**

Anharmonicity and phonon decay

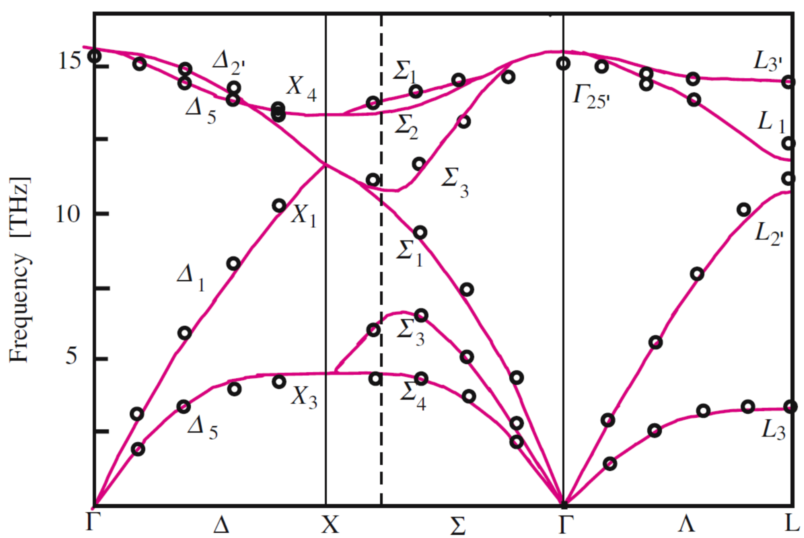
Low energy, low temperature: acoustic phonons, no umklapps

$v_\mathrm{T}|\mathbf{q}_1+\mathbf{q}_2| = v_\mathrm{T}|\mathbf{q}_1| + v_\mathrm{T}|\mathbf{q}_2|$ impossible (triangle inequality + $\omega_{\mathbf{q},\mathrm{T}}$ concave function)



Transverse acoustic phonons do not decay

$v_\mathrm{L}|\mathbf{q}_1+\mathbf{q}_2| = v_\mathrm{T}|\mathbf{q}_1| + v_\mathrm{T}|\mathbf{q}_2|$ possible, but $\dfrac{1}{\tau} \sim \omega_D \dfrac{\hbar\omega_D}{Ka^2}\left(\dfrac{\omega}{\omega_D}\right)^5$



Yu & Cardona, “Fundamentals of semiconductors”

LA phonon lifetime in silicon:

Frequency ν (THz)	Lifetime τ_a (ns)
7.5	0.0006
3.75	0.018
1.88	0.58
0.94	19

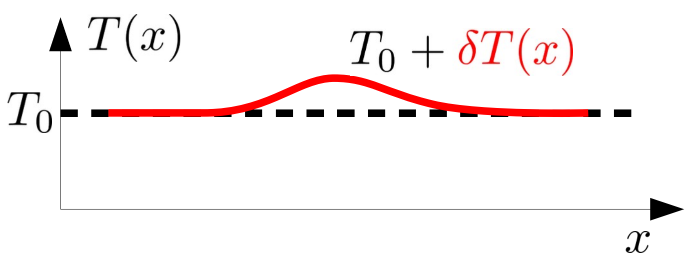
(from J. P. Wolfe, “Imaging Phonons”)

Goldstone modes are robust

Thermal conductivity

$$\frac{\partial \mathcal{E}(T)}{\partial t} = -\boldsymbol{\nabla} \cdot \mathbf{J}$$ heat current density

$$\mathbf{J} = -\kappa(T)\,\boldsymbol{\nabla} T$$ Fourier’s law (the current must vanish @ T = const)



Linearize the equation around T_0:

$$C_v(T_0)\,\frac{\partial \delta T}{\partial t} = \kappa(T_0)\,\nabla^2 \delta T$$ diffusion equation for temperature

specific heat

$$C_v(T) = \frac{\partial \mathcal{E}(T)}{\partial T}$$

thermal conductivity

$$\frac{\kappa}{C_v} \sim D \sim \frac{l^2}{\tau} = v^2\,\tau$$ phonon diffusion coefficient

$$l = v\tau$$ mean free path

$$\boxed{\kappa(T) \sim C_v(T)\,v^2\,\tau(T)}$$

Thermal conductivity

High temperatures $T \gg \Theta_D$: $\kappa \sim \frac{1}{a^3} \frac{v^2}{\omega_D} \frac{Ka^2}{T} \sim \frac{Ka}{\hbar} \frac{\Theta_D}{T}$ (Debye, 1929)

Low temperatures $T \ll \Theta_D$:

1. TA phonons $\tau = \infty$
2. LA phonons $\tau \propto 1/\omega^5$, but

$$\mathbf{q} = \mathbf{q}_1 + \mathbf{q}_2 + \cancel{\mathbf{b}}$$

no umklapps
momentum is conserved
energy current does not relax

A high-energy phonon needed to provide umklapp ⇨ $\kappa \propto e^{\Theta_D/T}$ (Peierls, 1929)

Phonon scattering on isotopic defects: $\frac{1}{\tau} \sim \omega_D \frac{n_\mathrm{d}}{n_0} \left(\frac{\Delta M}{M}\right)^2 \left(\frac{\omega}{\omega_D}\right)^4$ (Pomeranchuk, 1942)

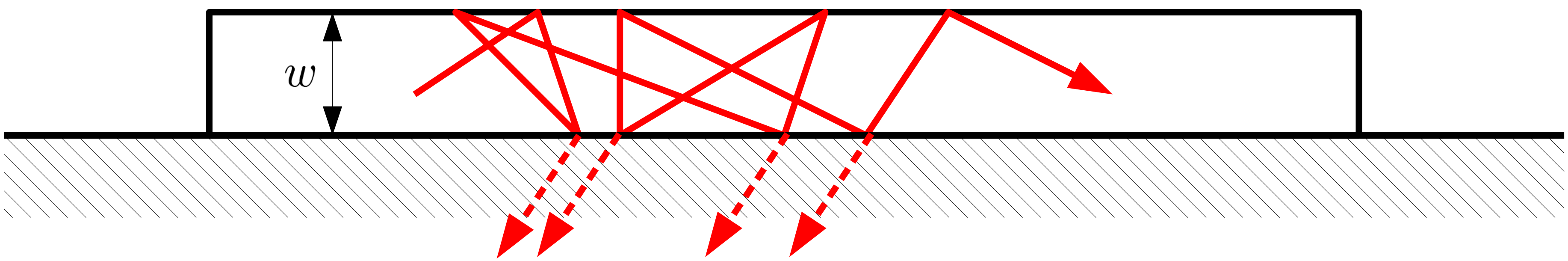
fraction of defective atoms

All phonon scattering mechanisms become very inefficient at low temperatures

Ballistic phonons

rough surface → diffuse scattering (Casimir, 1938)

scattering time $\tau \sim w/v$ ⇒ $\kappa(T) \sim C_v(T)\, vw$



escape to the substrate

area

Heat current density across the interface: $J_\perp = \dfrac{A}{R_\mathrm{K}} \Delta T$

Kapitza resistance

Acoustic mismatch model: wave refraction at a flat interface

Diffuse mismatch model: random scattering at a rough interface

Isotope and boundary effects

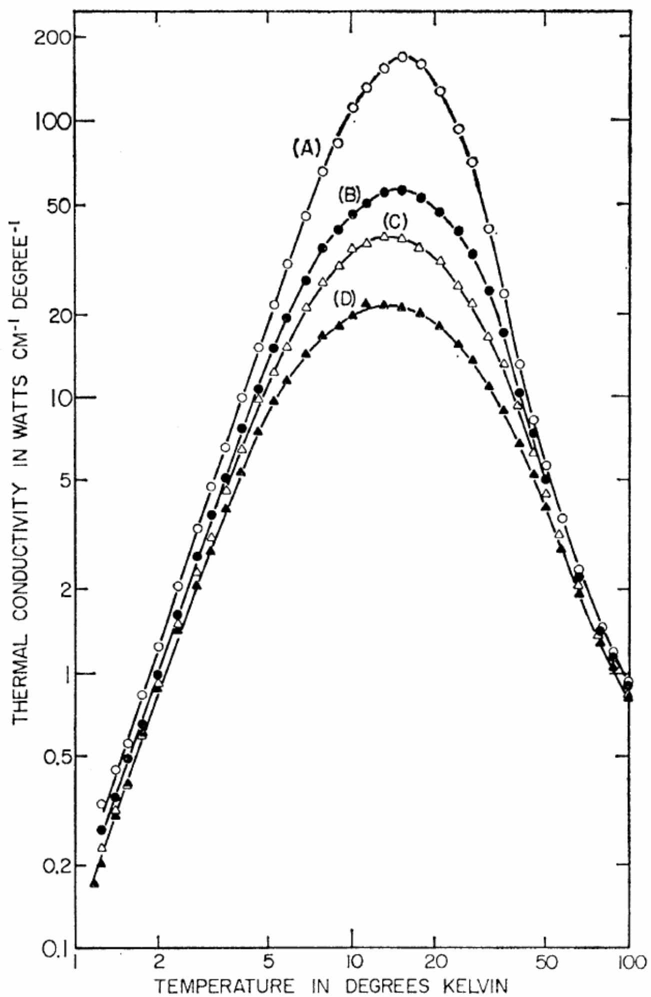


FIG. 4. Thermal conductivity of LiF showing the effect of isotopes. % ^{7}Li in LiF: (A) 99.99, (B) 97.2, (C) 92.6 (natural LiF), (D) 50.8. Mean crystal widths: (A) 7.25 mm, (B) 5.33 mm, (C) 5.44 mm, (D) 5.03 mm. Crystals A, B, and C were regrown

P. D. Thacher, Phys. Rev. **159**, 975 (1967)

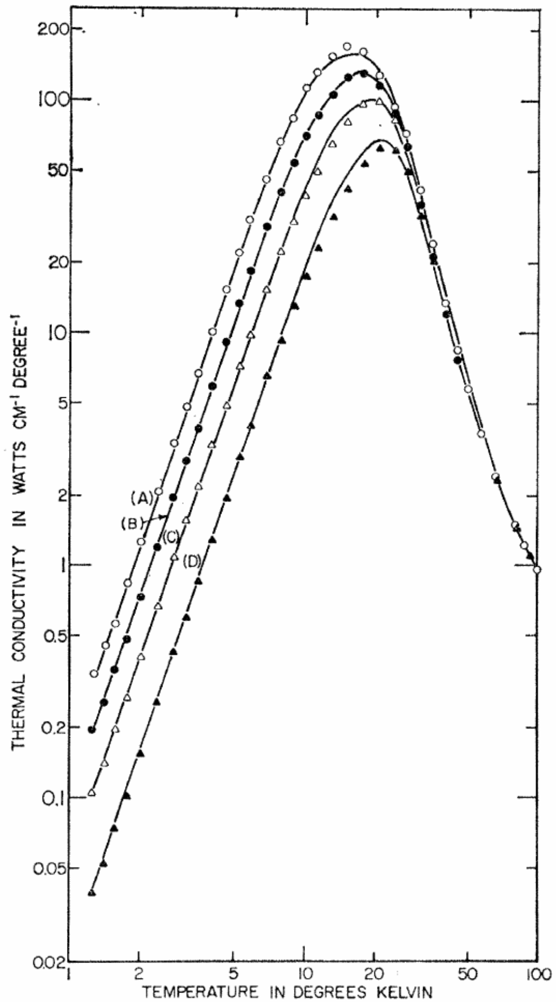


FIG. 1. Thermal conductivity of isotopically pure LiF showing the effect of boundaries for sandblasted crystals. Mean crystal widths: (A) 7.25 mm, (B) 4.00 mm, (C) 2.14 mm, (D) 1.06 mm.

Isotope and boundary effects

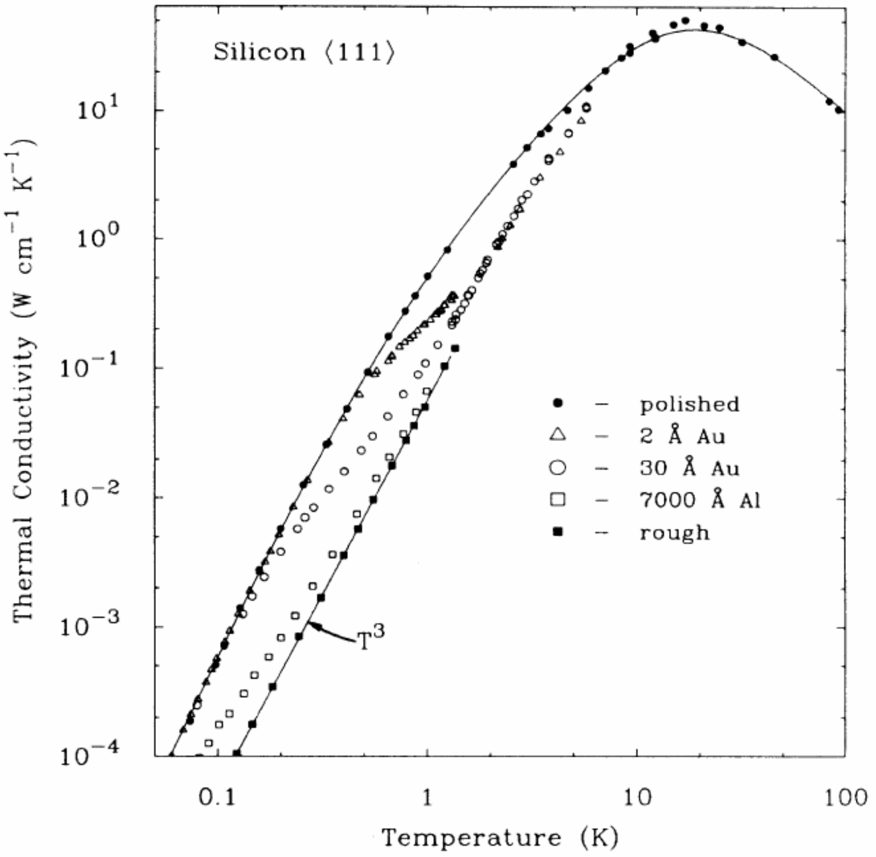


FIG. 5. Thermal conductivity of a pure silicon single crystal with different surface treatments. Top curve: Syton polished and cleaned; bottom: sandblasted. The intermediate curves were measured after metal films were deposited *(ex situ)* onto the polished and cleaned surfaces.

Klitsner & Pohl
Phys. Rev. B **36**, 6551 (1987)

Phonon kinetics in metals

Acoustic phonons in metals

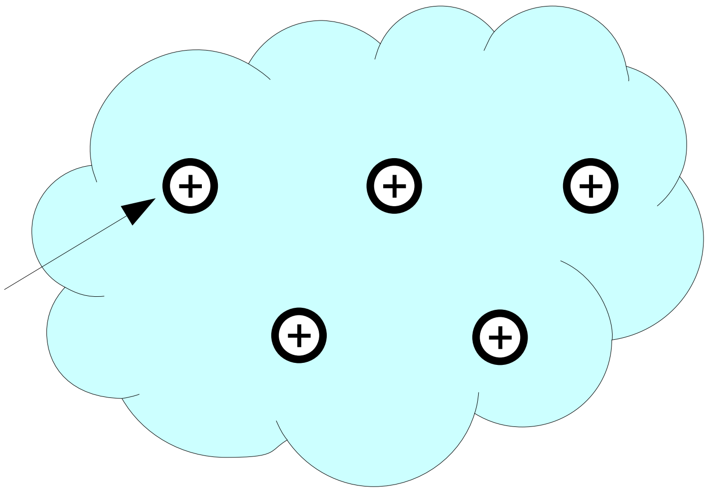
Atoms give away their valence electrons

Ions in electron jellium
instead of atoms with springs

$$M\,\frac{d^2\mathbf{u}_n}{dt^2} = -\frac{\partial W}{\partial \mathbf{u}_n}$$

from ions & electrons

charge $+Ze$
mass M
density n_i



Uniform system is electroneutral

Deformed system with ion displacements: $\mathbf{u}_n = \mathbf{u}(\mathbf{R}_n) = \mathbf{u}_\mathbf{q} e^{i\mathbf{q}\mathbf{R}_n - i\omega t}$

change in the ionic density $\dfrac{\delta n_\mathrm{i}(\mathbf{R})}{n_\mathrm{i}} = -\boldsymbol{\nabla}\cdot\mathbf{u}(\mathbf{R}) = -i\mathbf{q}\mathbf{u}_\mathbf{q}\,e^{i\mathbf{q}\mathbf{R} - i\omega t}$

Coulomb potential $\varphi(\mathbf{R}) = \displaystyle\int \frac{d^3\mathbf{R}'}{|\mathbf{R}-\mathbf{R}'|}\,Ze\,\delta n_\mathrm{i}(\mathbf{R}') = -\frac{4\pi Zen_\mathrm{i}}{q^2}\,i\mathbf{q}\mathbf{u}_\mathbf{q}\,e^{i\mathbf{q}\mathbf{R} - i\omega t}$

$$\omega^2 = \frac{4\pi n_\mathrm{i}(Ze)^2}{M} \sim \omega_D^2$$

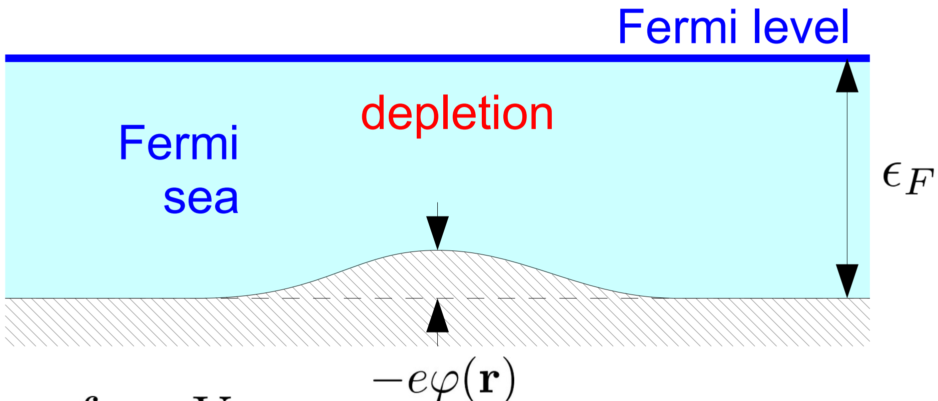
ionic plasma frequency,
not acoustic phonon

Screening by the Fermi sea

Electron density responds to the potential:

$$\delta n_{\mathrm{e}}(\mathbf{r}) \approx \nu e\varphi(\mathbf{r})$$

electronic density of states at the Fermi level



Fermi energy $\epsilon_F \sim \text{a few eV}$

Fermi momentum $p_F \sim 1\,\mathring{\mathrm{A}}^{-1}$

Fermi velocity $v_F \sim (\text{a few})\,\mathrm{eV}\,\mathring{\mathrm{A}}/\hbar \sim 10^6\ \mathrm{m/s}$

$$\nu \sim \frac{1}{(\text{a few})\,\mathrm{eV}\,\mathring{\mathrm{A}}^3}$$

Self-consistent potential from ions and electrons: screened Coulomb

$$-\nabla^2\varphi(\mathbf{r}) = 4\pi Ze\,\delta n_{\mathrm{i}}(\mathbf{r}) - 4\pi e\,\delta n_{\mathrm{e}}(\mathbf{r}) \Rightarrow \varphi(\mathbf{R}) = \int \frac{d^3\mathbf{R}'\,e^{-\kappa_D|\mathbf{R}-\mathbf{R}'|}}{|\mathbf{R}-\mathbf{R}'|}\,Ze\,\delta n_{\mathrm{i}}(\mathbf{R}')$$

$$\kappa_D \equiv \sqrt{4\pi e^2\nu} \sim 1\,\mathring{\mathrm{A}}^{-1}$$

inverse Debye (Thomas-Fermi) screening length

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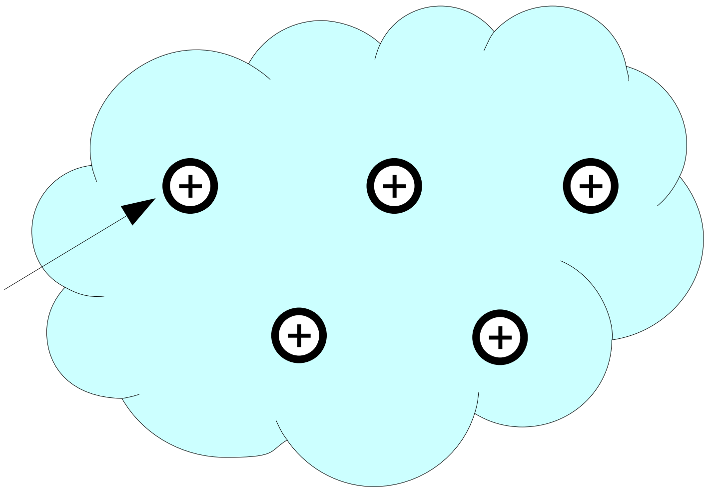

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change in the ionic density $\dfrac{\delta n_\mathrm{i}(\mathbf{R})}{n_\mathrm{i}} = -\boldsymbol{\nabla}\cdot\mathbf{u}(\mathbf{R}) = -i\mathbf{q}\mathbf{u}_\mathbf{q}\, e^{i\mathbf{q}\mathbf{R} - i\omega t}$

Screeneed Coulomb potential $\varphi(\mathbf{R}) = -\dfrac{4\pi Zen_\mathrm{i}}{q^2+\kappa_D^2}\, i\mathbf{q}\mathbf{u}_\mathbf{q}\, e^{i\mathbf{q}\mathbf{R} - i\omega t}$

$$\omega^2 = \frac{4\pi n_\mathrm{i}(Ze)^2}{M}\,\frac{q^2}{\cancel{q^2}+\kappa_D^2} \approx v_L^2 q^2 \qquad v_L = \sqrt{\frac{Z^2\rho}{M^2\nu}} \sim (\text{a few})\,\frac{\text{km}}{\text{s}}$$

Electron-phonon interaction

Born-Oppenheimer:

$W(\{\mathbf{u}_n\})$ from electronic ground state energy at fixed $\{\mathbf{u}_n\}$

$$M\,\frac{d^2\mathbf{u}_n}{dt^2} = -\frac{\partial W}{\partial \mathbf{u}_n}$$

basic assumption:
electrons follow adiabatically the nuclear motion

Validity: $\omega \ll E_1 - E_0$ electronic energy gap

Breaks down in any metal, semimetal, doped semiconductor

Electrons feel the potential

$$-e\varphi(\mathbf{r}) = \frac{n_\mathrm{i} Z^2}{\nu}\,\boldsymbol{\nabla}\cdot\mathbf{u}(\mathbf{r})\,e^{-i\omega t}$$

oscillating field

deformation potential ~ 10–20 eV

Phonon absorption by electrons

Electronic density response to an oscillating potential from the Kubo formula: $\Pi(\mathbf{q},\omega)$

Phonon decay rate:

$$\frac{1}{\tau} = -\omega\,\mathrm{Im}\,\Pi(\mathbf{q},\omega)\,\frac{n_\mathrm{i}Z^4/\nu^2}{2Mv_L^2} \sim \omega\sqrt{\frac{m}{M}}$$

The main mechanism of acoustic phonon decay in metals: **phonon absorption by electrons**

or escape to the substrate (Kapitza)

Decay rate due to anharmonicity:

$$\frac{1}{\tau} \sim \omega_D\sqrt{\frac{m}{M}}\left(\frac{\omega}{\omega_D}\right)^5$$

much weaker

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Inverse process: phonon emission by electrons (detailed balance)

Electron temperature T_{el}
Phonon temperature T_{ph}
$(T_\mathrm{el}, T_\mathrm{ph} \ll \Theta_D)$

Heat flow from electrons to phonons:

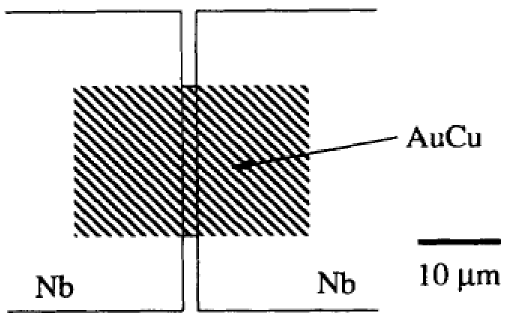
power per unit volume = $\Sigma\,(T_\mathrm{el}^5 - T_\mathrm{ph}^5)$

experimentally measurable coefficient

$$\int_0^\infty q^2\,dq\,\frac{\hbar v q}{e^{\hbar v q/T}-1}\,\frac{1}{\tau} \propto T^5$$

Phonon absorption by electrons

Wellstood, Urbina & Clarke,
PRB **49,** 5942 (1994)



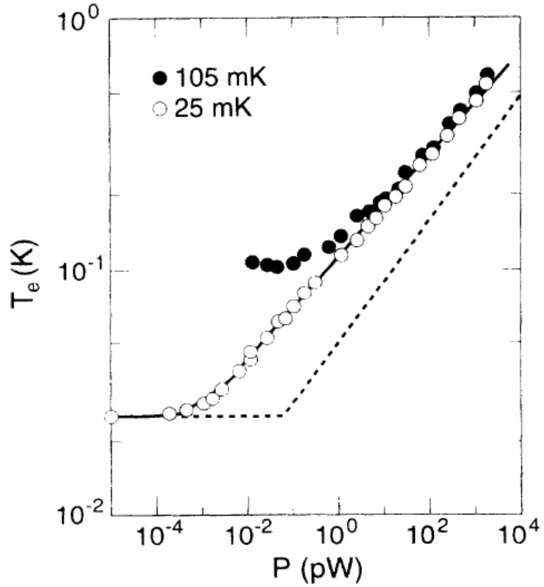


FIG. 8. Measured electron temperature T_e vs dissipated power for resistor 1 at two bath temperatures. The solid line is the fit of Eq. (4.1) to 25-mK data with $n = 4.87$. The dashed line is the "simple heating model."

Electron temperature T_{el}
Phonon temperature T_{ph}

Heat flow from electrons to phonons:

power per unit volume = $\Sigma \left(T_{\mathrm{el}}^5 - T_{\mathrm{ph}}^5\right)$

experimentally measurable coefficient

$$\int_0^\infty q^2\,dq\,\frac{\hbar v q}{e^{\hbar v q/T}-1}\,\frac{1}{\tau} \propto T^5$$

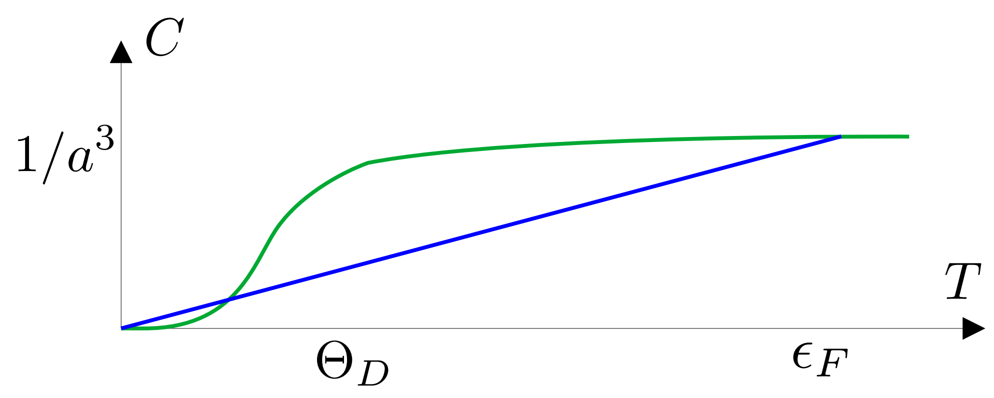
Specific heat and thermal conductivity

Phonons: $C_{\mathrm{ph}}(T \ll \Theta_D) \sim \frac{(T/\Theta_D)^3}{a^3}$ $\qquad C_{\mathrm{ph}}(T \gg \Theta_D) \sim \frac{1}{a^3}$

Electrons: $C_{\mathrm{el}}(T) = \frac{\partial}{\partial T}\, 2 \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3}\, \frac{\epsilon_{\mathbf{p}}}{e^{(\epsilon_{\mathbf{p}}-\epsilon_F)/T}+1}$

$$C_{\mathrm{el}}(T \ll \epsilon_F) = \frac{\pi^2}{3}\,\nu T \sim \frac{T/\epsilon_F}{a^3}$$

dominate below a few Kelvins



Superconductor: $C_{\mathrm{el}}(T \ll T_c) = \sqrt{2\pi}\,\nu\Delta \left(\frac{\Delta}{T}\right)^{3/2} e^{-\Delta/T}$

Specific heat and thermal conductivity

Phonons: $C_{\text{ph}}(T \ll \Theta_D) = \frac{2\pi^2}{15}\left(\frac{T^3}{(\hbar v_{\text{L}})^3} + \frac{2T^3}{(\hbar v_{\text{T}})^3}\right)$

Electrons: $C_{\text{el}}(T \ll \epsilon_F) = \frac{\pi^2}{3}\,\nu T$ dominate below a few Kelvins

Electronic thermal conductivity: $\kappa_{\text{el}} \sim C_{\text{el}}\, v_F^2 \tau_{\text{el}}$ dominates over phonons

much larger than sound velocity

Electric conductivity: $\sigma \sim e^2 \nu\, v_F^2 \tau_{\text{el}}$

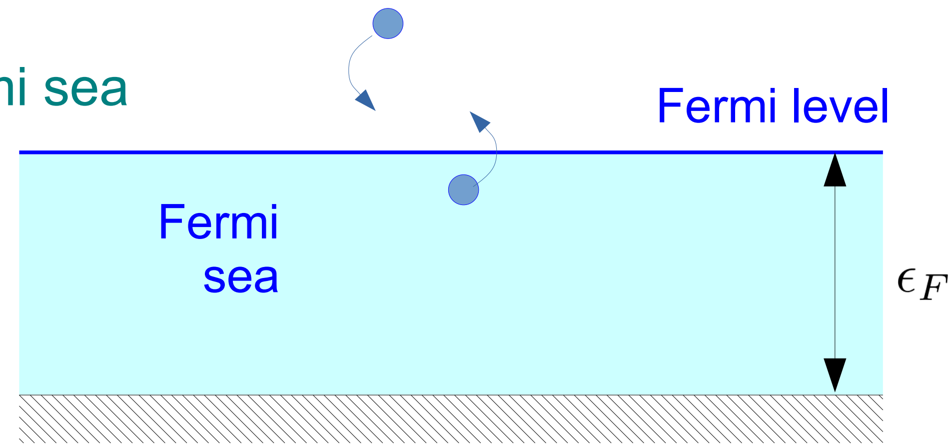
Wiedemann-Franz law: $\frac{\kappa}{\sigma} = \frac{\pi^2}{3}\,\frac{T}{e^2}$

Electron energy relaxation

Electron-electron collision:
kick another electron from the Fermi sea
(emit an *e-h* pair)

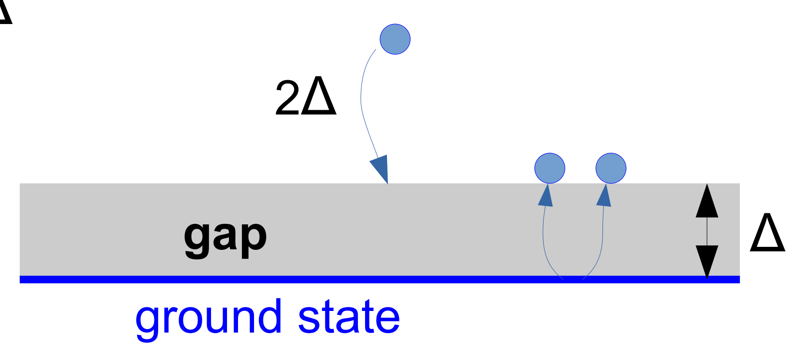
$$\frac{1}{\tau_{\mathrm{el}}} \sim \frac{(\epsilon - \epsilon_F)^2}{\hbar \epsilon_F}$$

(Landau & Pomeranchuk)



Superconductors: quasiparticle gap Δ

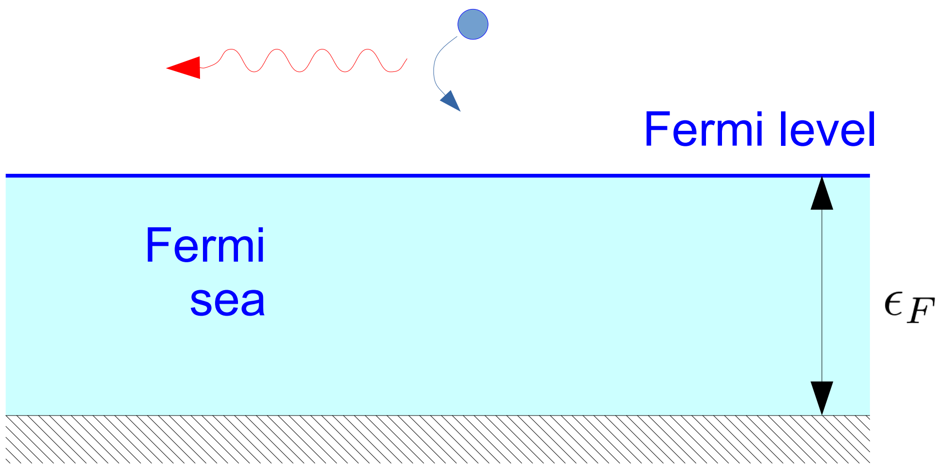
breaking a Cooper pair: cost 2Δ



Electron energy relaxation

Phonon emission

$$\epsilon_F \sim (\text{a few})\,\text{eV}$$
$$\hbar\omega_D \sim (\text{a few})\,10\,\text{meV}$$
$$\Delta \sim (\text{a few})\,100\,\mu\text{eV}$$
$$\frac{\hbar}{1\,\text{eV}} = 0.658\,\text{fs}$$

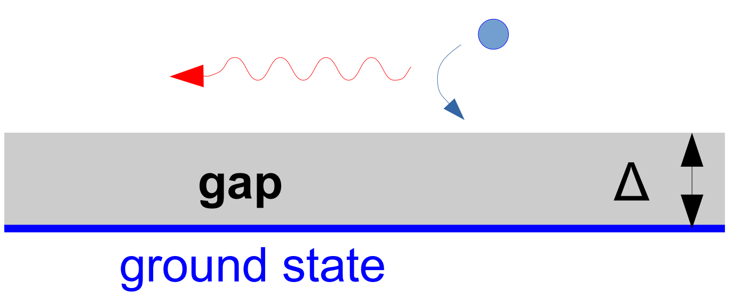


$\epsilon - \epsilon_F \gtrsim \hbar\omega_D$ | $\frac{1}{\tau_{\text{el}}} \sim \omega_D$

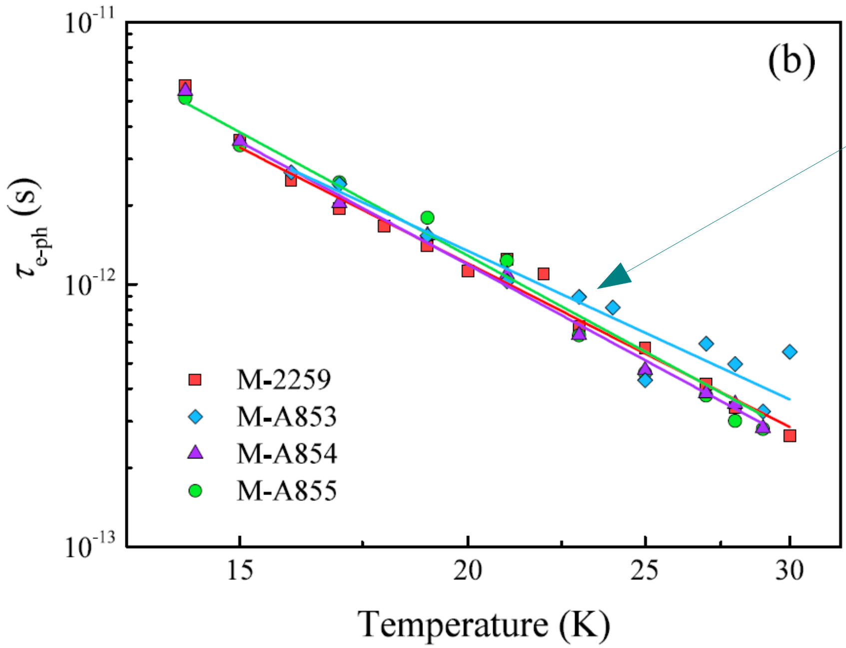
if $T_{\text{ph}} \gg \hbar\omega_D$, then $1/\tau_{\text{el}} \sim T_{\text{ph}}/\hbar$
random walk in energy

$\Delta \ll \epsilon - \epsilon_F \ll \hbar\omega_D$ | $\frac{1}{\tau_{\text{el}}} \sim \frac{(\epsilon-\epsilon_F)^3}{\hbar^3\omega_D^2}$

$\epsilon - \epsilon_F - \Delta \ll \Delta$ | $\frac{1}{\tau_{\text{el}}} \sim \frac{(\epsilon-\epsilon_F-\Delta)^{7/2}}{\hbar^3\omega_D^2\Delta^{1/2}}$



Electron energy relaxation



slopes between 3 and 4

clean electrons: $1/\tau_{\rm el} \propto T^3$

electrons scattering on impurities: $\dfrac{1}{\tau_{\rm el}} \propto T^4$

M. Sidorova *et al.*, PRB **102**, 054501 (2020)

Disordered NbN

Relaxation cascade in a detector

Overall picture

> 100 eV - cascade of atomic collisions

Kozorezov *et al.*, PHYSICAL REVIEW B **75**, 094513 (2007)

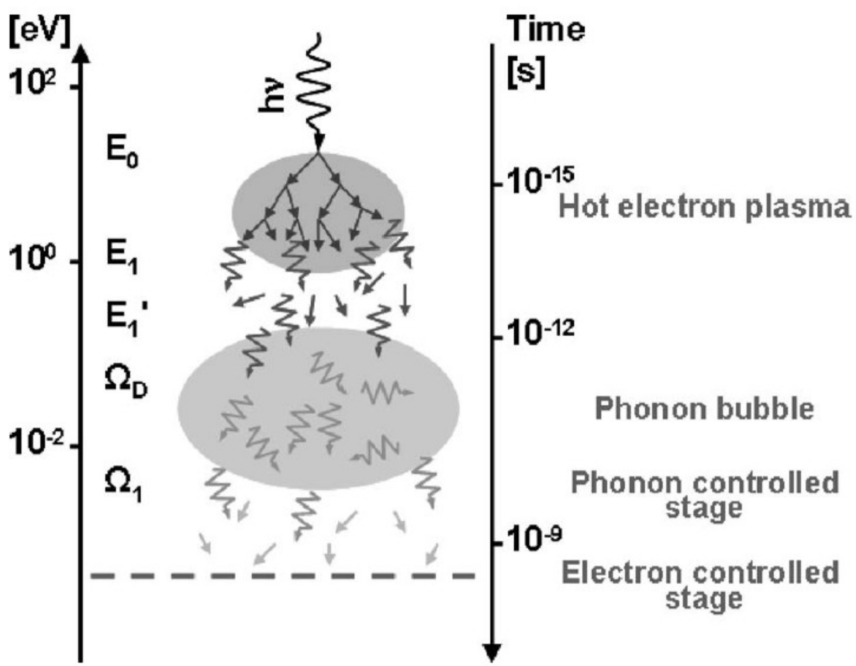
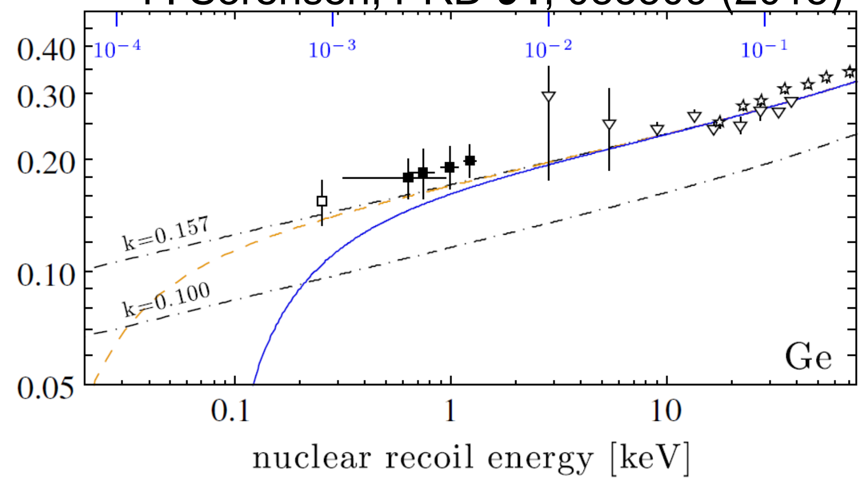


FIG. 1. Schematic picture of photoelectron energy down-conversion in a superconductor.

P. Sorensen, PRD **91**, 083509 (2015)



fraction of energy given to electrons by a fast Ge atom in a Ge crystal

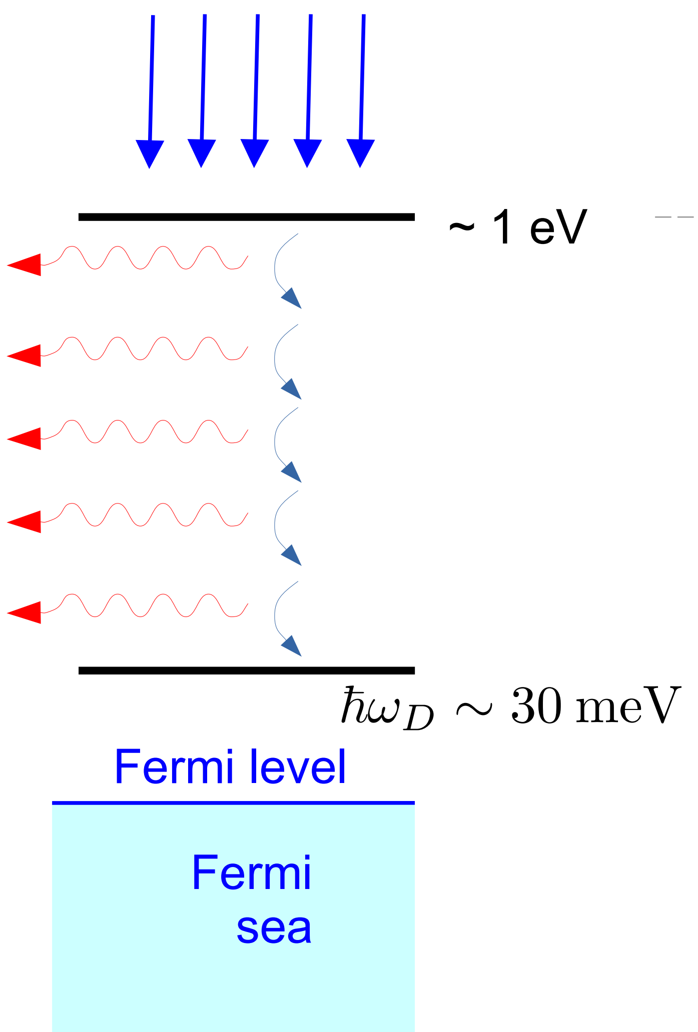
electronic plasmons (10–20 eV)

Landau damping

electron-hole pairs

within (a few) femtoseconds

Formation of the phonon bubble



Electron-hole pair emission rate		Phonon emission rate
$(\epsilon - \epsilon_F)^2/(\hbar\epsilon_F)$	$\gg$	ω_D
$(\epsilon - \epsilon_F)^2/(\hbar\epsilon_F)$	$\ll$	ω_D

Cascade emission of phonons with $\omega \sim \omega_D$

~ 1 picosecond

Phonon bubble

size ~ 10 nm

Most of the deposited energy is stored in the phonons $\omega \sim \omega_D$

Phonon down-conversion

phonon

escape to the substrate

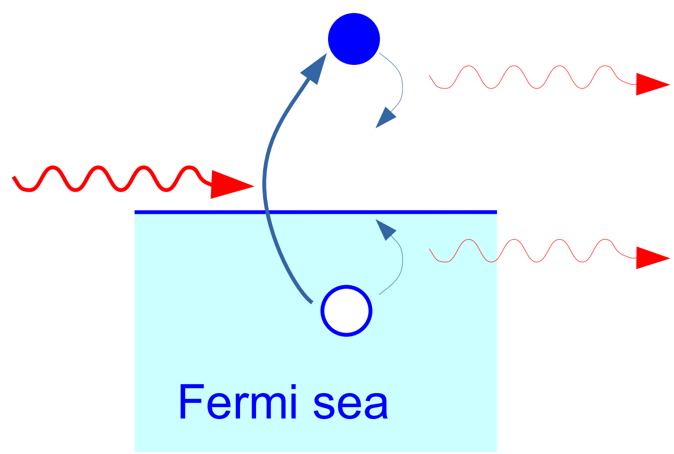
$$\frac{30\ \mathrm{nm}}{3\ \mathrm{km/s}} \sim 10\ \mathrm{ps}$$

produce electron-hole pair

$$1/\tau_{\mathrm{ph}} \sim \omega\sqrt{m/M}$$

electron and hole emit phonons

$$1/\tau_{\mathrm{el}} \sim (\epsilon - \epsilon_F)^3/(\hbar^3\omega_D^2)$$



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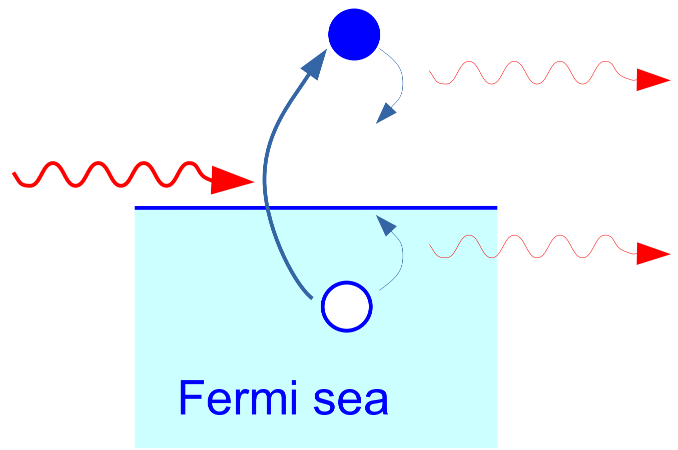
electron and hole emit phonons

$$1/\tau_{\mathrm{el}} \sim (\epsilon - \epsilon_F)^3/(\hbar^3\omega_D^2)$$

total
energy
conserved



Phonon down-conversion

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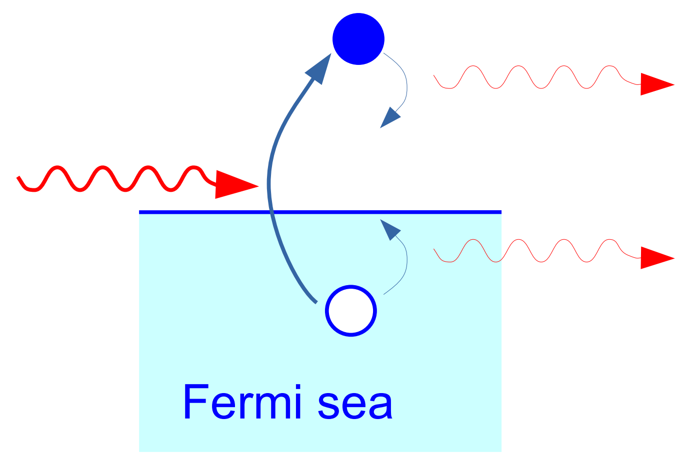
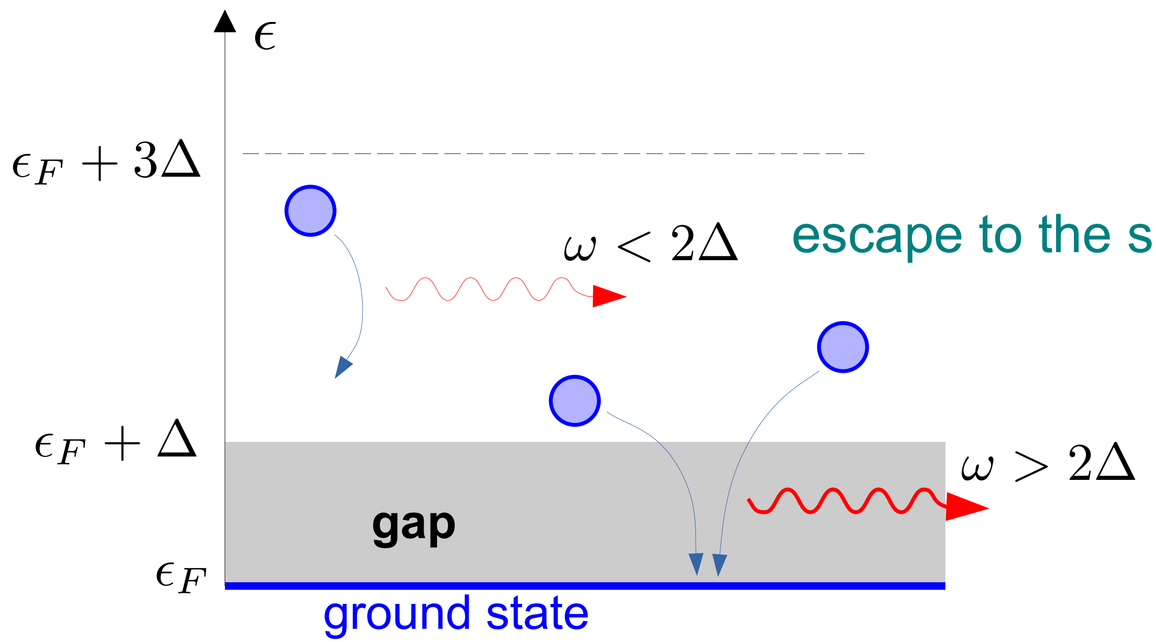


Down to ω ~ 2Δ
~ 1 nanosecond

pair-breaking threshold in a superconductor

Kozorezov *et al.*,
PRB **61**, 11807 (2000)

Quasiparticle cloud



escape to the substrate

escape to the substrate (> 10 ps)
break a Cooper pair (~ 1 ns)

To recombine,
two quasiparticles
must meet

Detect quasiparticle population:

1. Increase in the kinetic inductance
2. Increase in the dissipative conductivity

Cloud expansion:
quasiparticle diffusion

Useful textbooks

Ashcroft and Mermin, *Solid State Physics*

Ziman, *Electrons and Phonons: The Theory of Transport Phenomena in Solids*

Lifshitz & Pitaevskii, *Physical Kinetics*

Abrikosov, *Fundamentals of the Theory of Metals*

Yu & Cardona, *Fundamentals of Semiconductors*

Wolfe, *Imaging Phonons: Acoustic Wave Propagation in Solids*