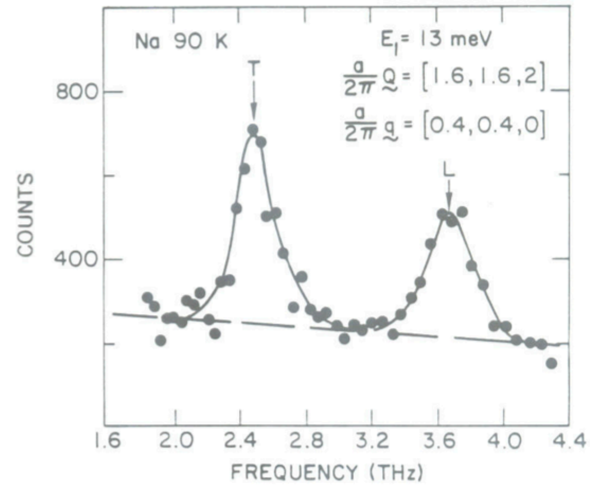
Inelastic Neutron scattering:

Probability of scatter includes zero and one-phonon terms (Fermi golden rule). (Also higher-order.)



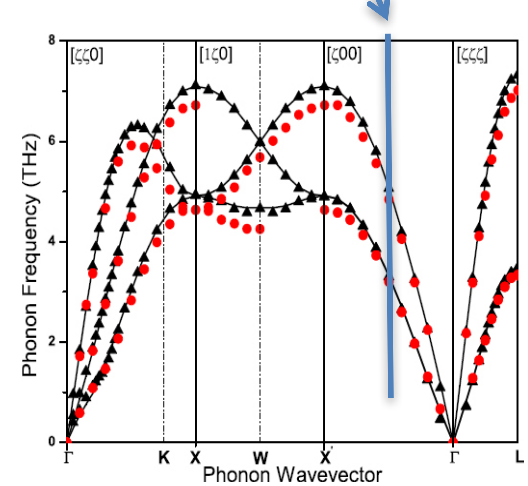
$$P \propto \left| \langle \psi | H_o + H_1 + \ldots | \psi \rangle \right|^2$$

Interaction of neutron with solid

$H_o \Rightarrow$ bragg scattering

Example, scanned energy transfer, giving phonon dispersion curves.

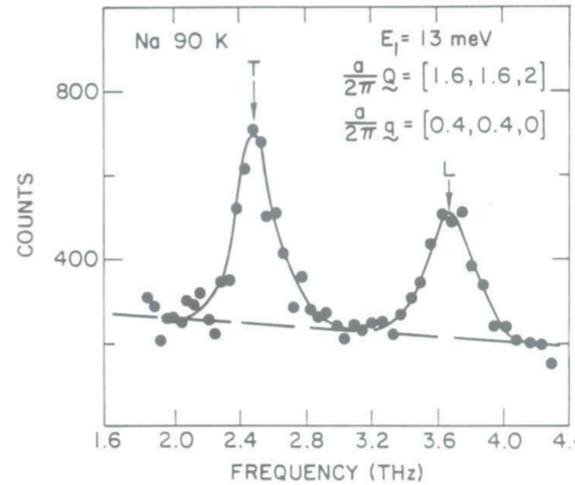
$H_1 \propto \hat{u} \quad (or\ Q_q)$ recall ~ sum of a and $a^\dagger$ (<u>One phonon term.</u>) gives isolated peaks.



H_2 and higher: broad background. (also, incoherent <u>static</u> atom displacements & impurities contribute broad signal.)

Neutron scattering:

Probability of scatter includes zero and one-phonon terms (Fermi golden rule). (Also higher-order.)

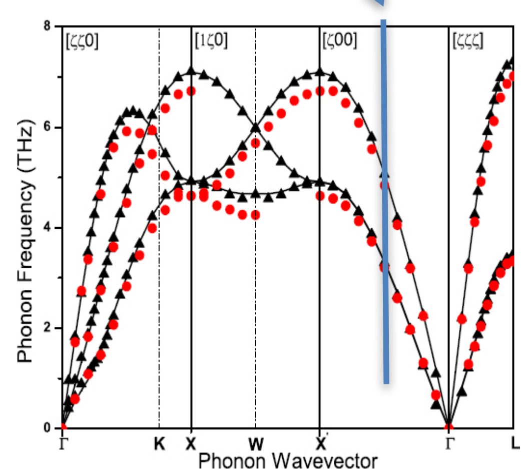


Selection rules:

$$\Delta\vec{k} = \vec{K} \pm \sum \vec{q}$$

$$\Delta\varepsilon = \pm \sum \hbar\omega_q$$

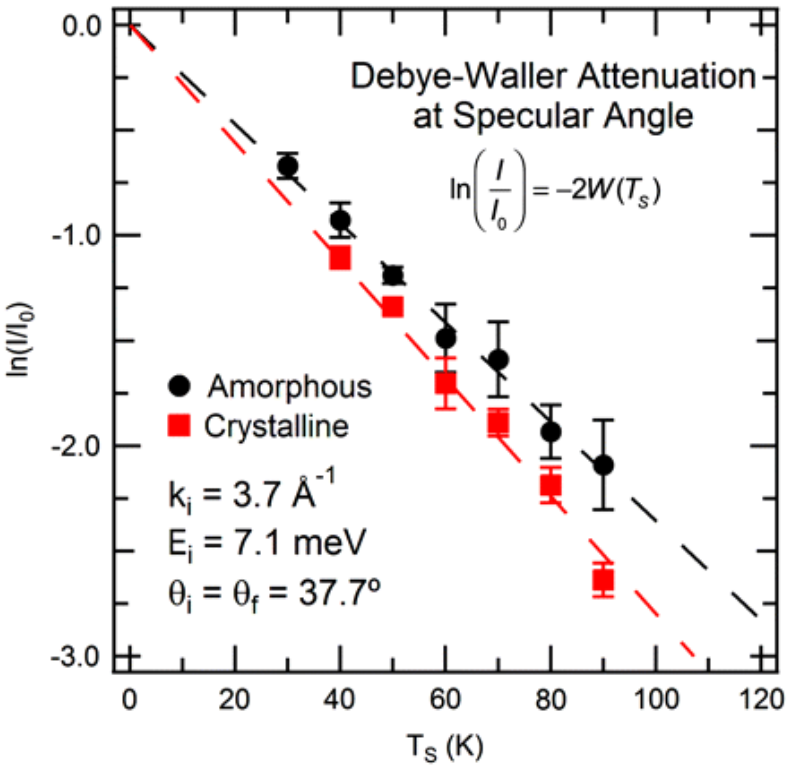
Example, scanned energy transfer, giving phonon dispersion curves.



Note we saw similar selection rules for photons;

- However Raman generally measures phonons at Γ.
- Resonant inelastic x-ray (RIXS) recently developed, capabilities somewhat similar to neutrons.

Bragg scatter intensity: Debye-Waller factor



Displaced atom $H \propto \hat{u} \quad (or\ q)$

Contribution of phonons:

Intensity = square amplitude: $I \propto \langle u^2 \rangle$

So, $\langle u^2 \rangle \propto \left|\langle \psi' | a | \psi \rangle\right|^2 etc.$

$\propto sum\ of\ n(T)$

Elastic scattering decrease vs. *T*

– appendix N.

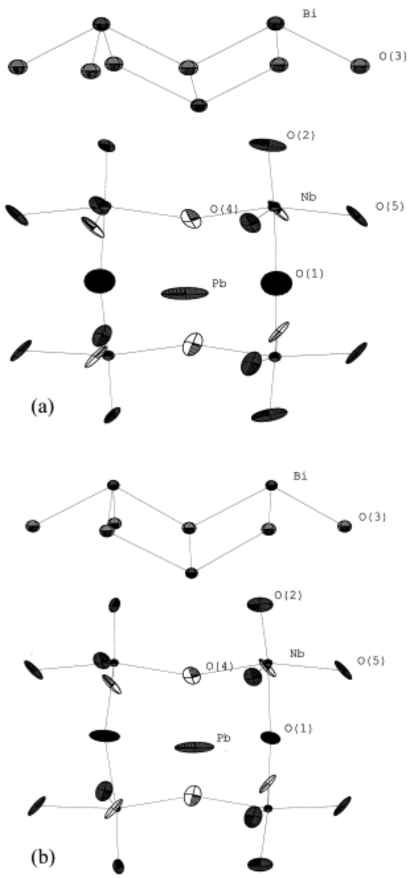
$$n = \frac{1}{e^{\hbar\omega/kT} - 1} \propto T, high\ T$$

<u>Debye-Waller Factor</u>: phonon scattering increases linear in *T*, high *T*; elastic peaks <u>decrease</u> initially linear in *T* (full solution is exponential drop).

(Appendix N of A&M)

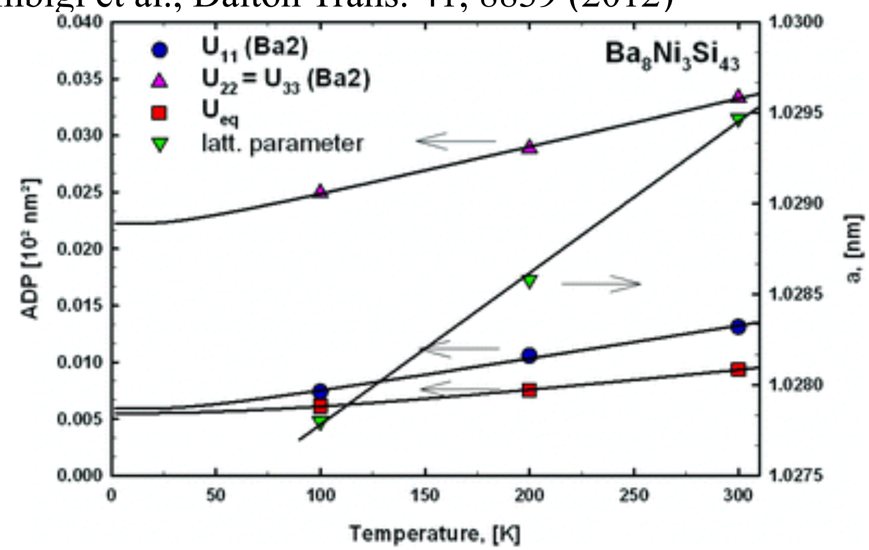
Xray analysis & displacement ellipsoids for $PbBi_2Nb_2O_9$ ferroelectric;
Ismunandar et al. Solid State Ionics 112, 281 (1998)

Generally static + dynamic disorder both reduce x-ray peaks. Often plotted as thermal displacement parameters.

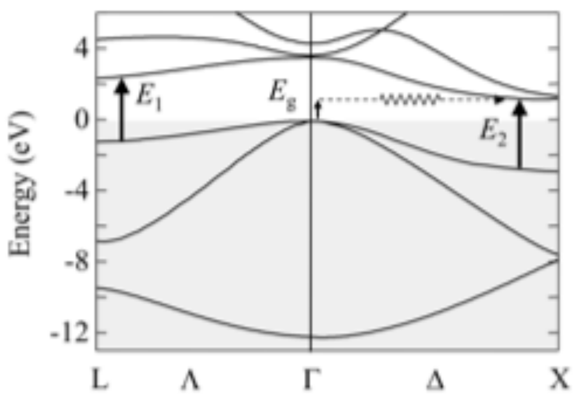


displacement parameter T dependence
Allows to resolve dynamic vs. random static (here $T \to 0$ disorder)
Falmbigl et al., Dalton Trans. 41, 8839 (2012)

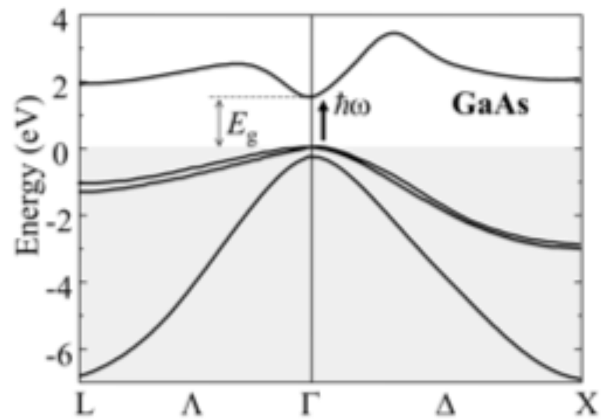
$\langle u^2 \rangle$



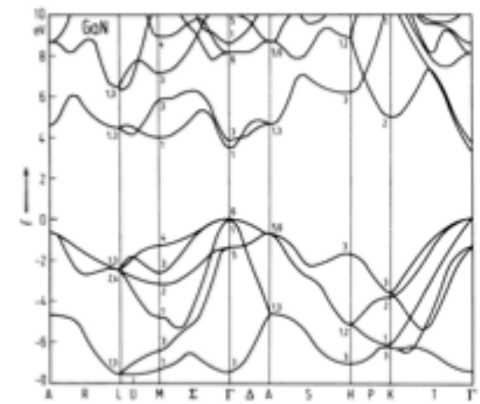
Semiconductors:



Silicon band structure

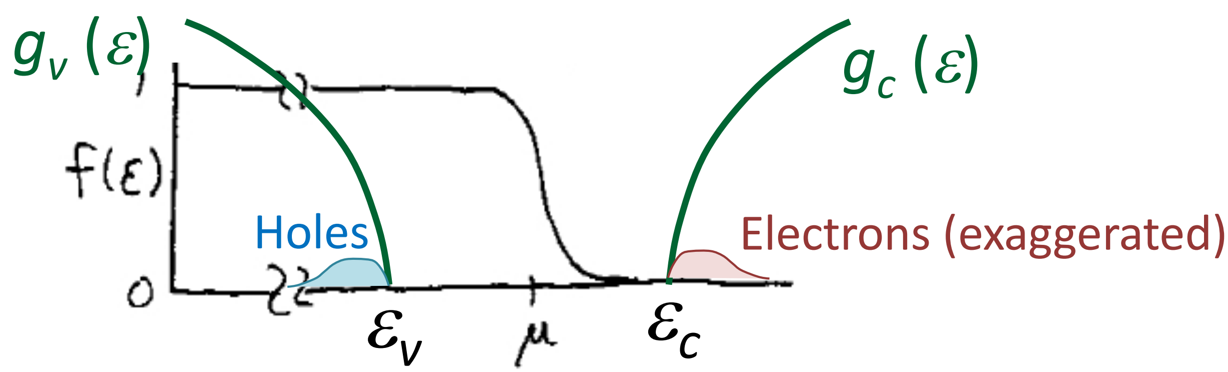


GaAs: zincblende (ZnS)



GaN: wurtzite

Material	Group IV			III-V							II-VI	
	Si	Ge	C	AlAs	GaAs	InAs	InP	GaSb	InSb	GaN	HgCdTe	ZnO
Bandgap (eV)	1.11	0.67	5.5	2.16	1.43	0.354	1.34	.726	0.17	3.4	0 – 1.47	3.4
Electron mass (or m_l)	0.98	1.64	1.1	0.1	0.063	0.027	0.073	0.042	0.014	0.19	~0	0.27
Electron mass (transverse)	0.19	0.082	0.22	-	-	-	-	-	-	-	-	-
light hole mass	0.16	0.044			0.082	0.026	0.089	0.05	0.015			
heavy hole mass	0.49	0.28	0.25		0.51	0.41	0.6	0.4	0.43	0.8		
Electron Mobility (cm^2/V.s)	1350	3900	2800	180	8500	40000	5400	3000	77000	500		
structure	diam	diam	diam	ZnS	ZnS	ZnS	ZnS	ZnS	ZnS	wurtzite	ZnS	wurtzite
Lattice Constant (Å)	5.43	5.66	3.57	5.66	5.65	6.06	5.87	6.09	6.48			



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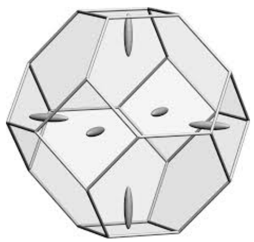
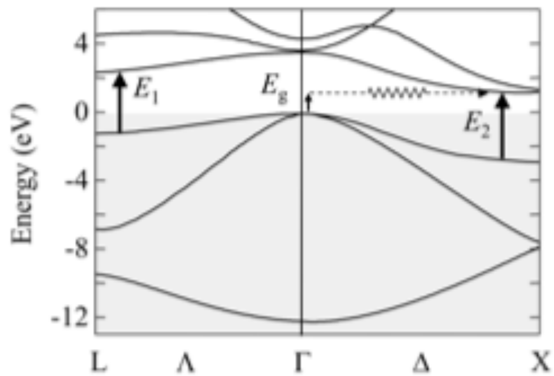
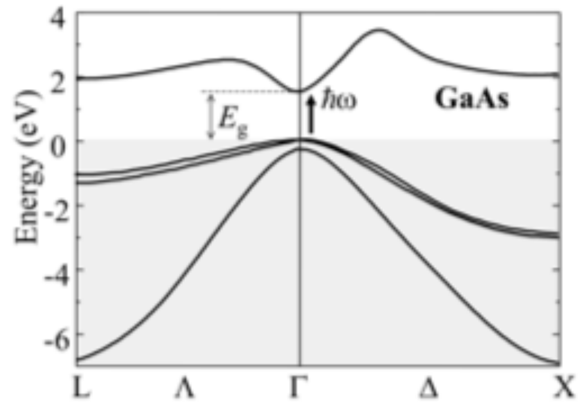


Silicon conduction-band pockets (M. Marder)



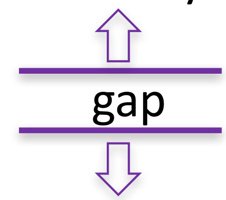
Silicon band structure



GaAs: zincblende (ZnS)

conduction bands

(nominally empty)



valence bands

(filled)

	Group IV			III-V							II-VI	
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Lattice Constant (Å)	5.43	5.66	3.57	5.66	5.65	6.06	5.87	6.09	6.48			

Si & Ge indirect gap
(poor optical behavior)

- AlAs, GaAs: matching lattice constants; red LED's, fast electronics (high mobility)
- n-InSb extremely high mobility / small mass
- $(In_{1-x}Ga_x)(As_{1-y}P_y)$: IR telecommunication lasers
- GaN blue/white LED's; $In_xGa_{1-x}N$ Blu-ray players

$Hg_{1-x}Cd_xTe$, Very long-wavelength IR detectors.
Original topological insulator.