PHY 745 Group Theory
11-11:50 AM MWF Olin 102

Plan for Lecture 22:

Symmetry of lattice vibrations

Chapter 11 in DDJ

1. **Lattice vibrations of LiF & elephants**
2. **Lattice vibrations of diamond structured materials**

Some materials for this lecture were taken from an electronic version of DDJ.

13	Fri: 02/10/2017	Chap. 5	Atomic orbitals	#11	02/13/2017
14	Mon: 02/13/2017	Chap. 6	Direct product groups	#12	02/15/2017
15	Wed: 02/15/2017	Chap. 7	Molecular orbital	#13	02/17/2017
16	Fri: 02/17/2017	Chap. 9	Introduction to Space Groups	#14	02/20/2017
17	Mon: 02/20/2017	Chap. 10	Group theory for the periodic lattice		
18	Wed: 02/22/2017	Chap. 10	Group theory for the periodic lattice		
19	Fri: 02/24/2017	Chap. 1-10	Review -- Distribute take-home exam		
20	Mon: 02/27/2017	Chap. 10	Space group representations		Exam
21	Wed: 03/01/2017	Chap. 11	Symmetry of vibrations		Exam
22	Fri: 03/03/2017	Chap. 11	Symmetry of vibrations		Exam Due
	Mon: 03/06/2017		*Spring break - no class*		
	Wed: 03/08/2017		*Spring break - no class*		
	Fri: 03/10/2017		*Spring break - no class*		
	Mon: 03/13/2017		*APS Meeting - no class*		
	Wed: 03/15/2017		*APS Meeting - no class*		
	Fri: 03/17/2017		*APS Meeting - no class*		
23	Mon: 03/20/2017				
24	Wed: 03/22/2017				

Comments:
- Enjoy your spring break
- Please use part of the week of March 13 to prepare your presentations for the end of April.

	Fri: 03/17/2017		*APS Meeting - no class*		
23	Mon: 03/20/2017				
24	Wed: 03/22/2017				
25	Fri: 03/24/2017				
26	Mon: 03/27/2017				
27	Wed: 03/29/2017				
28	Fri: 03/30/2017				
29	Mon: 04/03/2017				
30	Wed: 04/05/2017				
31	Fri: 04/07/2017				
32	Mon: 04/10/2017				
33	Wed: 04/12/2017				
	Fri: 04/14/2017		*Good Friday Holiday -- no class*		
34	Mon: 04/17/2017				
35	Wed: 04/19/2017				
36	Fri: 04/21/2017				
	Mon: 04/24/2017		Presentations I		
	Wed: 04/26/2017		Presentations II		

Example for LiF

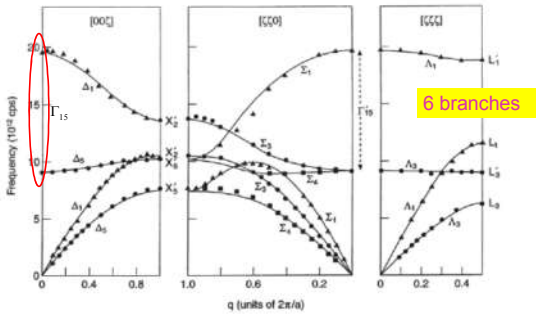

Figure 9.8 Measured phonon dispersion curves along three directions of high symmetry in LiF; the solid curves are a best least-squares fit of a parameter model [With permission from Fig. 4, Phys. Rev. *168*, 970 (1968)]. Notice that 10^{12} Hz = 4.137 meV.

Note that the splitting of the TO and LO vibrations for LiF is beyond the group theory analysis which predicts a single triply degenerate mode of symmetry Γ_{15}.

PHYSICAL REVIEW B VOLUME 43, NUMBER 9 15 MARCH 1991-II

***Ab initio* calculation of phonon dispersions in semiconductors**

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(Received 7 August 1990)

Lattice vibrations in polar crystals couple to electromagnetic fields, adding "non analytic" term to the dynamical matrix:

$$\tilde{C}^{\,\mathrm{na}}_{\alpha i,\beta j} = \frac{4\pi e^2}{\Omega} \frac{\sum_{\gamma} Z^*_{i,\gamma\alpha} q_\gamma \sum_{\nu} Z^*_{j,\nu\beta} q_\nu}{\sum_{\gamma,\nu} q_\gamma \epsilon^{\infty}_{\gamma\nu} q_\nu}$$

$$= \frac{4\pi e^2}{\Omega} \frac{(\mathbf{q}\cdot\mathbf{Z}^*_i)_\alpha (\mathbf{q}\cdot\mathbf{Z}^*_j)_\beta}{\mathbf{q}\cdot\vec{\epsilon}^{\,\infty}\cdot\mathbf{q}} ,$$

Brief digression concerning LO-TO phonon modes based on Grosso and Parravicini text

$$\ddot{\mathbf{d}}_n = -\omega_0^2\,\mathbf{d}_n + \frac{e^{*2}}{M^*}\mathbf{E}\,;$$

Resulting polarization density

$$\mathbf{P}_{\rm ion}(\mathbf{r},t) = \frac{N}{V}\,\mathbf{d}(\mathbf{r},t).$$

Coupling to an electric field

$$\ddot{\mathbf{P}}_{\rm ion} = -\omega_0^2\,\mathbf{P}_{\rm ion} + \frac{N}{V}\frac{e^{*2}}{M^*}\,\mathbf{E}\,.$$

$$= -\omega_0^2\,\mathbf{P}_{\rm ion} + \omega_0^2\,\frac{\varepsilon_s - \varepsilon_\infty}{4\pi}\,\mathbf{E}$$

Maxwell's equations

$$\begin{aligned} &\operatorname{div}\mathbf{D} = 0 \qquad &&\operatorname{div}\mathbf{B} = 0,\\ &\operatorname{curl}\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t} \qquad &&\operatorname{curl}\mathbf{H} = \frac{1}{c}\frac{\partial\mathbf{D}}{\partial t}. \end{aligned}$$

Longitudinal mode $\mathbf{P}_{\rm ion}(\mathbf{r},t) = \mathbf{P}_0\,e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}$ with $\mathbf{P}_0 \parallel \mathbf{q}$.

$\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0\,e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}$ with $\mathbf{E}_0 \parallel \mathbf{q}$.

Longitudinal case continued

The electric induction vector is defined as

$$\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}_{\rm el} + 4\pi\mathbf{P}_{\rm ion} = \varepsilon_\infty\mathbf{E} + 4\pi\mathbf{P}_{\rm ion}.$$

For longitudinal modes we have thus the following equations:

$$\begin{cases} \ddot{\mathbf{P}}_{\rm ion} = -\omega_0^2\,\mathbf{P}_{\rm ion} + \omega_0^2\dfrac{\varepsilon_s - \varepsilon_\infty}{4\pi}\mathbf{E}, \\ \operatorname{div}[\varepsilon_\infty\mathbf{E} + 4\pi\mathbf{P}_{\rm ion}] = 0. \end{cases}$$

Assuming $\mathrm{P}_{ion} = P_0 e^{-i\omega t}$

$$\begin{cases} -\omega^2 P_0 = -\omega_0^2 P_0 + \omega_0^2\dfrac{\varepsilon_s - \varepsilon_\infty}{4\pi}E_0\,, \\ \varepsilon_\infty E_0 + 4\pi P_0 = 0\,. \end{cases}$$

$$\textit{longitudinal modes}: \quad \omega^2 = \omega_0^2\frac{\varepsilon_s}{\varepsilon_\infty} \equiv \omega_{LO}^2 \quad \text{with} \quad E_0 = -\frac{4\pi}{\varepsilon_\infty}P_0\,.$$

Transverse modes

$$\mathbf{P}_{\text{ion}}(\mathbf{r},t) = \mathbf{P}_0 e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)} \quad \text{with} \quad \mathbf{P}_0 \perp \mathbf{q},$$

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0 e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)} \quad \text{with} \quad \mathbf{E}_0 \perp \mathbf{q}.$$

$$\text{curl}\,\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t},$$

$$\text{curl}\,\mathbf{H} = \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} = \frac{\varepsilon_\infty}{c}\frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c}\frac{\partial \mathbf{P}_{\text{ion}}}{\partial t},$$

$$\ddot{\mathbf{P}}_{\text{ion}} = -\omega_0^2 \mathbf{P}_{\text{ion}} + \omega_0^2 \frac{\varepsilon_s - \varepsilon_\infty}{4\pi}\mathbf{E},$$

$$-\nabla^2 \mathbf{E} = -\frac{\varepsilon_\infty}{c^2}\ddot{\mathbf{E}} - \frac{4\pi}{c^2}\ddot{\mathbf{P}}_{\text{ion}}.$$

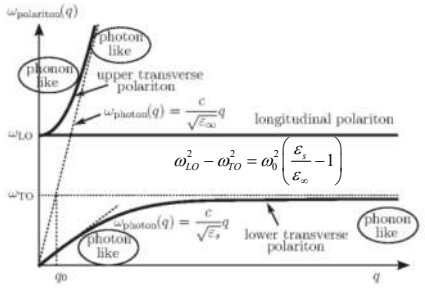
$$-\omega^2 P_0 = -\omega_0^2 P_0 + \omega_0^2 \frac{\varepsilon_s - \varepsilon_\infty}{4\pi} E_0$$

$$q^2 E_0 = \frac{\varepsilon_\infty}{c^2}\omega^2 E_0 + \frac{4\pi}{c^2}\omega^2 P_0$$

Transverse modes

After several steps we get two modes

$$\varepsilon_\infty \omega^4 - \left(\omega_0^2 \varepsilon_s + c^2 q^2\right)\omega^2 + \omega_0^2 c^2 q^2 = 0.$$



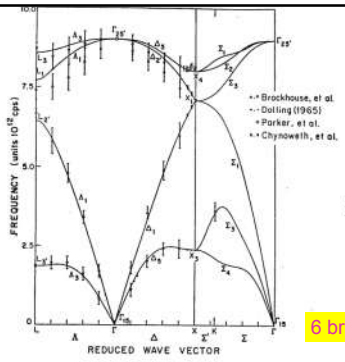
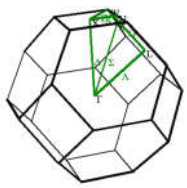


Figure 14.2: Phonon dispersion curves for Ge along certain high symmetry axes in the Brillouin zone. The data at the Γ point are from Raman scattering measurements and the data elsewhere in the zone are from neutron scattering experiments.

Ge (diamond structure)



6 branches

Notation for O_h symmetry

BSW	Molecular
Γ_1	A_{1g}
Γ_2	A_{2g}
Γ_{12}	E_g
Γ_{15}'	T_{1g}
Γ_{25}'	T_{2g}
Γ_1'	A_{1u}
Γ_2'	A_{2u}
Γ_{12}'	E_u
Γ_{15}	T_{1u}
Γ_{25}	T_{2u}

Symmetry of k=0 phonons in diamond structure

	$\{E\|0\}$	$\{8C_3\|0\}$	$\{3C_2\|0\}$	$\{6C_4^1\|\tau\}$	$\{6C_4\|\tau\}$	$\{i\|\tau\}$	$\{8iC_3\|\tau\}$	$\{3iC_2\|\tau\}$	$\{6iC_4^3\|0\}$	$\{6iC_4\|0\}$
$\chi_{\text{a.s.}}$	2	2	2	0	0	0	0	0	2	2

Decomposition of $\chi_{\text{atom sites}}$ into irreducible representations of O_h leads

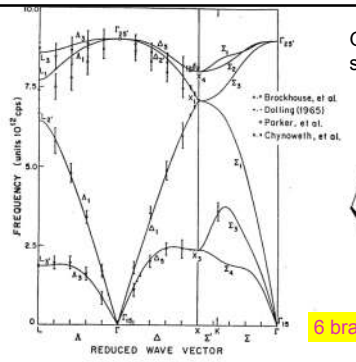
$$\chi_{\text{a.s.}} = A_{1g} + A_{2u} \text{ or } \Gamma_1^+ + \Gamma_2^-.$$

$$\chi_{\text{lattice modes}} = \chi_{\text{a.s.}} \otimes \chi_{\text{vector}} = (A_{1g} + A_{2u}) \otimes T_{1u} = T_{1u} + T_{2g} = \Gamma_{15}^- + \Gamma_{25}^+$$

Analysis of phonons for k>0 in diamond structure from Bouckaert, Smoluchowski, and WIgner:

TABLE VII. *Compatibility relations between* Γ *and* Δ, Λ, Σ.

Γ_1	Γ_2	Γ_{12}	Γ_{15}'	Γ_{25}'
Δ_1	Δ_2	$\Delta_1\Delta_2$	$\Delta_1'\Delta_3$	$\Delta_2'\Delta_3$
Λ_1	Λ_2	Λ_3	$\Lambda_2\Lambda_3$	$\Lambda_1\Lambda_3$
Σ_1	Σ_4	$\Sigma_1\Sigma_4$	$\Sigma_2\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_3$
Γ_1'	Γ_2'	Γ_{12}'	Γ_{15}	Γ_{25}
Δ_1'	Δ_2'	$\Delta_1'\Delta_2'$	$\Delta_1\Delta_3$	$\Delta_2\Delta_3$
Λ_2	Λ_1	Λ_3	$\Lambda_1\Lambda_3$	$\Lambda_2\Lambda_3$
Σ_2	Σ_3	$\Sigma_3\Sigma_3$	$\Sigma_1\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_4$



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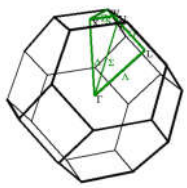
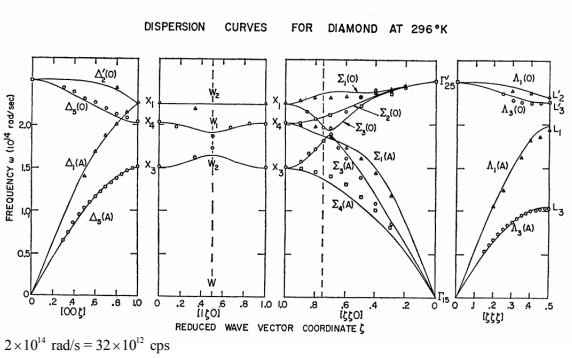
Ge (diamond structure)



6 branches

Phys. Rev. 158, 805-808 (1967)



2×10^{14} rad/s = 32×10^{12} cps

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Lattice Dynamics of Diamond*

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and
G. Dolling and R. A. Cowley
Chalk River Nuclear Laboratories, Chalk River, Ontario, Canada
(Received 9 December 1966)

The first two authors have measured the dispersion curves for phonons whose wave vector lies along the symmetry lines Σ and Z in the Brillouin zone. The measurements were made by the method of inelastic neutron scattering. With the aid of these new results the latter two authors have determined the shell-model parameter δ which could not be determined from the previously measured dispersion curves along the lines Δ and Λ. A figure is given which summarizes all the measured dispersion curves of diamond and gives the most recently calculated shell-model fit to the data. Because of the large size of this parameter δ, it was necessary to recompute some of the thermodynamic and optical properties of diamond previously reported by the last two authors elsewhere. Thermodynamic quantities such as the Debye temperature were very little affected, but some of the critical-point frequencies used in the analysis of the two-phonon infrared absorption spectrum had to be altered. A corrected table of critical points is given.