

Structure and Dynamics

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Syllabus

1. The 32 point groups

- Symmetry operators and elements
- Point groups, notation, and stereographic projections
- Point groups of simple molecules

2. Molecular vibrations

- Vibrational modes
- Infra-red spectroscopy
- Raman spectroscopy

3. The 230 space groups

- The crystal lattice, basis, and fractional coordinates
- Symmetry operators of a 3D crystal
- Screw axes and glide planes
- The 230 space groups and their Wyckoff positions

4. Reciprocal space

- The reciprocal lattice
- The structure factor
- The Laue Class and Friedel's Law
- Measuring distances and angles in non-orthonormal spaces

5. Phonons and electrons

- Vibrations of a 1D chain
- Vibrations of a 3D crystal
- Thermal expansion
- The symmetry of electron bands

6. X-ray diffraction

- X-ray scattering from an electron, atom, and a perfect crystal
- Determining the lattice parameters
- Determining the space group
- Determining the atomic fractional coordinates

7. X-ray diffraction: Experiments

- The Ewald sphere
- Single crystal diffraction in reflection
- Single crystal diffraction in transmission
- Powder diffraction
- Anomalous x-ray diffraction

8. Measuring phonons

- Inelastic neutron scattering
- Triple axis spectroscopy
- Time-of-flight spectroscopy

9. Displacive phase transitions

- Ferroelectric phase transitions
- Neumann's principle and domains
- Ferroelastic phase transitions
- Antiferroic phase transitions
- The order parameter and soft phonon modes

10. Landau theory

- The Landau free energy and symmetry invariants
- Second order phase transitions
- Susceptibility and the specific heat
- First order phase transitions
- Secondary order parameters

Bibliography

Core text:

Structure and Dynamics by Martin Dove, Oxford University Press.

For further details on x-ray diffraction:

Elements of Modern X-ray Physics by Jens Als-Nielsen and Des McMorrow, Wiley.

For further details on the application of group theory in physics (advanced - graduate level):

Group Theory in Quantum Mechanics by Volker Heine, Dover.