



INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION



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SPRING COLLEGE ON AMORPHOUS SOLIDS
AND THE LIQUID STATE
14 April - 18 June 1982

VIBRATIONAL STATES IN AMORPHOUS MATERIALS

Outline of lectures

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These are preliminary lecture notes, intended only for distribution to participants.
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SPRING COLLEGE ON AMORPHOUS SOLIDS AND THE LIQUID STATE.

VIBRATIONAL STATES IN AMORPHOUS MATERIALS.

6 lectures by Giuseppe Zerbi
Polytechnic of Milano.

Outline

- 1) Local and overall structures of aggregates of atoms or molecules.
Short and long range order in amorphous or partially amorphous materials. Predictions of structures based on atom-atom potentials. Limitations of such methods. When is a material amorphous? Experimental problems for structure determinations.
- 2) Examples of various kinds of amorphous materials, with the emphasis on organic materials. From molecules to one-dimensional crystals (polymers) and to tridimensional crystals. Examples from small molecules to biological systems. Structural evolution of structures with time. From resonance normal modes to relaxation phenomena. Time scales of mobilities in solid materials.
- 3) Group theory in molecules and solids. Local and overall mechanical and electrical symmetry in organic systems. Basic concepts.
- 4) The vibrational levels of coupled harmonic oscillators. The double harmonic approximation and resonance normal modes. What do we know on interatomic potentials in covalent systems? Theory and experimental determination of potentials.

Lattice dynamics of perfect crystals. Selection rules for optical spectra of molecules and crystals.

- 5) Lattice dynamics of partially disordered or fully amorphous materials. Density of vibrational states. Numerical methods for the calculations of $g(\omega)$. Localized and collective vibrational states. Optical and neutron spectra. Electrical and mechanical localization.
- 6) A guided tour. A few examples of recent works on lattice dynamics of amorphous materials and their relevance in various fields of physics and material science.

References.

A collection of references on the various problems and examples discussed during the lectures can be found in:

G.Zerbi "Molecular Vibrations of High Polymers", Applied Spectroscopy Reviews 2, 193 (1969).

G.Zerbi "Defects in Organic Crystals-Numerical Methods" in "Lattice Dynamics and Intermolecular Forces". Academic Press. (1975).

G.Zerbi "Advances in Chemistry Series; American Chemical Society, (1982) in press.

G.Zerbi "Vibrations of Very large Molecules" in "Advances in Infrared and Raman Spectroscopy" (Clark and Hester Eds) Heyden, (1982) in press.

G.Zerbi "Limitations of Force Constant Calculations in Large Molecules" in "Modern Methods in Vibrational Spectroscopy" (Orville Thomas, Barnes Eds) Elsevier (1977).

P.C. Painter, M.M.Coleman and J.L. Koenig, The theory of Vibrational Spectroscopy and its applications to Polymeric Materials, Wiley (New York) (1982)