Paper-15C

Condensed Matter Physics Lab and Computational Condensed Matter Physics

Group A: Condensed Matter Physics Lab

List of Experiments:

1. Determination of band gap of a semiconductor sample using UV-VIS spectroscopy.
2. Determination of magnetoresistance of a given semiconductor for different magnetic fields.
3. Determination of precise lattice parameter and grain size of crystalline materials by X-Ray powder diffractometer.
4. To study the temperature dependence of the Hall coefficient for metal/semiconductor.
5. Preparation of nanocrystalline powder specimen by chemical route & its size analysis.
6. Determination of Band gap of a given semiconductor material by four probe technique.
7. Measurement of variation of microhardness of selected specimens.
8. Study of colour centers and thermoluminiscence of alkali halides.
9. Variation of grain size and porosity of sintered/thin film specimens sintered at different temperatures by optical microscope.
10. Dispersion relation in a periodic electrical circuit: an analog of monatomic and diatomic lattice vibration.

- Hands on experience: Visit to facilities in and around Kolkata and outside Kolkata (subject to availability of accommodation).

Group B: Computational Condensed Matter Physics

Quantum mechanical modeling of materials: Hartree-Fock and Density Functional Theory. Kohn-Sham equation, Exchange-Correlation energy functionals. Hellmann-Feynman theorem. Atomic Pseudopotentials, Basis Sets: Plane Waves and Augmented Basis sets. Plane Wave based DFT calculations. Simplified Approaches to the electronic problem: Tight binding Methods; Slater-Koster approach. Atomistic modeling of materials: Interatomic Potential semi-empirical to many-body system, Classical force fields. Monte Carlo and Molecular dynamics simulations; Hybrid Quantum Mechanics - Molecular Mechanics (QM-MM) method. Ehrenfest, Born-Oppenheimer & Car-Parrinello molecular dynamics.

Reference Books:

1. Quantum Theory of Molecules and Solids, J.C. Slater, Vol IV

(McGrawHill, New York, 1974).

2. Electronic structure and properties of solids, W.A. Harrison (Freeman, 1980).

3. "Theory of inhomogeneous electron gas", S Lundqvist and N.H. March, (Plenum, New York, 1983)

4. "Electronic Structure: Basic Theory and Practical Methods", Richard M. Martin (Cambridge University Press, 2004)