Annexure 14.3

Avinashilingam Institute for Home Science and Higher Education for Women
Coimbatore
Department of Physics
Ph. D. Physics
21PHPH03D Crystal Growth and X-ray Crystallography
(Applicable for Ph.D. Part time scholar admitted in August 2021)

Name of the Scholar : **Ms. V. Bhuvaneswari (21PHPHP001)**
Name of the Supervisor : **Dr. N. S. Rajeswari** **No. of Credits: 5**

Course Objectives:

1. To understand the fundamentals and theories of crystal growth.
2. To learn experimental methods of crystal growth
3. To understand x-ray crystallography and other characterizations.

Unit 1: ***Fundamentals of Crystal Growth*** **21 Hrs**

Classification of crystal growth methods – Basic steps: Generation, transport and adsorption of growth reactants – Nucleation: Kinds of nucleation –Classical theory of nucleation: Gibbs Thomson equations for vapour and solution – Kinetic theory of nucleation – Becker and Doring concept on nucleation rate – Energy of formation of aspherical nucleus – Statistical theory on nucleation: Equilibrium concentration of critical nuclei,Free energy of formation

Unit 2*: Theories of Crystal Growth* **21 Hrs**

An introductory note to Surface energy theory, Diffusion theory and Adsorption layer theory –Concepts of Volmer theory, Bravais theory, Kossel theory and Stranski"s treatment – Two-dimensional nucleation theory: Free energy of formation, Possible shapes and Rate of nucleation – Mononuclear, Polynuclear and Birth and Spread models – Modified Birth and Spread model –Crystal growth by mass transfer processes: Burton, Cabrera and Frank (BCF) bulk diffusionmodel, Surface diffusion growth theory - Formation and thermodynamics of cocrystals.

Unit 3: ***Experimental Crystal Growth-Part-I:*** **21 Hrs**

Melt Growth Techniques:

Basics of melt growth – Heat and mass transfer – Conservative growth processes: Bridgman-Stockbarger method – Czochralski pulling method – Kyropolous method – Non-conservative processes: Zone-refining – Vertical and horizontal float zone methods – Skull melting method –Vernueil flame fusion method.

Unit 4:*Experimental Crystal Growth-Part-II:* **21 Hrs**

Solution Growth Techniques.Growth from low temperature solutions: Selection of solvents and solubility – Meir"s solubility diagram – Saturation and supersaturation – Metastable zone width – Grọwth by controlled evaporation of solvent, slow cooling of solution and temperature gradient methods– Crystal growth in Gel media: Chemical reaction and solubility reduction methods – Growth from hightemperature solutions: Flux growth Principles of flux method – Choice of flux – Growth by slowevaporation and slow cooling methods – Hydrothermal growth method. Solid growth: mechano-chemical method of crystallization.

Unit 5:*X –Ray Crystallography and other characterizations* **21 Hrs**

Concept of reciprocal lattice, construction of the diffracted wave vectors in the reciprocal lattice, Theory of X –ray Diffraction by crystals, powder Diffractometer, Recording and interpretation of powder patterns, single crystal techniques. Intensities of Diffracted X-rays and structural analysis, elementary theory of X-ray scattering by a single electron and by a single atom, atomic scattering factor. FTIR, UV-vis spectrometry, NLO studies, Polarization measurements, refractive index and etching studies - Kinetics and thermodynamics of co-crystallization with aromatic acids.

References: Total **105Hrs**

1. ***Michael M.Woolfson, An introduction to X-ray crystallography, Cambridge University press (1970).***
2. ***Brice, J.C., Crystal growth processes, Halstesd press, John Wiley &Sons, New York (1986). William H.Zacharisan, Theory of X-ray diffraction in crystals, John Wiley &Sons, New York (2004).***
3. ***P. Ramaswamy& P. ChandanaRghavan, Crystal growth Technique. KRU Publications, (2001).***
4. ***J.W. Mullin, Crystallization*, Elsevier Butterworth-Heinemann, London , (2004).**
5. ***AB.R. Pamplin, Crystal Growth* ,Pergamon Press, Oxford (1975).**

Course Outcomes:

1. Learn the fundamentals of crystal growth and apply the same in crystal growth
2. Acquire the knowledge of theories of crystal growth
3. Acquire the knowledge of melt growth techniques
4. Acquire the knowledge of solution growth techniques and apply the same to synthesis crystal
5. Acquire and apply the knowledge of x-ray crystallography and other required characterization techniques to identify the applications of crystals.