

Preface

Editorial on the Special issue on “Synthesis, Characterization and Properties of Nanostructures: Computational and Experimental Approach”

Reducing the dimension of matter domains down to the nanometer scale, confines the electronic and vibrational wavefunctions resulting in unique properties and opens a wide range of potential applications in domain as optics, mechanics, electrical, magnetic devices, reactivity and biomedicine. Nanostructures, characterized by at least one dimension in the nanometer range are considered to constitute a bridge between single molecule and bulk counterpart. The challenges for the so called nanotechnologies are to achieve perfect control of nanoscale-related properties, which obviously requires correlating the parameters of the synthesis process with the resulting nanostructures. Nanostructures are also ideal for computer simulation and modeling. In computations related to nanomaterials one deals with a spatial scaling from few nanometer to few micrometer and a time scaling from few femto-second (fs) to 1 second with the limit of accuracy going beyond 1 kcal mol^{-1} .

This special issue of solid state phenomena documents novel computational and experimental approaches summoned to resolve questions on growth of nanostructures, its characterization and modeling. Motivated by the increasing need to synthesize and understand the properties of materials at nanoscale this special issue is timely and a step toward improving our knowledge of how nanomaterials are useful for modern technologies.

The special issue contains a collection of ten original review/papers including the reviews concerned with experimental approaches, theoretical analysis and numerical models. Seven papers are related to growth and characterization of nanomaterials while three papers deal theoretical approaches for understanding their properties. Another positive point of this special issue is the one common aim of several of these papers to achieve a deeper understanding of the underlying functionality of the properties of nanomaterials. The special issue has been divided in two sections namely the *Computational Nanomaterials* and *Experimental Nanomaterials*. The special issue contains three extensive topical review articles. Contributions appear in alphabetical order of their first authors in each section.

The paper by Lu *et al* aims to develop better understanding of the size dependent interface energy of nanomaterials. The classic thermodynamics as a powerful theoretical tool is used to model different bulk interface energies in the computations of the size dependence of coherent energy of atoms within nanocrystals. This exhaustive review may lead to improve insight into the understanding of surface and interface energy of nanomaterials of low dimensional materials in different shapes with different chemical bond natures.

Maiti examines the electron transport properties of some molecular wires and an unconventional disordered thin film and persistent current in metallic Rings and Cylinders under the frame work of tight-binding approach in his two of his articles. The model calculations provide a physical insight into the behavior of electron conduction across a bridge system. The characteristic properties of persistent current strongly depend on total number of electrons, chemical potential, randomness and total number of channels.

The paper by Acharya reports the microscopic analysis of track etched polymeric membranes produced by bombardment of energetic ions on polymer membranes. The track results due to the energy loss during the formation of loosely bound passage in membrane. The Atomic Force Microscopy (AFM) used for the characterization gives the size and distribution of

the pores. The pore size is observed in nano regime and the pore density was found to depend on the irradiation dose.

The ultimate objective of the paper by Ding *et al* is to prepare a ZnO thin film for the high optical transmittance in the visible region and strong absorption in ultraviolet region. The ZnO film is prepared from sol-gel precursors using electrospray method. The surface images obtained from AFM showed the compact ZnO films composed of wurtzite ZnO nanoparticles.

The review article by Dutta and Tyagi aims to better understand the inorganic phosphor materials for solid state white light generation. Various examples are discussed based on oxide, fluoride, nitride, sulfide and phosphate based host lattices. The important concepts like CIE coordinates and color correlated temperature (CCT) are also discussed. Eu^{3+} -doped NaYF_4 and YOF nanocrystallites were seen to be good red emitters.

The paper by Mehta *et al* discusses the study of the dielectric properties of thin films of multiferroic compound $\text{Sr}[(\text{Mg}_{0.32}\text{Co}_{0.02})\text{Nb}_{0.66}]\text{O}_3$ (SMCN) prepared by Pulsed Laser Deposition Technique (PLD). The dielectric properties show enhanced ϵ' values compared to bulk and decrease in ac susceptibility with temperature suggesting promising applications in alternative technologies for the switching devices. Technologically important two step activation energy is also observed in the film of SMCN.

The aim of Parekh *et al* is to synthesize the monodispersed magnetite and cobalt ferrite nanoparticles via non-aqueous route. The characterization techniques used reveals the size distribution less than 5 % and particles of spherical shape. The magnetic moment obtained at room temperature is higher than that obtained earlier using other techniques.

The work of Singhal *et al* reports the electronic structure study of Mn doped ZnO diluted magnetic semiconductor by using x-ray absorption spectroscopy for its possible use for future spin-electronic applications. The changes in the electronic structure are correlated with the observed magnetic properties. They observed that the most of the Mn ions of the ferromagnetic samples are in divalent state.

Yadav proposes a simple citrate gel process to prepare magnetoelectric nanocomposite. TEM observation showed that the average particles size is around 40 nm. The variation of the dielectric constant and the dielectric loss with frequency showed dispersion in the low frequency range. The large values of M_E coefficients are attributed to low coercivity, large magnetization and small crystallite size of constituent phases.

It is hoped that the present selection of contributions is of interest to the scientists working in the area of nanoscience and that it will contribute to the dynamic and rapidly expanding field of nanoscience and nanotechnology particularly with regards to growth, characterization and modeling.

Our heartfelt thanks are due to all the contributors for the submission of their valuable work and the referees of the papers for sparing their valuable time. We especially thank the Editorial Board of Solid State Phenomena for their support in bringing out this special topical volume and all the members of the TRANS TECH PUBLICATIONS LTD office for their efforts throughout the publication process.

Prafulla K. Jha and Arun Pratap (Guest Editors)