

ΤΜΗΜΑ ΦΥΣΙΚΗΣ

Γενικό Σεμιναρίο Τμηματός Φυσικής

PHYSICS COLLOQUIUM

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3rd Floor Seminar Room

"An integrated method for nanoscale analysis of solid matter based on transmission electron microscopy techniques"

Thomas Kehagias

Aristotle University of Thessaloniki, Department of Physics

<u>Abstract</u>

Interfacial engineering, implicit defect analysis and deep apprehension and control of the related structural mechanisms in the atomic scale are prerequisites for the construction of innovative nanostructured materials. Transmission electron microscopy (TEM) methods provide a steady, time-tested basis for the systematic experimental analysis of nanostructural features of advanced materials. However, in modern understanding of a thorough structural analysis, experimental information has to be mutually combined with complex simulation and computational techniques in an integrated manner.

Well-known TEM-based techniques and theoretic calculations have been complemented and brought together to constitute an integrated framework of interfacial and defect analysis in thin film materials systems. These comprise: a) Conventional TEM, electron diffraction and high-resolution TEM (HRTEM) for the experimental analysis of linear and extended defects, such as misfit, threading and partial dislocations, stacking faults and inversion domains. b) Quantitative HRTEM (qHRTEM) including the geometric phase analysis (GPA), the peak finding (PF) and the projection methods, image filtering and fast Fourier transform (FFT) analysis, in order to quantify strain and deformation fields around defected structures. c) Elasticity and topological theory for the identification of admissible defect/interface atomic configurations. d) Empirical interatomic potential calculations and density functional theory (DFT) based ab initio calculations for modeling of the energetically favorable defect/interface structures. The resultant models are implemented in simulations of the experimental HRTEM images. Simulated images are then compared with the corresponding experimental ones by the use of PF and pattern registration procedures.

Further quantification of the TEM experimental results can be realized by means of analytical methods provided in TEM, such as energy dispersive X-ray spectroscopy (EDX), Z-contrast imaging and electron energy loss spectroscopy (EELS).

The abovementioned integrated methodology is illustrated in a series of up-to-date applications on 0-, 1and 2-dimensional (quantum dots and nanoparticles, nanowires and quantum wells) nanostructures of the III-Nitride system, i.e. GaN, AIN, InN and their ternary and quaternary alloys grown on various substrates.