My Recent Research Interests

Regarding my research interests, in brief, I have recently been working on two main projects:

(1) Silicon Nancrystals:

It has been shown by Munir Nayfeh and coworkers [1] that the integration of a high-quality film of silicon nanoparticles (coated with hydrogen) of 1-nm size directly onto the silicon solar cells improves power performance up to 67 % in the UV and up to 10% in the visible. Subsequently, great interest has been focused on such subject as to explore the novel material in solar-energy applications. We have started a project last summer 2009 (during my visit to KFUPM, Dhahran, Saudi Arabia) in which we studied the electronic and optical properties of silicon nanocrystals versus size, coating and atomic relaxation. Density-Functional Theory (DFT) was used for the relaxation of nanocrystals and the tight-binding (TB) method was used to calculate the band-gap energy and oscillator strength (which is proportional to the absorption). We have demonstrated that the coating would result not only in the saturation of the dangling bonds but also the clearance of the gap from trap states. The size of the particle controls the bandgap through the quantum confinement. One of our two manuscripts has been recently accepted for publication in "J. Luminescence" [2]. As a future work, one may consider studying the Si nanocrystals coated with oxygen rather than hydrogen and see the effects on the electronic structure and the oscillator strength.

(2-A) GaInN alloys:

The energy bandgap of zincblende GaN and InN are respectively: 3.50 eV and 0.71 eV. The lattice mismatch between these two materials is relatively high (of about 10%). The alloys of these two materials ($Ga_{1-x}In_xN$) are of great interests for both photonics and telecommunication applications. Three unusual characteristics are found in these alloys: (i) They possess a rather strong bowing character; (ii) The bowing parameter is composition dependent and (iii) They exhibit a strong Stokes shift between emission and absorption spectra. I have studied these alloys and a single-author paper is just appeared online in "J. Alloys & Compd." [3].

(2-B) Alloyed GaInN/GaN Multiple-Quantum Wells (MQWs):

The previous project is just the first step toward the modeling of the recent Photoluminescence data obtained by Prof. A. Yoshikawa (Chiba University, Japan). The PL data shows the effect of well composition within the limit of very fine well thickness. I need to extend the basis set of the Hamiltonian from sp^3s^* with the inclusion of spin-orbit (SO) coupling effects into $sp^3s^*d^5$ with SO interaction effects for a better representation of the conduction bands of both GaN and InN. Then, I plan to use my program for the MQWs, which is already well tested but what remains is the extension of the basis set of the Hamiltonian to include the models famous tight-binding models of Professor Bassani and coworkers [4]

References:

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[2] "Origins of visible-light emissions in hydrogen-coated silicon nanocrystals", N. Tit, Z.H. Yamani, J. Graham and A. Ayesh, J. Lumin. 130, 2226 (2010).

[3] "Nitrogen-electronegativity-induced bowing character in ternary zincblende $Ga_{1-x}In_xN$ Alloys", N. Tit, J. Alloys Compd. 503, 529 (2010).

[4] J.M. Janco, F. Bassani, F. Della Sala and R. Scholz, Appl. Phys. Lett. 81, 25 (2002).