Thermodynamic, Electronic and Optical Properties of Quantum-Dots and Quantum-Well Nanocrystals : Effects of Interdiffusion

[a)]K. Masuda-Jindo [b)]R. Kikuchi and [c)]Vu Van Hung

[a)]Department of Materials Science and Engineering, Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama 226-8503, Japan
[b)] Materials Science and Mineral Engineering, University of California, Berkeley, CA 94720-1760, USA
[c)]Hanoi National Pedagogic University, km8 Hanoi-Sontay Highway,Hanoi, Vietnam

Recently, there has been a great interest in the self-assembled semiconductor quantum dots and nanocrystals in conjunction with the applications of wet chemical techniques to optoelectronic devices, biological labels, etc.. In the present study, the atomistic, elastic, electronic and optical properties of the nanoscale materials are investigated by using an ab initio molecular dynamics (TBMD) method [1] and temperature dependent lattice Green's function (LGF) method [2,3]. The path probability method (PPM) in the statistical physics is also used to study the influence of the interface disorder on the electronic properties of the semiconductor nanostructures [1]. It is shown that the interface interdiffusion influences quite significantly the electronic and optical properties of semiconductor heterostructures. The influence of interdiffusion on the excitonic transition energies in semiconductor nanocrystals is demonstrated both for core-shell and quantum-dot-quantum well nanosrystals. The critical layer thickness h_c for the generation of misfit dislocations depends significantly on the interface disorder (increase of h_c) at the semiconductor heterostructures. We also investigate the effects of strain in quantum dots caused by the differences of the lattice constants (dot and substrate materials) on both the self-organization mechanisms and the electro-optical properties using the LGF method. The calculation results are compared with those obtained by the continuum elasticity theory (finite element method).

[1] K. Masuda-Jindo and R. Kikuchi, International Journal of Nanoscience, **1**, (2002) 357-371
[2] K. Masuda-Jindo, V. V. Hung and P. D. Tam, Phys. Rev., **B67** (2003) 094301-1
[3] K. Masuda-Jindo, V. V. Hung, J. Phys. Soc. Jpn., **73** (2004) 1205-1215